Hydroacoustic signal classification using support vector machines

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Abstract. Kernel-based algorithms such as support vector machines (SVMs) are state-of-the-art in machine learning for pattern recognition. This chapter introduces SVMs and describes a specific application to hydroacoustic signal classification. Long-range, passive-acoustic monitoring in the oceans is facilitated by propagation properties for underwater sound. In particular, the deep sound (SOFAR, Sound Fixing and Ranging) channel can act as a waveguide for underwater signals. In this chapter, SVMs are employed for classifying hydroacoustic signals recorded by the sensor network for verification of the Comprehensive Nuclear-Test-Ban Treaty. Constraints in the early signal processing chain and limited data require tailored kernel functions and careful SVM model selection. We demonstrate how problem-specific kernel functions can increase classifier performance when combined with efficient gradient-based approaches for optimizing kernel and SVM regularization parameters.

1 Introduction

While the fundamental scientific principles behind many of the earth-monitoring systems in operation today have been well known for decades, sensor hardware and sensor deployment are steadily evolving further. Simultaneously, advances in data transmission and storage leave their own and distinct marks on the field. Today vast amounts of raw data are routinely being collected and transferred. One key challenge on the receiving end is to reliably extract knowledge that is both meaningful and yet sufficiently condensed, in order to facilitate human (or other) interpretation of the information flow. This especially holds for systems performing real-time monitoring. In general, we obtain information about real-world processes in the form of non-linear, noisy, multidimensional signals. Both the underlying phenomenon itself as well as all aspects of the signal processing and transmission chain are in general too complex to be fully captured

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by a physical model. Therefore, best practice data processing and analysis rules have to be inferred from observations and validated empirically. Here *machine learning* comes into play, which is a branch of computer science and applied statistics covering software that improves its performance on a given task based on sample data or experience. This chapter considers *supervised learning* for classification, which refers to automatically assigning signals to predefined categories. In the supervised learning scenario, the learning machine is provided with sample input-output pairs during a preparational training phase. The learner's task then is to infer from the training data a function that relates any admissible input (not only those seen during training) to a corresponding output. Such a function is called the learner's hypothesis. We demand that all examples used for training as well as later for testing be generated independently of each other by the same probability distribution. Relying on this assumption, the learner should choose a hypothesis which with high confidence will perform accurately on unseen test data. One central challenge in any supervised learning task is to settle a trade-off between on the one hand well fitting the hypothesis to the training examples, and on the other hand hedging against *overfitting*, which occurs when overly adapting to misleading peculiarities of the training data. Section 2 formally introduces the supervised learning task, regularized risk minimization, and support vector machines (SVMs) for classification. We introduce SVMs step by step from linear classification to the full kernelized case. This chapter emphasizes aspects deemed relevant to practitioners and at the same time strives to include a reasonably systematic overview over regularized risk minimization, SVM classification, and SVM model selection. The application of these concepts is illustrated through a classification task in acoustic remote sensing. We learn to discriminate signals stemming from the verification network for the Comprehensive Nuclear-Test-Ban Treaty (CTBT). The CTBT's permanently installed International Monitoring System (IMS) consists of several hundred geophysical sensors and relies on four different monitoring technologies. In particular we are concerned with distinguishing explosive-like and non-explosive signals recorded by the IMS underwater sensor network. Section 3 provides background on the IMS as well as preprocessing routines relevant to the application. We then approach the actual problem of CTBT hydroacoustic signal classification by drawing on the generic concepts established earlier. Section 4 concludes this chapter.

2 Supervised learning and support vector machine classification

We next formalize the supervised learning and classification task. In the standard setting, we have obtained training data S from the same data generating process to which we intend to apply the trained learning machine. The data S consists of N exemplary input-output pairs $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $1 \leq i \leq N$. The input and output domains $\mathcal{X}$ and $\mathcal{Y}$ can in general be any (non-empty) sets. Given S, the output of a learning machine is a prediction function or hypothesis $h : \mathcal{X} \to \mathcal{Y}$

from the input set $\mathcal{X}$ to the output set $\mathcal{Y}$. For each possible input $x \in \mathcal{X}$ we present to h, it will yield its hypothesis $h(x) \in \mathcal{Y}$ of what output value should most likely be associated with x. It is not sufficient to learn the training data by heart. We rather want h to perform as well as possible for the entirety of input values in $\mathcal{X}$, and especially for those that occur often. When we know the true label y of a sample x, we can compare it to the learner's prediction $h(x)$. Feeding both to a *loss function* L

$$\begin{aligned} L \,:\, \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_0^+, \\ \text{with the property: } L(h(x), y) = 0 \text{ for } h(x) = y \ , \end{aligned} \tag{1}$$

assigns a "cost" to predicting $h(x)$ instead of y. Formally the goal of supervised learning may now be expressed as finding a function h that minimizes the overall cost, or *risk* $\mathcal{R}_p$, when evaluated over the entire probability distribution $p(x, y)$ underlying our data generating process:

$$h = \arg\min_{\hat{h} \in \mathcal{H}} \mathcal{R}_p(\hat{h}) = \arg\min_{\hat{h} \in \mathcal{H}} \int_{\mathcal{X} \times \mathcal{Y}} L(\hat{h}(x), y) \, \mathrm{d}p(x, y) \ , \tag{2}$$

where $\mathcal{H}$ would ideally be the space of all (measurable) functions mapping from $\mathcal{X}$ to $\mathcal{Y}$. A hypothesis minimizing eq. (2) is called a *Bayes optimal* solution, the according risk the *Bayes risk* of p, and both depend on p and the loss function employed. Note that the Bayes risk is not necessarily zero. This is easy to see for finite $\mathcal{X}$. If an input pattern $x \in \mathcal{X}$ can belong to two different classes – $p(x, y_1) > 0$ and $p(x, y_2) > 0$ for different $y_1, y_2 \in \mathcal{Y}$ – the best possible hypothesis still can map x only to one class and will inevitably make mistakes. In practice, non-zero Bayes risk frequently occurs in the case of noisy input signals, signals describing the underlying process incompletely, or uncertain labels.

Clearly, if we knew the underlying distribution p, we would have complete knowledge about the data generating process. But p usually is unknown. Thus for all practical purposes the overall risk $\mathcal{R}_p$ can neither be computed nor optimized directly, even if the integrals in eq. (2) were tractable. One step towards optimizing eq. (2) is to replace $\mathcal{R}_p$ by the equivalent quantity restricted to the training data. This defines the *empirical risk* $\mathcal{R}_S$ on S,

$$\mathcal{R}_S(\hat{h}) = \frac{1}{N} \sum_{i=1}^{N} L(\hat{h}(x_i), y_i) \ , \tag{3}$$

which is simply the average loss on the training data. A minimizer of $\mathcal{R}_S$ is a hypothesis as consistent with the training examples as possible. Minimum empirical risk can for example be achieved by a function that reproduces the labels of all training examples and merely returns one single, arbitrary output for all other possible inputs. Evidently this would be a poor prediction function, and a better objective than to just minimize eq. (3) over all functions is needed.

2.1 Regularized risk minimization

A hypothesis h should not solely reflect peculiarities of the given training data, but work well for examples previously unencountered. What kind of quantity can

assist us – without knowing more about the data generating distribution than S – in automatically deciding which hypothesis may have *overfitted* to the training data and which may *generalize* well to unseen data? It is not only intuitive to look for a simple hypothesis still yielding a reasonably low empirical risk, but a range of according theorems in statistical learning theory (e.g., [34, 39]) formalize and justify this concept. These theorems typically provide bounds on the risk in the following form. If of all functions in a certain function or hypothesis space $\mathcal{H}$, h is the minimizer of $\mathcal{R}_S$, then with probability of at least $1-\delta$ it will hold that $\mathcal{R}_p(h) \leq \mathcal{R}_S(h) + B(N, \delta, \mathcal{H})$. The function B bounds the extent to which the true risk might exceed the empirical risk. An increase in both the number of training examples N as well as the uncertainty δ leads to a decrease in B. Most importantly, B increases with the complexity of $\mathcal{H}$. We argue that any function $B_{N,\delta}(\mathcal{H})$ which permits inequalities like the above provides a measure of the complexity of a function space $\mathcal{H}$ – and therefore simplicity of a hypothesis class can be (non-uniquely) defined in precise ways. Such theorems confirm that if we permit the minimizer of $\mathcal{R}_S$ to be highly complex, this expressive power might be exploited for overfitting on the training data rather than be helpful in producing better hypotheses. We thus want to enforce the preference that if the learning machine suggests a more complex hypothesis, it should have a very good justification in terms of – sufficiently – high associated decrease in training error. The hypothesis spaces considered in this chapter can be endowed with a norm $\| \ \|_{\mathcal{H}}$ serving as a measure of complexity of a hypothesis. Then we can express the aforementioned tradeoff within the *regularized risk minimization* paradigm, in which h is found by minimizing the regularized risk $\mathcal{P}_S$,

$$\mathcal{P}_S(\hat{h}) = \|\hat{h}\|_{\mathcal{H}} + C \sum_{i=1}^{N} L(\hat{h}(x_i), y_i) \ . \tag{4}$$

Here $C \in \mathbb{R}^+$ is the so-called *regularization parameter* and balances the preference for low training error (right summand) against keeping the hypothesis simple (left summand), where complexity is assumed to correlate to the norm in $\mathcal{H}$, cf. [34, 39].

2.2 Support vector machines

In general a multitude of supervised learning algorithms exist, which may or may not fall into the framework of regularized risk minimization presented in the previous section. We in this chapter focus on support vector machines (SVMs, [7, 29]), which are most commonly used for classification, but also applicable to regression and density estimation tasks. Support vector machines can be seen as composed of building blocks from originally different areas of research and for example are linked to functional analysis and convex optimization. We next introduce SVMs step by step as composition of concepts, namely straightforward linear classification seeking for large separating margins; allowing for margin violations in a regularized risk minimization framework; and non-linear classification via kernel functions, which replace the scalar product in the original input space by a scalar product in another, unrealized feature space.

2.3 Linear classification

From now on we for clarity assume that all inputs are represented by an m-dimensional, real-valued feature vector $x \in \mathbb{R}^m = \mathcal{X}$. Further we restrict our considerations to two-class or binary classification and set $\mathcal{Y} = \{-1, 1\}$. A two-class hypothesis function $h : \mathcal{X} \to \{-1, 1\}$ with a linear decision boundary can be realized through an affine linear *decision function* $f : \mathcal{X} \to \mathbb{R},\ f(x) = \langle x, w\rangle + b$ by taking the sign of f:

$$h(x) = \mathrm{sgn}(f(x)) = \mathrm{sgn}(\langle x, w\rangle + b) \ . \tag{5}$$

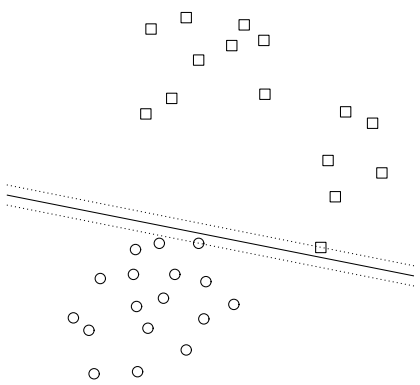
Here the weight vector $w \in \mathcal{X}$ lies in the same space as the input data, $b \in \mathbb{R}$ is a real-valued offset term, and sgn() is the standard signum function except for an argument of zero, in which case it returns +1. The decision boundary is the subspace of all points x for which $\langle x, w\rangle + b = 0$. For two-dimensional input, this subspace is a line, and a hyperplane of dimension $m - 1$ in general. The vector w is perpendicular to the decision boundary. With an offset or bias term of zero, $b = 0$, the decision surface passes through the origin. For $b \neq 0$ the decision surface is shifted from 0 by a distance of $\frac{b}{\|w\|}$.

The quantity $y_i(\langle w, x_i\rangle + b) = y_i f(x_i)$ is positive if the i-th pattern (x_i, y_i) is classified correctly by the hypothesis $\mathrm{sgn}(f(x))$. We call this quantity the *functional margin* of (x_i, y_i) with respect to the linear decision boundary induced by (w, b). The *geometric margin* of (x_i, y_i) with respect to the linear decision boundary induced by (w, b) is given by $y_i f(x_i)/\|w\|$. The absolute value of the geometric margin is the distance of x_i from the decision boundary in the input space. A collection S of N two-class data points is called linearly separable if there exists a linear classifier (w, b) separating both classes without error. This implies $y_i(\langle w, x_i\rangle + b)/\|w\| \geq \rho > 0$ for all $1 \leq i \leq N$. The largest ρ for which this holds true defines the geometric margin of the linear classifier (w, b) with respect to S. Its value is determined by the data point having the smallest margin. In the following, we will not explicitly distinguish between functional and geometric margin when the meaning is clear from the context.

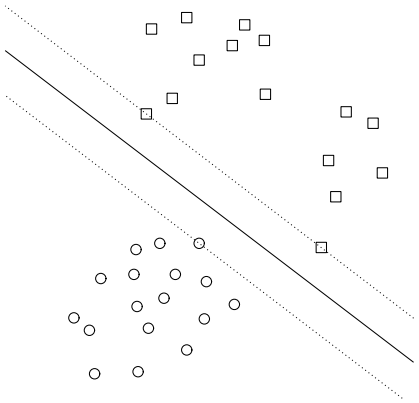
2.4 Linear support vector machines

We first introduce large-margin support vector machine classification for linearly separable data. Figure 1 shows a separable two-class problem in two dimensions, and in the upper left a "barely separating" hyperplane. Intuitively we see that this hypothesis is quite vulnerable, as already little noise on samples close to the boundary would lead to their misclassification. Therefore, *hard margin* SVMs for separable training data S yield a hypothesis for which the smallest margin of a training data point – the distance between the decision hyperplane and the closest data point in S – is maximal. It can be shown that solving the optimization problem

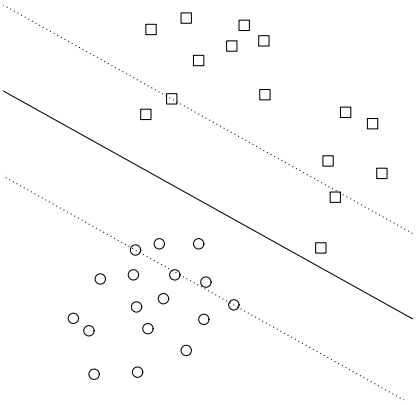
$$\begin{aligned} \text{minimize}_{w,b} \quad & \frac{1}{2}\langle w, w\rangle \\ \text{subject to} \quad & y_i(\langle w, x_i\rangle + b) \geq 1 \ , \ \ 1 \leq i \leq N \ , \end{aligned} \tag{6}$$



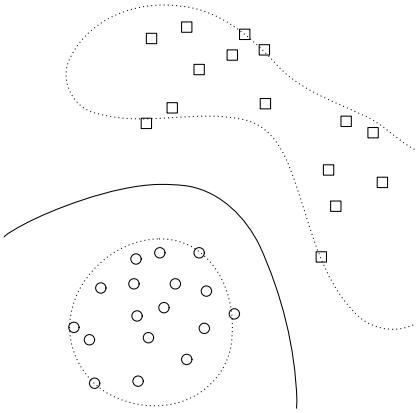
(a) Linear separation by a small margin.



(b) The linear large-margin solution.



(c) Also allowing for margin violations.



(d) Non-linear separation with outliers.

Fig. 1: Example of linearly separable two-class data, and different hypotheses for a discrimination boundary between them. Subfigure (a) shows a hypothesis (bold line) that might have been proposed by an algorithm not maximizing the margin (distance to dotted lines) between samples and the discrimination boundary. In subfigure (b) a maximum-margin solution found by the linear hard-margin SVM of eq. (6) is shown. We can expect the solution in subfigure (a) to be less reliable when classifying data from the same generating distribution. The third subfigure shows the hypothesis produced by a soft-margin SVM using $C = 0.3$ in objective (7). Note that its different slope and position could not have been reached through objective (6). Subfigure (d) shows a curved decision surface obtained by solving the canonical, non-linear SVM optimization problem (10), using $C = 3$ and a radial basis function kernel (cf. Section 2.5) with $\gamma = 0.5$. While (a) clearly is not a large-margin classifier, all three hypotheses in (b, c, d) are valid solutions to the full SVM optimization problem. Solution (b) can be seen as a special case of (c) with a strong preference against margin violations expressed through a large regularization parameter. Both linear solutions are further special cases of the non-linear one, using the scalar product in the original feature space as kernel function. In other words, (b, c, d) have all been obtained by solving the SVM optimization problem (10) for different choices of the regularization parameter C and kernel function k.

leads to a decision function with a geometric margin of $\frac{1}{\|w\|}$, so that the objective of problem (6) exactly ensures a hypothesis with maximum margin [29]. The term "hard margin" refers to the fact that the constraints in eq. (6) strictly enforce a functional margin of at least one for each training pattern, which implies correct classification of all examples. Applied to the previous example in Figure 1, the large-margin objective (6) generates the hypothesis shown in the upper right. In practice few datasets are linearly separable in the input space. But even for those, it may be beneficial to allow for misclassification of training patterns if in turn a more appealing hypothesis can be established with respect to the overall data. Obviously, if the Bayes risk is non-zero and the pool of training data sufficiently large, the Bayes optimal hypothesis makes errors on the training data. We thus want to allow for *margin violations*, that is, for training patterns (x_i, y_i) for which $y_i(\langle w, x_i\rangle + b) < 1$. This includes misclassified patterns, for which $y_i(\langle w, x_i\rangle + b) < 0$ indicates that they lie on the "wrong" side of the hyperplane. We for these reasons return to the concept of regularized risk minimization established in Section 2.1. To make usable an objective of the form of eq. (4), a loss function $L(h(x), y)$ has to be chosen. For classification we would ideally like to use the 0-1-loss, which returns 0 for correct classification, $h(x) = y$, and 1 otherwise. Incorporating the non-convex 0-1-loss into eq. (6) would however complicate the optimization procedure by voiding convexity of the overall problem. For this reason SVMs commonly rely on the *hinge loss* $L(f(x), y) = \max(0, 1 - yf(x))$ defined on the SVM decision function f as a convex *surrogate loss function*. Introducing the possibility for margin violations into eq. (6) and penalizing them by the hinge loss yields

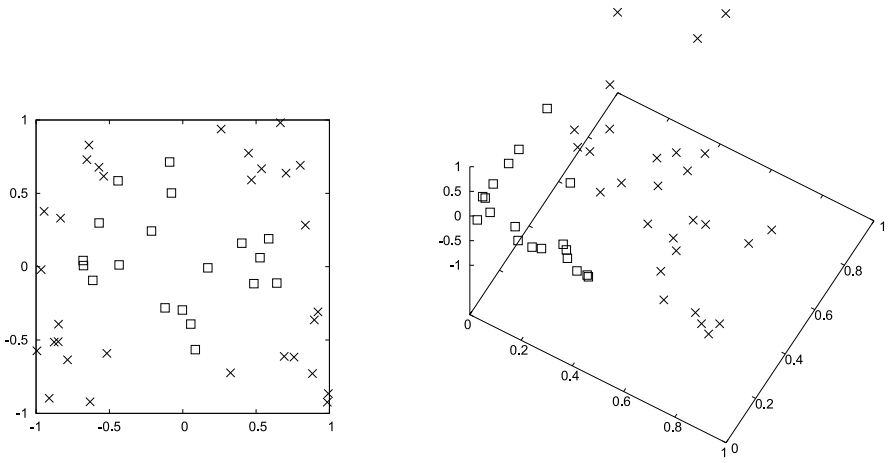
$$\begin{aligned} \text{minimize}_{\xi,w,b} \quad & \frac{1}{2}\langle w, w\rangle + C\sum_{i=1}^{N}\xi_i \\ \text{subject to} \quad & y_i(\langle w, x_i\rangle + b) \geq 1 - \xi_i \ , \ 1 \leq i \leq N \\ & \xi_i \geq 0 \ , \ 1 \leq i \leq N \ . \end{aligned} \tag{7}$$

Problem (7) is the linear *soft margin* SVM optimization problem. Each variable $\xi_i \geq 0$ measures the margin violation of pattern (x_i, y_i). Their sum accounts for all violations of the separability paradigm by exactly the sum of the corresponding hinge loss, which in turn is penalized within the objective function. The lower left of Figure 1 shows the result of solving eq. (7) for $C = 0.3$. While the difference on the toy dataset is not drastic, it exemplifies the fact that eq. (7) allows for solutions not reachable through eq. (6). The hard-margin solution can however still be obtained by letting C tend to infinity. We are now only an additional step short of obtaining the canonical non-linear SVM formulation as we will also employ in the experimental Section 3.

2.5 Kernelized support vector machines

Solving problem (7) will yield a regularized large-margin hypothesis, however always using a linear decision function. This can be a disadvantage, for example

when imagining a two-dimensional classification problem in which samples of one class all lie within a circle around the origin, and samples of the second class surround them in a ring-like fashion, as illustrated on the left of Figure 2. SVMs



(a) Using (x_1, x_2) as representation

(b) Using $(x_1^2, x_2^2, \sqrt{2}x_1x_2)$

Fig. 2: Example of an embedding into a feature space that turns linearly non-separable data into linearly separable data. Squares and crosses indicate examples of two different classes. The feature map $\phi : \mathbb{R}^2 \to \mathbb{R}^3$ changes the representation of input patterns (x_1, x_2) to $(x_1^2, x_2^2, \sqrt{2}x_1x_2)$.

incorporate non-linear hypotheses by implicitly transforming the input data to an unrealized, possibly high- or infinite-dimensional dot product space via kernel functions. In this feature space, different from the input space, SVMs perform linear classification. This in general gives rise to non-linear decision surfaces in the original input space. From another angle, one might imagine subjecting the input data to a non-linear transformation and only then solving problem (7) for the transformed input. In the right of Figure 2, the result of carrying out such a non-linear transformation from the input space into a higher-dimensional space is shown. If the new feature space however is of high dimension, carrying out computations dimension-wise is time-consuming, and the transformation might be as well. Instead, we use the fact that a solution w of eq. (7) admits a representation of the form $w = \sum_i^N \alpha_i x_i$ with $\alpha \in \mathbb{R}^N$ [9, 31]. In other words it is guaranteed that the solution is a linear expansion of the training examples.

Substituting into (7) yields

$$\begin{aligned} \text{minimize}_{\xi,\alpha,b} \quad & \frac{1}{2}\sum_{i,j=1}^{N}\alpha_i\alpha_j\langle x_i, x_j\rangle + C\sum_{i=1}^{N}\xi_i \\ \text{subject to} \quad & y_i\Big(\sum_{j=1}^{N}\alpha_j\langle x_j, x_i\rangle + b\Big) \geq 1-\xi_i \ , \ 1 \leq i \leq N \\ & \xi_i \geq 0 \ , \ 1 \leq i \leq N \ . \end{aligned} \tag{8}$$

Looking at problem (8) we see that the objective is solely formulated in terms of scalar products between training examples. Were the examples mapped to another dot product space $\mathcal{F}$ by the map $\phi : \mathbb{R}^m \to \mathcal{F}$ before solving eq. (8), each occurrence of $\langle x_i, x_j\rangle$ would simply have to be replaced by $\langle\phi(x_i), \phi(x_j)\rangle_{\mathcal{F}}$. In order to allow for efficient computation of the dot product in $\mathcal{F}$, we can use a function $k : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ with $k(x_i, x_j) = \langle\phi(x_i), \phi(x_j)\rangle_{\mathcal{F}}$. More importantly one can proceed the other way around and specify a kernel k in order to solve problem (8) in another dot product space. The theory of reproducing kernels [1, 2, 29] establishes the requirements k has to fulfill in order to be sure that substituting $k(x_i, x_j)$ for the scalar product will actually correspond to solving problem (8) in some valid dot product space. The only condition on a symmetric function k is that k must be *positive definite*, in the sense that for every collection of points from $\mathcal{X}$, the matrix K of kernel entries between these points, $K_{ij} = k(x_i, x_j)$, must be positive definite. In detail, for a non-empty input set $\mathcal{X}$ and a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ the following holds:

$$\forall\, n \in \mathbb{N},\ x, z, x_1, \ldots, x_n \in \mathcal{X},\ c_1, \ldots, c_n \in \mathbb{R} :$$
$$k(x, z) = k(z, x) \ \wedge \ \sum_{i,j=1}^{n} c_i c_j k(x_i, x_j) \geq 0$$

$$\Rightarrow$$

$$\exists\ (\mathcal{F},\ \phi : \mathcal{X} \to \mathcal{F}) \ : \ \forall\, x, z \in \mathcal{X} \quad k(x, z) = \langle\phi(x), \phi(z)\rangle_{\mathcal{F}} \ . \tag{9}$$

Equation (9) states an equivalence between a kernel function k and a scalar product in some dot product space $\mathcal{F}$ as long as k is symmetric and positive definite. We list commonly used families of positive definite kernels below. Completing the kernelization of the SVM optimization problem, we state the final objective which allows for both misclassified training examples as well as non-linear decision surfaces using kernel functions:

$$\begin{aligned} \text{minimize}_{\xi,\alpha,b} \quad & \frac{1}{2}\sum_{i,j=1}^{N}\alpha_i\alpha_j k(x_i, x_j) + C\sum_{i=1}^{N}\xi_i \\ \text{subject to} \quad & y_i\Big(\sum_{j=1}^{N}\alpha_j k(x_j, x_i) + b\Big) \geq 1-\xi_i \ , \ 1 \leq i \leq N \\ & \xi_i \geq 0 \ , \ 1 \leq i \leq N \ . \end{aligned} \tag{10}$$

Problem (10) constitutes the canonical SVM optimization problem [7]. The decision function f of an SVM is linear in the kernel-induced feature space. In the original input space the SVM's final hypothesis h takes the form

$$h(x) = \operatorname{sgn}(f(x)) = \operatorname{sgn}\left(\sum_{i=1}^{N} \alpha_i k(x, x_i) + b\right) . \tag{11}$$

The lower right of Figure 1 shows a classifier obtained from eq. (10) using $C = 3.2$ and a radial basis function kernel of $\gamma = 0.5$ (see below). The solution would differ considerably for different values, and even more so for other kernel function families. The final SVM hypothesis does not depend on correctly classified training examples with a distance to the decision hyperplane larger than the safety margin. Their coefficients α_i will hence be zero. All samples with non-zero coefficients α_i will lie on the margin or violate it (i.e., have $y_i f(x_i) = 1$ or $y_i f(x_i) < 1$, respectively). These are called *support vectors*, and only they contribute to the sum in eq. (11). This *sparsity property* of SVMs reduces the computational burden when evaluating the hypothesis on unseen examples.

2.5.1 Kernel functions

The question arises how to choose a proper kernel function. We first introduce two families of kernels commonly used for real-valued input vectors.

Polynomial kernel. For a non-negative, real-valued offset parameter c and a positive integer exponent d, the function $k(x, z) = (\langle x, z\rangle + c)^d$ is a kernel on real-valued input vectors $x, z \in \mathbb{R}^m$. For $c = 0$ and $d = 1$ it reduces to the standard scalar product.

Gaussian kernel. A general Gaussian kernel on real-valued input vectors $x, z \in \mathbb{R}^m$ is given by $k(x, z) = e^{-(x-z)^T Q(x-z)}$, where Q is a positive definite $m \times m$ matrix. The most common variant is the radial basis function (RBF) kernel using a positive scaling of the identity matrix I, $Q = \gamma I$, $\gamma \in \mathbb{R}^+$, which introduces γ as single free parameter. A theoretically appealing property of RBF kernels is that they fulfill a necessary condition for an SVM to be *universally consistent* [35]: an SVM using an RBF kernel will under mild conditions converge to the Bayes optimal hypothesis as the collection of training examples grows. Another variant is the automatic relevance detection (ARD) kernel, for which $Q_{ij} = \delta_{ij}\gamma_i$, with Kronecker delta δ. The ARD kernel owes its name to the fact that learning values for the m positive parameters $\gamma_i \in \mathbb{R}^+$ can provide insight into the relevance of individual features for classification. As a drawback, the ARD kernel introduces as many free parameters as there are input space dimensions. However, efficient parameter optimization has been demonstrated for both the ARD and the general Gaussian kernel ([14, 15], also see Section 2.7).

Individual application domains, for example in biology or natural language processing, can require the use of highly specific and task-tailored kernel functions.

Their design and analysis often constitutes an active area of research of its own (e.g., [13, 30]). Positive definite kernels further exhibit convenient closure properties in the sense that several operations between kernels again yield a valid kernel [2]. For two kernels k_1 and k_2 their product $k_1 \cdot k_2$ and sum $k_1 + k_2$ is positive definite. Similarly, all following operations on a kernel k retain positive definiteness: scaling by a positive constant to ak, $a \in \mathbb{R}^+$; taking k as exponent e^k; or normalizing k to $k_n(x,z) = k(x,z)/\sqrt{k(x,x)k(z,z)}$. Further, closure under sum and product also imply closure under direct sum and direct product: let $k_a(x,z)$ be a kernel on $A \times A$ and $k_b(u,w)$ a kernel on $B \times B$. Then kernels $k((x,u),(z,w))$ on $(A \times B) \times (A \times B)$ are both given by $k_a(x,z) \cdot k_b(u,w)$ and $k_a(x,z) + k_b(u,w)$. This for example is useful when working with combinations of features from different domains.

Convolution kernels. Not a standard choice of kernel function as such, we list Haussler's convolution kernel[4] [18] in preparation for an application in Section 3. Suppose the input space $\mathcal{X} = \mathbb{R}^m$ can be split up into g subspaces. For simplicity, we assume that these subspaces are equal and write $\mathcal{X} = \mathcal{S}^g$. This yields a partitioning of an input vector x into g sub-vectors $x^{(i)} \in \mathcal{S} = \mathbb{R}^{(\frac{m}{g})}$, $1 \leq i \leq g$, of equal length. Further assume that we have g corresponding sub-kernels $k^{(i)} : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ defined on the subspace $\mathcal{S}$. By the above composition rules we can construct a composite kernel on $\mathcal{X} \times \mathcal{X}$ by for example adding all sub-kernels, $k(x,z) = \sum_i k^{(i)}(x^{(i)}, z^{(i)})$, or multiplying them, $k(x,z) = \prod_i k^{(i)}(x^{(i)}, z^{(i)})$. The convolution or ANOVA kernel k_D of order D, $D \in \{1, \ldots, g\}$, generalizes from these two exemplary compositions by viewing both as sums over all possible monomials (multiples excluded) of degree D:

$$k_D(x,z) = \sum_{1 \leq j_1 < \cdots < j_D \leq g} \prod_{d=1}^{D} k^{(j_d)}(x^{(j_d)}, z^{(j_d)}) \ . \tag{12}$$

Here the sum runs over all possibilities to draw unique subsets of size D from $\{1, \ldots, g\}$. Clearly the convolution kernel k_D is the direct sum kernel for $D = 1$ and the direct product kernel for $D = g$. In general, k_D yields the sum of all monomials (multiples excluded) of order D.

2.6 SVM optimization

One of the canonical approaches to SVM optimization, that is, to solving problem (10), is to derive the corresponding *dual program* via Lagrange multipliers [7, 39]. The resulting constrained quadratic optimization problem would be solvable using off-the-shelf methods, but highly efficient tailored methods have been derived. Decomposition methods for SVMs [21, 25] are iterative algorithms

[4] The special form of convolution kernel as we consider here has also been studied in [28, 39] as ANOVA kernels. We refer the reader to Haussler's overarching construction as the most systematic one.

that operate on a fixed subset of (usually two) variables per iteration. It is generally accepted that such solvers have a runtime complexity between quadratic and cubic in the number of training examples [21]. When working with large datasets, fast solvers specialized on linear kernels can be employed, at the cost of purely linear decision functions (e.g., [10, 33]). Alternatives that also support non-linear kernels are *online* SVM solvers (e.g., [3]), which aim for an approximate solution.

2.6.1 SVM execution

In general, the hypothesis put forth by an SVM is *sparse*: it only depends on the fraction of training examples that are support vectors. SVM execution can thus be faster than for example naive implementations of nearest neighbor classification. It has however been shown that the number of support vectors itself grows linearly with the number of training examples if the Bayes risk is non-zero [36]. A number of different approaches have been proposed for approximating the final solution when classification speed is important (e.g., [24, 32]).

2.7 Model selection

Maybe the most important aspect in SVM usage is that of model selection – the process of choosing the regularization parameter C and a kernel function family as well as values for the kernel parameters. A multitude of methods for hyperparameter selection exist. Most of them optimize an approximation of, bound on, or heuristic substitute for the generalization error, that is, for eq. (2) using the 0-1-loss. We present the standard method, grid search on the cross-validation error, together with a gradient-based maximum-likelihood approach better suited for kernels with more than a few parameters.

2.7.1 Direct search

One common estimator of the generalization error is the n-fold cross-validation error. By partitioning the available training data S into n different parts or *folds*, one obtains n possibilities for training a classifier on $n-1$ parts of S. The average of the n validation errors on each remaining single evaluation fold is the n-fold cross-validation error (CV-n). It can be shown that the CV-n is a slightly biased estimator of the generalization error [17], and choices of $n = 5$ or $n = 10$ have proven reasonable in practice. Because CV-n is not differentiable, the hyperparameter space is generally probed at multiple locations using some direct (zeroth-order) search heuristic.

Grid search. The most common SVM model selection procedure, grid search, defines a multi-dimensional grid of points in the hyperparameter search space, where the grid points may for example be spaced evenly on a linear or logarithmic scale. For each point on the grid, n SVMs are trained (each on a different

set of $n-1$ folds) using the corresponding hyperparameter vector. The parameter combination yielding lowest CV-n over the entire grid is in turn chosen to train the final classifier, now using all data in S. Due to the curse of dimensionality, CV-n gets prohibitive for more than a few free SVM hyperparameters. Sometimes variations such as nested grid search are employed, where the grid resolution iteratively increases while focusing around the previously best point. Beyond grid search, more elaborate direct search techniques, such as evolution strategies, have successfully been applied to SVM model selection [11, 19].

2.7.2 Gradient-based model selection

A lot of research has been devoted to developing and evaluating differentiable estimates of, bounds on, or heuristic substitutes for the generalization error (see e.g. [5]). Even if such an objective is not convex (i.e., does not prevent gradient-based optimizers from getting stuck in suboptimal local minima) gradient descent is still appealing. First, the directional information provided by the gradient guides the search. Second, the derivative of the objective might be faster to evaluate at a given point in the hyperparameter space than training n SVMs for CV-n. As a consequence, gradient-based approaches can have significant advantages over direct search, especially when the parameter space has more than a few dimensions.

Maximum-likelihood model selection. We present one recent gradient-based model selection algorithm which has been shown to outperform several established methods on a large benchmark set [15]. The classification error in general is a non-differentiable quantity with respect to the parameters of a deterministic hypothesis. In contrast, assume a probabilistic classifier approximating the probability $P(y \mid x)$ of observing class $y \in \mathcal{Y}$ given input $x \in \mathcal{X}$ by some model $\hat{P}(y \mid x)$, where $\hat{P}$ depends smoothly on its parameters and the hyperparameters of the learning algorithm. A typical approach for learning these parameters is maximizing the *logarithmic likelihood function* $\mathcal{L} = \sum_{(x_i,y_i)\in S} \log \hat{P}(y_i \mid x_i)$ with respect to the adaptive parameters, which can be done using gradient ascent.

Learning a model of $P(y \mid x)$ is a more general and therefore usually more difficult task than "just" learning a hypothesis for classification. While a perfect model gives the Bayes optimal hypothesis by $h(x) = \arg\max_{y\in\mathcal{Y}} P(y \mid x)$, a bad model leads to bad classification results. In the SVM framework one therefore searches for a proper hypothesis directly without estimating $P(y \mid x)$. This at the same time prevents us from using the maximum-likelihood approach for model selection as described above. Therefore, Glasmachers and Igel [15] use a probabilistic interpretation of the output of an already trained SVM solely for the purpose of model selection. They follow an approach by Platt [26], who proposed to estimate class membership probabilities $P(y = +1 \mid f(x))$ from SVM decision functions f by fitting a simple sigmoid $\sigma_{r,s}(f(x)) = 1/(1+\exp(s\cdot f(x)+r))$ around f, where $s \in \mathbb{R}^-$ and $r \in \mathbb{R}$ are the scaling and offset parameter, respectively. This fitting can be done by gradient-based optimization of a cross-validation

estimate of the likelihood. For an SVM decision function f, a sigmoid $\sigma_{r,s}$ around f, and validation data S' the likelihood is:

$$\mathcal{L}(S', \sigma_{r,s}, f) = \sum_{\substack{(x',y')\in S' \\ y'=+1}} \log \sigma_{r,s}(f(x')) + \sum_{\substack{(x',y')\in S' \\ y'=-1}} \log\left(1 - \sigma_{r,s}(f(x'))\right) \quad . \quad (13)$$

In [15], this quantity is optimized with respect to the kernel parameters and the regularization parameter C of the SVM using gradient ascent. This requires the kernel function to depend smoothly on its parameters. The derivative of the SVM with respect to its hyperparameters and the kernel can be computed using the procedure proposed in [22]. It has to be stressed that the probabilistic interpretation of the SVM output is a heuristic, because the SVM (on purpose) does not aim at learning proper probabilities. However, the probabilistic interpretation is solely used to guide model selection. In practice, this maximum-likelihood approach to SVM model selection achieves state-of-the-art results and especially performs well when optimizing flexible kernels on small datasets [15].

The model selection algorithms described in this chapter are all available as part of the open source machine learning library Shark [20].

2.8 Summary

To conclude our introduction to support vector machines for classification we emphasize the following properties of these powerful learning machines:

+ *Convex optimization.* When all of an SVM's hyperparameters are fixed, SVM training corresponds to solving a convex quadratic optimization problem, which is free from suboptimal local extrema. In other words, SVMs always return some best solution possible given a fixed set of hyperparameters.
+ *Consistency.* Under relatively mild conditions, standard SVMs are known to be universally consistent. As the number of training examples increases, the SVM solutions converge to the Bayes optimal hypothesis, which is the best classifier possible given the data generating distribution [35].
+ *Kernel trick.* As long as a kernel function can be defined between them, the input patterns may be arbitrary elements. For example text documents, graphs, or trees can directly serve as input to an SVM if a valid kernel function between them is defined. Kernel-based algorithms in general can be seen as elegantly separating the general part of a learning machine from the problem specific part. The kernel function (as well as the regularization parameter) allows for incorporation of domain-specific prior knowledge into the learning process, which is necessary to achieve well generalizing hypotheses.
∘ *Model selection problem.* Support vector machines – as most other learning machines – are not parameter-free in the sense that they do not intrinsically determine all entities their behavior is influenced by. The regularization parameter and a kernel function with additional free parameters must be specified externally. However, there cannot be a "universal" learning machine that excels across all possible problems (e.g., [4]). That is, one has to

incorporate prior knowledge to tailor a learning machine to some given task. For SVMs this includes choosing the SVM hyperparameters such as a proper family of kernel functions.

- *Multi-class classification.* There is no canonical extension of the binary SVM formulation (10) to multi-class problems with $|\mathcal{Y}| > 2$. Many application studies in the multi-class case rely on training and combining a number of binary machines. At the same time, several multi-class SVM formulations exist that solve the multi-category classification task in one joint optimization problem [8, 23, 40]. These all have different properties and require solvers distinct from those used for purely binary problems.

- *Training and execution time.* Training time in general is between quadratic and cubic in the number of training examples and additionally influenced by input dimension and kernel function [21]. Evaluating an SVM on an unseen example benefits from the sparseness property and is linear in the number of support vectors times the number of operations per kernel function evaluation. If the Bayes risk is non-zero, the number of support vectors scales linearly with the number of training examples [36]. Several extensions or modifications have been proposed to reduce training and execution times. The latter can be achieved, for instance, by approximating the SVM solution after training [27, 37].

In summary, consistency and convexity constitute convenient theoretical advantages that provide certain guarantees on the solution obtained by an SVM. In order for a practitioner to obtain truly meaningful results however, some familiarity with the model selection problem and standard techniques to approach it are essential. While SVM learning for non-standard domains – such as trees, graphs, or text – is well supported conceptually, this often gives rise to highly expertized fields of research in itself.

3 Hydroacoustic signal classification

We consider an application task of hydroacoustic signal classification using remote sensor data from the Comprehensive Nuclear-Test-Ban Treaty verification network.

3.1 Nuclear-Test-Ban verification

International arms control treaties must be verifiable with high confidence. A verification regime is a set of technological and administrative measures that discourages attempts towards treaty violation from the start by making actual violations detectable with high probability. The Comprehensive Nuclear-Test-Ban Treaty (CTBT) is an international agreement banning all nuclear explosions. As of 2011, it awaits formal ratification by nine further states before it will enter into force. Since 1996, the *Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization* (CTBTO) is tasked with building up a

global verification system for operation under the treaty. Nuclear weapons have been detonated underground, underwater, and in different altitudes of the atmosphere. While the latter two forms are banished under the Partial Nuclear Test Ban Treaty of 1963, the CTBT would also forbid, and hence require verification against, underground tests.

3.1.1 The International Monitoring System

At the heart of the CTBT's verification regime lies the *International Monitoring System* (IMS), a network of 321 geophysical monitoring stations positioned around the entire globe. Both the sensor technologies they employ as well as their locations have been defined by the treaty and its annexes. Any additional on-site inspection would be limited to an area of 1000 square kilometers through the treaty, which poses implicit constraints on the localization performance of the IMS. The IMS relies on four different monitoring technologies to achieve its goal [16, 38]. In full operation around 15 gigabyte of incoming data are expected each day, mostly transmitted in real time through a global VSAT satellite network. The largest subnetwork of 170 seismic stations, including arrays for enhanced detection capability, measures seismic energy traveling through the earth. Further, 60 infrasound stations record low-frequency pressure variations in the atmosphere, and 11 hydroacoustic stations measure energy transmitted through the world's oceans. These three sensor types constitute the so-called *waveform technologies*. While the analysis of waveform data can indicate that a detected event might not be of natural origin, the fourth sensor network, radionuclide measurements, can provide valuable evidence for a certain event being a nuclear explosion rather than an earthquake, chemical explosion, or other source not violating the treaty.

3.1.2 Hydroacoustic monitoring

The hydroacoustic network's main purpose is to monitor the oceans for underwater nuclear tests. The main signature of a test would be water pressure waves generated by the underwater explosion. Other sources of underwater sound are natural events like iceberg calving, suboceanic earthquakes, underwater volcanoes, and marine mammals. Man-made events include intentional or accidental chemical explosions (for example in military exercises or dynamite fishing), seismic air-gun surveys, and marine vessels. As a secondary use case, the hydroacoustic network can also contribute to processing of signals originating from the continents. Conceptually, global hydroacoustic monitoring relies on a natural phenomenon of underwater sound propagation. The deep sound channel (DSC) or SOFAR (sound fixing and ranging) channel is a certain depth region in the ocean around a minimum in the vertical sound speed profile. While local channel depths vary from close to the ocean's surface to around 1200 meters below, the DSC as a whole exhibits waveguide properties for underwater sound on a global scale. Due to this phenomenon, the relatively small number of IMS hydroacoustic stations is sufficient for global ocean coverage. The IMS hydroacoustic

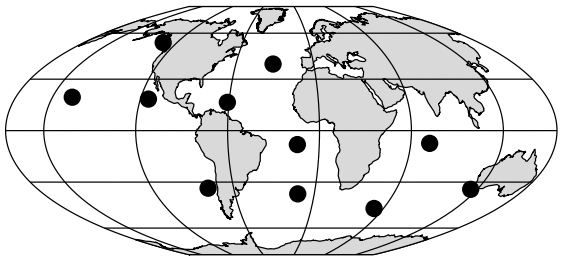


Fig. 3: Locations of hydroacoustic stations defined by the treaty.

network consists of 11 stations. Six of these use hydrophones placed underwater at the local deep sound channel axis, and five use seismometers residing near the coastline of steep-sloped oceanic islands. Figure 3 shows the locations of all hydroacoustic stations as defined by the treaty. Every on- and offshore station consists of several individual sensors, facing different sides of the island which hosts the communication infrastructure.

We classify signals recorded by IMS in-ocean hydrophones, learning to label them as either having explosive or non-explosive signature. Information about sensor or source location is not taken into account, and also no assumption is made that the same signal might have been recorded by multiple sensors. As a consequence, we solve a classical classification task as if all signals had been obtained independently and identically distributed through a single sensor.

3.2 Preprocessing

We want to evaluate the baseline potential of SVM hydroacoustic signal classification while relying on as few as possible modifications of the existing processing pipeline. We hence use for representation a set of pre-calculated features provided by the CTBTO's Provisional Technical Secretariat. The raw sensor data were sampled at 250 Hz and from the outset filtered into eight partially overlapping frequency bands between 1 and 100 Hz. Table 1 shows the filter band lower and upper frequency limits. In each band, detection and feature extraction are

Table 1: List of the eight frequency bands used for feature extraction.

	Frequency filter bands [Hz]							
Lower limit	1	2	3	6	8	16	32	64
Upper limit	2	80	6	12	16	32	64	100

carried out independently, but according to the same algorithm. Within the continuous data stream, a detection algorithm for each band monitors if the ratio of

a short-term average (10s window) to long-term average (150s window) exceeds a station-specific threshold. If detections in different frequency bands occur close enough in time, they are grouped into a signal, which is hence defined by one or more contemporaneous detections across frequency bands. For each signal a fixed set of 16 identically calculated features is extracted from every band with an associated detection. The union of all extracted features then serves as representation of the event which triggered the detections. Each event is thus represented by $\ell \cdot 16$ real numbers with $\ell \in \{1, \ldots, 8\}$. As a consequence the feature sets of any two given signals can differ and need not even overlap. The 16 features extracted in every frequency band are listed in Table 2. They can be

Table 2: Features extracted from each band with a detection.

Temporal	Energy	Statistical	Cepstral Peak (2x)
Peak Time	Peak Level	Time Spread	Position
Mean Arrival	Total Energy	Skewness	Level
Total Duration	Average Noise	Kurtosis	Variance
Zero Crossing Rate			

grouped into (i) time-related, (ii) energy-related, (iii) statistical moments, and (iv) cepstral features. The power cepstrum is a good indicator of periodicity in the signal's power spectrum, that is, the presence of harmonics. For this reason cepstral features may be good indicators of the bubble pulses possibly accompanying underwater explosions. They are also in general considered to well separate the propagation Green's function from the source function. The cepstral features listed in Table 2 were calculated in two variants, once from a low-pass filtered and once from a detrended spectrum.

3.3 Classifying incomplete data

The classification task described above falls into the group of missing data problems (e.g., [12]). For such it is common to consider a missingness matrix $R \in \{0, 1\}^{mN}$ of the same size as the matrix formed by all feature vectors $x_i \in S$. Each of its Boolean entries $R_{ij} \in \{0, 1\}$ indicates whether the corresponding feature x_{ij} is present in the sample x_i or not. The missingness matrix R of given training data S is then often interpreted as one specific instance or draw from an underlying *missingness distribution* p_R, just as S is assumed to be drawn from a data generating distribution p. This presumes that the missing values actually existed and would have been observable, but were for some reason not obtained. Such missing data problems are often grouped according to three possible relations between these two generating distributions. If p_R is completely independent of p, the data is coined *missing completely at random* (MCAR). A situation where p_R depends on p, but is conditionally independent of all missing values is termed *missing at random* (MAR). For all other relations between p_R

and p one speaks of data *missing not at random* (MNAR). In addition there are cases where a feature's absence is not simply due to non-observation, but the entity to be observed was undefined or did not exist for some reason. This is referred to as *structural absence*. CTBT hydroacoustic data constitute a mixture of features being MNAR and structurally absent.

The most convenient way to deal with samples holding missing values is to eliminate them from the training data, or to discard all features which exhibit missing values. Since the missingness ratios in the hydroacoustic data are high across both features and samples, and incomplete test cases with possibly unencountered missingness pattern have to be classifiable, neither is a viable option. In general, deletion can significantly bias both classifier and results, and hence a wide range of more systematic approaches have been suggested, see for example [12] for a review. Among these, imputation techniques are the most common, where missing values are filled in according to some heuristic. Traditional imputation techniques include constant value imputation (for example imputing zero or the mean feature value), and guessing a good imputation value, possibly through regression or by using the value of another example that is similar in some sense. More elaborate techniques include for example multiple imputation, a Monte Carlo technique for which an imputation model first has to be specified. Then multiple complete datasets are generated by sampling from the imputation model, analysis is carried out on each of the imputed datasets and then combined into one final result. In maximum-likelihood based approaches, an underlying model for the data generating process is assumed and its parameters estimated from the available data. Besides imputation, learning algorithms can also be modified to directly deal with incomplete input. For example, an elegant SVM variant by Chechik et al. avoids imputation by altering the margin interpretation for samples with values that are structurally absent [6].

In practice it is often tedious to identify among all possible approaches one that performs well on a given application problem. In addition, many of the above methods have been formulated for MAR and MCAR settings rather than MNAR or structural absence which are relevant for CTBT hydroacoustic data. We here use a straightforward approach and impute a single value of zero for all missing values. For many features in Table 2, this would constitute a physically or statistically plausible continuation for the limit case of a zero-threshold detector. For example peak and total energy as well as skewness of a non-present signal might be well represented by zero. For others, such as the average noise level, zero cannot be seen as a logical continuation and our choice is far from ideal. In addition to zero-imputation, we use the "flag" approach which was found to be a well-performing baseline method in [6]. For each of the eight frequency bands, a Boolean variable is added to the imputed feature set, indicating whether or not that band has been detected and its features extracted. We further extend this "flag" approach by using kernel functions which have a bipartite structure, with one sub-kernel operating on the Boolean missingness representation and another on the real-valued, imputed features.

3.3.1 Heterogeneous kernel functions

Let S_r denote the zero-imputed hydroacoustic training data and x_r one of its samples, a 128-dimensional real-valued vector. Then we write x_b for the corresponding missingness vector of eight Booleans indicating whether the features of each band are present or not. Thus each sample $x = (x_b, x_r)$ is represented by a vector in a 136-dimensional joint feature space $\mathcal{X}$, which is the Cartesian product $\mathcal{X}_b \times \mathcal{X}_r$ of the space of the according Boolean and real-valued feature vectors. In order to allow the machine to incorporate information held by the Boolean and real values differently we employ kernel functions with a *bipartite structure*, where one sub-kernel k_b operates on the Boolean features $x_b \in \mathcal{X}_b$ and another sub-kernel k_r on their real counterparts $x_r \in \mathcal{X}_r$. On $\mathcal{X}_r$ we employ a standard radial basis function (RBF) kernel $k(x_r, z_r) = e^{-\gamma\|x_r - z_r\|^2}$. For $\mathcal{X}_b$, a polynomial kernel $k(x_b, z_b) = (\langle x_b, z_b\rangle + c)^d$ is used. When combining the sub-kernels k_b and k_r into one joint kernel k through a function f,

$$k : (\mathcal{X}_b \times \mathcal{X}_r) \times (\mathcal{X}_b \times \mathcal{X}_r) \to \mathbb{R} \ , \ \ k(x, z) = f(k_b(x_b, z_b), k_r(x_r, z_r)) \ , \qquad (14)$$

f must be of such a form that the overall kernel k remains positive definite. Recalling the kernel composition rules of Section 2.5, we consider two intuitive possibilities. First, a direct product kernel

$$k_p(x, z) = (\langle x_b, z_b\rangle + c)^d \cdot e^{-\gamma\|x_r - z_r\|^2} \ , \qquad (15)$$

and a weighted direct sum kernel

$$k_s(x, z) = (\langle x_b, z_b\rangle + c)^d + we^{-\gamma\|x_r - z_r\|^2} \qquad (16)$$

with weighting factor $w \in \mathbb{R}^+$. The structure of k_p and k_s stresses the similarity of features across all bands on the one hand and inherent differences between the Boolean and real-valued features on the other.

Independent of the combination of k_b and k_r, we might desire an overall kernel family that is more suitable for our hydroacoustic application task. Especially given that underwater signal propagation is frequency-dependent, the overall kernel could better account for the fact that the input vector concatenates information from eight different frequency bands. Mirroring the steps above, we view $\mathcal{X}$ as the Cartesian product of the band-wise feature spaces: $\prod_{i=1}^{8}(\mathcal{X}_b^{(i)} \times \mathcal{X}_r^{(i)})$. For each band's subspace $\mathcal{X}^{(i)}$ a *band-wise bipartite direct product kernel* $k^{(i)}$ can in analogy to eq. (15) be defined as

$$k^{(i)}(x^{(i)}, z^{(i)}) = k_b^{(i)} \cdot k_r^{(i)} = (\langle x_b^{(i)}, z_b^{(i)}\rangle + c)^d \cdot e^{-\gamma^{(i)}\|x_r^{(i)} - z_r^{(i)}\|^2} \ . \qquad (17)$$

Here the polynomial kernel parameters c and d are chosen identical across all sub-kernels $k^{(i)}$. The RBF bandwidth parameters $\gamma^{(i)}$ are however allowed to vary from band to band since we expect different feature distributions across the frequency bands. Note that in each sub-kernel (17) the Boolean sub-kernel operates on two single Boolean values only. The corresponding scalar product

can hence only yield one (if both samples have a detection in band i) or zero (if only one or none of them do). In the special case of $c = 0$ this has the effect of switching on or off the contribution of the overall sub-kernel: if two samples both have detections for band i, $k^{(i)}$ returns the RBF kernel evaluation between their real-valued features in band i. If only one or none hold detections in band i, $k^{(i)}$ returns zero. For this reason, and because it would introduce again more hyperparameters, we consider the direct product kernel (15) on the subspaces $\mathcal{X}^{(i)}$ rather than the weighted direct sum kernel (16). For combining all sub-kernels $k^{(i)}$ into one overall kernel, both addition and multiplication are feasible options. As seen in Section 2.5, convolution kernels allow for multiplication as well as addition of sub-kernels and also cover an intermediate range by varying the integer degree D as single free parameter. The convolution kernel k_D of degree D on the eight sub-kernels $k^{(i)}$ is

$$k_D(x, z) = \sum_{1 \le j_1 < \cdots < j_D \le 8} \prod_{d=1}^{D} k^{(j_D)}(x^{(j_D)}, z^{(j_D)}) \ . \tag{18}$$

With equations (15, 16, 18) we have three candidate families of kernels for the imputed, Boolean-augmented data S on $\mathcal{X}$. All three kernels have as free parameters the real-valued polynomial offset $c \in \mathbb{R}_0^+$ and integer degree $d \in \mathbb{N}^+$. For eq. (15) and (16) the RBF kernels introduce the bandwidth $\gamma \in \mathbb{R}^+$ as single parameter, while eq. (18) holds one RBF parameter $\gamma^{(i)} \in \mathbb{R}^+$ for each frequency band. An SVM using kernel (18) has 11 free kernel parameters plus the SVM regularization parameter C. In the following we describe our experimental setup, including the model selection procedure to determine these SVM hyperparameters.

3.4 Experiments

In total 778 expert-labeled samples were available for classifier training, validation and testing. Of these, less than 5% had values for all 128 features, while 91% of samples held values for the most common frequency band between 6 and 12 Hz. For all experiments described below we obtained the test error as an average over five different splits into 80% training and 20% test data. Within each of these 80% of training data we for all SVM classifiers used another "inner" 5-fold cross-validation procedure for SVM model selection. The best hyperparameters were used to re-train an SVM on the entire 80% before obtaining the test error on the remaining 20% of test data. For the direct sum and direct product kernel, we conducted simple grid search on the five-fold cross-validation error CV-5 to find the best values for c, d, (w), γ, and C. For the convolution kernel grid search is far from feasible and we employed the maximum-likelihood based approach described in Section 2.7.2. We optimized the real-valued parameters only and repeated this for different combinations of integer values for the kernel parameters d and D.

3.5 Results

We compared SVMs using the three candidate kernels (15, 16, 18) on the zero-imputed and Boolean-augmented dataset S to two baseline methods which operated on the zero-imputed, but not Boolean-augmented dataset S_r only. Table 3 shows the results obtained. In the first column, *LDA* refers to a baseline linear discriminant analysis [17]. The SVM baseline classifier *svm* used one single RBF kernel and was optimized by grid search as well. The three entries *svm-s*, *svm-p*, and *svm-c* all operated on the zero-imputed and Boolean-augmented training data S, and correspond to the candidate SVMs with a direct sum kernel (eq. 16), direct product kernel (eq. 15), and convolution kernel of degree one (eq. 18), respectively. In summary, all SVMs performed better than the linear approach, and the two bipartite kernels from eqs. (15, 16) were on par with the baseline RBF kernel not having access to the Boolean-encoded missingness pattern. Additionally passing the Boolean indicators to the baseline *svm* did not influence its performance. The convolution kernel of degree one, which corresponds to summing up all band-wise sub-kernels, performed best among all approaches. With increasing degree however, error rates tended to increase as well. At the highest value of $D = 8$, which corresponds to multiplying all band-wise sub-kernels, the test error with 5.9% was higher than that of LDA.

Table 3: Average classification test errors for the binary case.

	Classifier				
	LDA	svm	svm-s	svm-p	svm-c
Error [%]	5.2	4.9	4.9	4.8	4.3

It should be noted that SVMs allow to control the trade-off between sensitivity and specificity, or false positive and false negative rates, by penalizing positive and negative misclassification differently through two different values for the regularization parameter C. Table 3 should hence be seen as ranking the different approaches at some generic operation point rather than providing actual error rates for the practical application. It might be desirable to operate such a classifier at high sensitivity at the cost of more false alarms having to be rejected during human analyst review.

4 Summary

We introduced support vector machines (SVMs) as one specific approach to solving supervised classification tasks. Motivated by the concept of regularized risk minimization we iteratively refined the SVM optimization problem from linear large-margin classification to the canonical kernelized case. Emphasizing several properties of SVMs relevant to practitioners, we in particular discussed the

model selection problem and two approaches towards it: simple grid search as well as one gradient-based method for hyperparameter selection. In the second part of the chapter, we described an exemplary application task of classifying hydroacoustic signals recorded by the sensor network for verification of the Comprehensive Nuclear-Test-Ban Treaty. We combined information from different frequency bands via task-specific kernel functions also incorporating information about a sample's missingness pattern. This custom classifier, in combination with parameter optimization through a maximum-likelihood approach to model selection, showed improved performance over baseline linear methods as well as support vector machines using standard kernels.

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