Kernel Pre-Training in Feature Space via \( m \)-Kernels

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Abstract

This paper presents a novel approach to kernel tuning. The method presented borrows techniques from reproducing kernel Banach space (RKBS) theory and tensor kernels and leverages them to convert (re-weight in feature space) existing kernel functions into new, problem-specific kernels using auxiliary data. The proposed method is applied to accelerating Bayesian optimisation via covariance (kernel) function pre-tuning for short-polymer fibre manufacture and alloy design.

1 Introduction

The kernel trick \( \{2\} \{17\} \{3\} \) is well known in machine learning and provides an elegant means of encapsulating a combined feature map (non-linear map \( \varphi: \mathbb{R}^n \rightarrow \mathbb{R}^d \) from input space into feature space) and inner product into a simple function \( K: \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \) that effectively hides the feature map: starting from a positive definite kernel \( K \) one can prove that there exists an associated (implicit) feature map \( \varphi \) such that \( K(x, x') = <\varphi(x), \varphi(x')> \), all without knowing (or needing to know) what form \( \varphi \) actually takes. This allows the (implicit) use feature maps of essentially arbitrary complexity at little or no additional computational cost.

While elegant, the kernel trick is not magic. Typically the kernel \( K \) is selected from a set of “standard” kernels to minimise cross-fold error, test-set error, log-likelihood or similar. In so doing one is essentially picking a feature map from a bag of “standard” feature maps. The result of this process is a feature map (not known but implicitly defined by a kernel) that may, barring an extremely unlikely perfect match scenario, be viewed as the least-worst of the available maps. Techniques such as hyper-parameter tuning, multi-kernel learning \( \{10\} \{1\} \) etc aim to improve on this situation by fine-tuning the kernel (and hence the implicit feature map) or combining kernels (and hence the combining the feature maps implicit in them). However one is still limited in the space of reachable feature maps, and there is no clear interpretation of such techniques from a feature-space perspective.

Our motivation is as follows: suppose the “best” kernel \( K \) for a given dataset \( D \), found using standard techniques, has associated with it an (implicit) feature map \( \varphi \). As the least-worst option, this map will have many individual features \( \varphi_i(x) \) in it that are highly relevant to the problem at hand, which we would like to emphasise, but also some features \( \varphi_j(x) \) that are either not relevant or actively misleading which we would like to suppress or remove. This implies three questions: (a) how can

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we identify the (ir)relevant features, (b) how can we amplify (or suppress) features to obtain a better feature map and (c) how can we do steps (a) and (b) without direct access to the feature map \( \varphi \) (whose existence we infer from the positive definiteness of \( K \) but whose form we do not know)?

To address question (a) we use standard machine-learning techniques. If we apply for example a support vector machine (SVM) [2] method (or similar) equipped with kernel \( K \) to learn either from dataset \( D \) or some related dataset \( D_0 \), then the answer we obtain takes the form of the representation \( \alpha_1, \alpha_2, \ldots \) of a weight vector \( w = \sum_i \alpha_i \varphi(x_i) \) in feature space. Assuming a reasonable “fit” the weights \( w_i \) will be larger in magnitude for relevant features and smaller for irrelevant ones.

To address questions (b) and (c) we borrow concepts from reproducing kernel Banach space (RKBS) theory [4, 21, 6] and \( \ell^p \)-norm regularisation [16, 15] - in particular \( m \)-kernels (tensor kernels [15], moment functions [4]) - and prove that it is possible to adjust the magnitudes of individual features without explicitly knowing the feature map. We show that, if \( K \) is a kernel with implied feature map \( \varphi \), and \( \alpha_0, \alpha_1, \ldots \) implicitly define a weight vector \( w = \sum_i \alpha_i \varphi(x_i) \) in feature space (with larger \( |w_i| \) implying greater relevance), then we may perform a kernel re-weighting operation:

\[
    K(x, x') = \langle \varphi(x), \varphi(x') \rangle \rightarrow K^w(x, x') = \langle w \odot \varphi(x), w \odot \varphi(x') \rangle
\]

that converts a kernel \( K \) (whose implied feature map \( \varphi \) containing both relevant and irrelevant features) into a kernel \( K^w \) with implicit features \( w_i \varphi_i \) that emphasises relevant features (larger \( |w_i| \)) and suppresses irrelevant or misleading ones (smaller \( |w_i| \)), as shown in figure 1. That is, we may pre-tune (re-weight) our kernel to “fit” a particular problem, adjusting the implicit feature map in a principled manner without any explicit (direct) knowledge of the feature map itself.

To achieve this in section 2.1 we describe \( m \)-kernels (tensor-kernels [15] [16], moment function [4]) formally, and then in section 3 introduce a new concept, free kernels, which are families of \( m \) kernels embodying the same underlying feature map over a range of \( m \) (examples are given in table 1). We then formally prove how \( m \)-kernels may be re-weighted in theorem 1 to emphasise/suppress features, and in section 4 develop an algorithm (algorithm 1) that utilises the concept of kernel re-weighting to tune kernels by suppressing irrelevant features and emphasising important ones.

We demonstrate our method on accelerated Bayesian Optimisation (BO [13]). By pre-tuning the covariance function (kernel) of the Gaussian Process (GP [14]) using auxiliary data we show a speedup in convergence due to better modelling of our function. We consider (1) new short polymer fibre design using micro-fluid devices (where auxiliary data is generated by an older, slightly different device) and (2) design of a new hybrid Aluminium alloy (where auxiliary data is based on 46 existing patents for aluminium 6000, 7000 and 2000 series). In both cases kernel pre-tuning results in superior performance.

Our main contributions are:

- Introduction of the concept free kernels: families of \( m \)-kernels whose corresponding (implied) feature weights and maps are independent of \( m \) (definition 1, section 3).
- Construction of a range of \( m \)-kernel analogues of standard kernels (table 1).
- Development of kernel re-weighting theory: a method of tuning free kernels to adjust implied feature weights (theorem 1, section 3).
- Design of an algorithm using kernel re-weighting for pre-tuning of kernels to fit data (algorithm 1, section 4).

Figure 1: Geometry of kernel re-weighting in feature space, 2-dimensional example.
1.1 Notation

Sets are written $A, B, \ldots$; with $\mathbb{Z}_+ = \{1, 2, \ldots\}$, $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$, $\mathbb{Z}_+ = \mathbb{Z}_+ \cup \{\infty\}$. Column vectors are bold lower case $\mathbf{a}, \mathbf{r}$. Matrices are bold upper case $\mathbf{W}$. Element $i$ of vector $\mathbf{a}$ is $a_i$. Element $i, j$ of matrix $\mathbf{W}$ is $W_{i,j}$, $\mathbf{a}^T$ is the transpose, $\mathbf{a} \odot \mathbf{b}$ the elementwise product, $\mathbf{a}^\odot \mathbf{b}$ the elementwise power, $|\mathbf{a}|$ the elementwise absolute value, $\text{sgn}(\mathbf{a})$ the elementwise sign, and $\text{sum}(\mathbf{a}) = \sum_i a_i$. $\mathbf{1}$ a vector of 1s and $\mathbf{0}$ a vector of 0s. The Kronecker product is $\mathbf{a} \otimes \mathbf{b}$. The inner-product $\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a}^\odot \mathbf{b} = \sum_i a_i b_i$. The elementwise absolute value, $|\mathbf{a}| = \sqrt{\mathbf{a}^\odot \mathbf{a}}$. Matrices are bold upper case $\mathbf{A}$.

2 Problem Statement and Background

The kernel trick is well known in machine learning. A (Mercer) kernel is a function $K : (\mathbb{R}^d)^m \to \mathbb{R}$ for which there exists a corresponding feature map $\varphi : \mathbb{R}^d \to \mathbb{R}^d$, $d \in \mathbb{Z}_+$, such that $\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$:

$$K(\mathbf{x}, \mathbf{x}') = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \rangle$$

(1)

Geometrically, if $\theta(\mathbf{x}, \mathbf{x}')$ is the angle between $\varphi(\mathbf{x})$ and $\varphi(\mathbf{x}')$ in feature space:

$$K(\mathbf{x}, \mathbf{x}') = ||\varphi(\mathbf{x})||_2 ||\varphi(\mathbf{x}')||_2 \cos \theta(\mathbf{x}, \mathbf{x}') = \sqrt{K(\mathbf{x}, \mathbf{x})}\sqrt{K(\mathbf{x}', \mathbf{x}')}
\cos \theta(\mathbf{x}, \mathbf{x}')$$

(2)

so $K(\mathbf{x}, \mathbf{x}')$ is a measure of the similarity of $\mathbf{x}$ and $\mathbf{x}'$ in terms of their alignment in feature space. For a normalised kernel such as the RBF kernel this simplifies to $K(\mathbf{x}, \mathbf{x}') = \cos \theta(\mathbf{x}, \mathbf{x}')$.

In practice a kernel $K$ is usually selected from a set of well-known kernels, (e.g. the polynomial kernel $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\odot \mathbf{x}')^p$ or an RBF kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$), possibly with additional hyper-parameter tuning and/or consideration of kernel combinations (e.g. multi-kernel learning $[10][11]$). However the resulting kernel (and the feature map implied by it) may still be viewed as a “least-worst fit” from a set of readily available feature maps.

In the present paper we show how the feature map implied by a given kernel $K$ may be tuned, in a principled manner, to make it better fit the data. Using techniques from reproducing kernel Banach spaces $[4][2][6]$ and $\ell^p$-norm regularisation $[16][15]$ to show how kernels can be pre-trained or re-weighted by scaling the features of the feature map $\varphi$ embodied by a kernel $K$:

$$K(\mathbf{x}, \mathbf{x}) = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}) \rangle \rightarrow K^\mathbf{w}(\mathbf{x}, \mathbf{x}) = \langle w \odot \varphi(\mathbf{x}), w \odot \varphi(\mathbf{x}) \rangle$$

(3)

to emphasise important features (in feature space) over unimportant features. The geometry of this operation is shown in figure $[4]$, important features can be emphasised or amplified, while irrelevant or misleading features are de-emphasised.

2.1 $m$-Kernels

A number of generalisations of the basic concept of kernel functions arise in generalised norm SVMs $[12][13]$, reproducing kernel Banach-space (RKBS) theory $[4][2][6]$ and $\ell^p$-norm regularisation $[16][15]$. Of interest here is the $m$-kernel (tensor kernel $[16]$, moment function $[4]$), which is a function $K : (\mathbb{R}^n)^m \to \mathbb{R}$ for which there exists an (unknown) feature map $\varphi : \mathbb{R}^n \to \mathbb{R}^d$ such that:

$$K(\mathbf{x}, \mathbf{x}', \ldots, \mathbf{x}''') = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}'), \ldots, \varphi(\mathbf{x}''') \rangle_m \quad \forall \mathbf{x}, \mathbf{x}', \ldots, \mathbf{x}''' \in \mathbb{R}^n$$

(4)

(so Mercer kernels are 2-kernels). Discussion of the properties of $m$-kernels may be found in $[15][16][4]$. Examples of $m$-kernels include:

- **$m$-inner-product kernels**: By analogy with the inner-product kernels it may be shown $[15]$ that, given $k : \mathbb{R} \to \mathbb{R}$ expandable as a Taylor series $k(\chi) = \sum_i \xi_i \chi^i$, the function:

$$K(\mathbf{x}, \mathbf{x}', \ldots, \mathbf{x}''') = k(\langle \mathbf{x}, \mathbf{x}', \ldots, \mathbf{x}''\rangle_m)$$

(5)

is an $m$-kernel if and only if all terms in the series are non-negative.

- **$m$-direct-product kernels**: Similarly for any Taylor-expandable $\kappa : \mathbb{R} \to \mathbb{R}$, $\kappa(\chi) = \sum_i \rho_i \chi^i$, with non-negative terms the function:

$$K(\mathbf{x}, \mathbf{x}', \ldots, \mathbf{x}''') = \prod_i \kappa(x_i, x_i', \ldots x_i''')$$

(6)

is an $m$-kernel (a special case of a Taylor kernel $[15]$).
A canonical application of \( \varphi \) (representor theorem) and hence:

Let \( \text{Definition 1 (Free kernels)} \) related domains. We begin with the following definition:

### 2.2 \( p \)-Norm Support Vector Machines

A canonical application of \( m \)-kernels is the \( p \)-norm support vector machine (SVM) (\( \ell^p \)-SVM \[16\], max-margin \( \ell^p \) moment classifier \[4\]). Let \( \mathcal{D} = \{ (x_i, y_i) \in \mathbb{R}^d \times \mathbb{Y} | i \in \mathbb{Z}_N \} \) be a training set. Following \[16\] the aim is to find a sparse (in \( w \)) trained machine:

\[
g(x) = w^T \varphi(x) + b
\]

(7)

where \( \varphi: \mathbb{R}^n \to \mathbb{R}^d \) is implied by a \( 2q \)-kernel \( K \) to fit the data. \( w \in \mathbb{R}^d, b \in \mathbb{R} \) are found by solving the \( p \)-norm SVM training problem, where \( 1 < p \leq 2 \) is dual to \( 2q \) (i.e. \( \frac{1}{p} + \frac{1}{2q} = 1 \)):

\[
\min_{w, b} R_p(w, b, \xi) = r \left( \frac{1}{p} \|w\|_p^p + \frac{C}{N} \sum_{i \in \mathcal{Z}_N} E(y_i, g(x_i)) \right)
\]

(8)

where \( r \) is strictly monotonically increasing, \( E \) is an arbitrary empirical risk function, and the use of \( p \)-norm regularisation with \( 1 < p \leq 2 \) encourages sparsity in \( w \) in feature space. Following \[16\] \[15\]:

\[
w = \sum_{i_1, \ldots, i_{2q} \in \mathcal{Z}_N} \alpha_{i_1} \alpha_{i_2} \cdots \alpha_{i_{2q}} \varphi(x_{i_1}) \odot \varphi(x_{i_2}) \odot \cdots \odot \varphi(x_{i_{2q}})
\]

(9)

(representor theorem) and hence:

\[
g(x) = \sum_{i_1, \ldots, i_{2q} \in \mathcal{Z}_N} \alpha_{i_1} \alpha_{i_2} \cdots \alpha_{i_{2q}} K(x, x_{i_1}, x_{i_2}, \ldots, x_{i_{2q}}) + b
\]

(10)

where \( K \) is a \( 2q \)-kernel with implied feature map \( \varphi \) (the \( m \)-kernel trick). Moreover we may completely suppress \( w \) and construct a dual training problem entirely in terms of \( \alpha \) \[15\] \[16\] - e.g. if \( \mathbb{R} = \mathbb{Y} \), \( E(y, g) = \frac{1}{2}(y - g)^2 \) (ridge regression), the dual training problem is:

\[
\min_{\alpha} \frac{1}{2D} \sum_{i_0, i_1, \ldots, i_{2q-1} \in \mathcal{Z}_N} \alpha_{i_0} \alpha_{i_1} \cdots \alpha_{i_{2q-1}} K_{i_0, i_1, \ldots, i_{2q-1}} + \frac{N}{2C} \alpha^T \alpha - y^T \alpha
\]

such that:

\[ 1^T \alpha = 0 \]

(11)

where \( K_{i_0, i_1, \ldots, i_{2q-1}} = K(x_{i_0}, x_{i_1}, \ldots, x_{i_{2q-1}}) \). Similar results, analogous to the “standard” SVMs (e.g. binary classification) may be likewise constructed \[15\] \[16\] \[4\].

### 3 Making Kernels from \( m \)-Kernels - Free Kernels and Kernel Re-Weighting

In the present context we wish to leverage the additional expressive power of the \( m \)-kernels to directly tune the feature map to suit the problem (or problems) at hand. In particular we will demonstrate how kernels may be pre-tuned or learnt for a particular dataset and then transferred to other problems in related domains. We begin with the following definition:

**Definition 1 (Free kernels)** Let \( \bar{m} \in 2\mathbb{Z}_+ \). A free kernel (of order \( \bar{m} \)) is a family of functions \( K_m : (\mathbb{R}^n)^m \to \mathbb{R} \) indexed by \( m \in \bar{m} \mathbb{Z}_+ \) for which there exists an (unweighted) feature map \( \vartheta : \mathbb{R}^n \to \mathbb{R}^d \) and feature weights \( \tau \in \mathbb{R}^d \) (\( d \in \mathbb{Z}_+ \)), both independent of \( m \), such that \( \forall m \in \bar{m} \mathbb{Z}_+ \):

\[
K_m(x, x', \ldots, x'''') = \left\{ \tau^2, \vartheta(x), \vartheta(x'), \ldots, \vartheta(x''') \right\}_{m+1}
\]

(12)
For fixed \( m \in m\mathbb{Z}_+ \), a free kernel of order \( m \) defines (is) an \( m \)-kernel with implied feature map:

\[
\varphi_m(x) = \tau^{2/m} \odot \vartheta(x)
\]

(13)

We assume free kernels of order 2 throughout unless otherwise specified. Note that the \( m \)-inner-product and \( m \)-direct product kernels are free kernels (it is straightforward to show that they have implied feature map \( \vartheta(x) = \otimes \delta_{\alpha}(x)^{\alpha} \) and implied feature weights, respectively, \( \tau^{inner} = \sum_{i_0,i_1,\ldots,i_n-1} \delta_{\alpha}(x)^{\alpha} \) and \( \tau^{direct} = \sum_{i_0,i_1,\ldots,i_n-1} \rho_{\alpha}(x)^{\alpha} \)). It follows that all of the kernels in table [1] are free kernels. Given a free-kernel \( K_m \) of order \( m \in 2\mathbb{Z}_+ \), we have the following key theorem that enables us to re-weight or tune the kernel:

**Theorem 1** Let \( K_m \) be a free kernel of order \( m \) with implied feature map \( \vartheta \) and feature weights \( \tau \); and let \( E = \{(x_i,\alpha_i) : x_i \in \mathbb{R}^n, \alpha_i \in \mathbb{R} \} \) and \( q \in \mathbb{Z}_+ \). Then the function \( K^E_m \) defined by:

\[
K^E_m(x_i,\ldots,x_{jm+q})(x_i,\ldots,x_{jm+q}) = \sum_{j_1,j_2,\ldots,j_{m+q}} \alpha_{j_1} \cdot \alpha_{j_2} \cdots \alpha_{j_{m+q}} \cdot \varphi_2(x_{j_1}) \odot \varphi_2(x_{j_2}) \odot \cdots \odot \varphi_2(x_{j_{m+q}})
\]

defines a free kernel of order \( m \) with implied feature map \( \vartheta^E = \vartheta \) and weights \( \tau^E_2 = w^2 \), where:

\[
w = \sum_{i_1,i_2,\ldots,i_{jm+q}} \alpha_{i_1} \alpha_{i_2} \cdots \alpha_{i_{jm+q}} \varphi(x_{i_1}) \odot \varphi(x_{i_2}) \odot \cdots \odot \varphi(x_{i_{jm+q}})
\]

and we note that \( w \) has the form of the representation \( \vartheta \) of \( w \) in a \( p \)-norm SVM, \( \frac{1}{p} + \frac{1}{mq} = 1 \).

**Proof:** This result follows from definition [1] by substitution and application of equation (13).

| 4 The Kernel Pre-Tuning Algorithm |

Having established our theoretical results we arrive at the core of our method - an algorithm for tuning kernels using re-weighting (theorem [1]) to fit a dataset. Our algorithm is detailed in algorithm [1] and illustrated in figure [2]. It is assumed that we are given a dataset \( D_0 = \{(x_{i_0},y_{i_0}) \in \mathbb{R}^n \times \forall |i| \in Z_{N_0}\} \) from which to infer feature relevance, and a free kernel \( K_m \). Then, assuming \( m = 2, q = 1 \) for simplicity, we proceed as follows:

1. The free kernel \( K_m \) defines a two-kernel \( K_2 \) for \( m = 2 \), implying feature map \( \varphi_2 \) by (13).
2. Train an SVM using \( K_2 \) and \( D_0 \) to obtain \( \alpha_0, \alpha_1, \ldots \) and hence \( E = \{(\alpha_i, x_i) | i \in Z_{N_0}\} \), implying weights \( w = \sum_i \alpha_i \varphi_2(x_i) \) in feature space by theorem [1].
3. Using \( K_m \) and \( E \), construct re-weighted kernel \( K^E_2 \) using (14), where \( K^E_2 \) has implied feature map \( w \odot \varphi_2 \) by theorem [1].

In the more general case \( m \in 2\mathbb{Z}_+, q \in \mathbb{Z}_+ \) a \( p \)-norm SVM (\( \frac{1}{p} + \frac{1}{mq} = 1 \)) generates a sparse weight vector \( w \), but the concept is the same. Note that at no point in this process do we need to explicitly know the implied feature map or weights - all work is done entirely in kernel space.

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1 The RBF kernel has unweighted feature map \( \vartheta(x) = \| \varphi_{\exp}(x) \|^2 \theta^\exp(x) \) and weights \( \tau = \tau^\exp \), where \( \varphi_{\exp}, \theta^\exp, \tau^\exp \) are the feature map \( m = 2 \), unweighted feature map and weights of the exponential kernel.
Algorithm 1 Kernel Tuning (re-weighting) Algorithm.

**input** Dataset \( D_q \), free kernel \( K_m \) of order \( m \in 2\mathbb{Z}_+ \), order \( q \in \mathbb{Z}_+ \).

Train a \( p \)-norm SVM (\( \frac{1}{p} + \frac{1}{mq} = 1 \)) with \( D_q \) with \( mq \)-kernel \( K_{mq} \) (\( K_m \) with \( m = mq \)) to get \( a_{0q} \).

Construct re-weighted free-kernel \( K_{m}^E \) of order \( m \) using the definition:

\[
K_m^E(x, \ldots, x^{m'}) = \sum_{i_1=1}^{N} \ldots \sum_{i_{mq}=1}^{N} \alpha_0 i_1 \alpha_0 i_2 \ldots \alpha_0 i_{mq-1} \alpha_0 j_1 \ldots \alpha_0 j_{mq-1} \ldots \sum_{i_1=1}^{N} \ldots \sum_{i_{mq}=1}^{N} \alpha_0 i_1 \alpha_0 i_2 \ldots \alpha_0 i_{mq-1} \alpha_0 j_1 \ldots \alpha_0 j_{mq-1} \ldots \]

5 Application: Accelerated Bayesian Optimisation

In this section we present a practical example of the application of kernel pre-tuning via re-weighting, namely accelerated Bayesian Optimisation.

Bayesian Optimisation (BO) [13] is a form of sequential model-based optimisation (SMBO) that aims to find \( x^* = \arg \max_x f(x) \) with the least number of evaluations for an expensive (to evaluate) function \( f : \mathbb{R}^n \to \mathbb{R} \). It is assumed that \( f \sim \text{GP}(0, K) \) is a draw from a zero mean Gaussian Process (GP) [14] with covariance function (kernel) \( K: (\mathbb{R}^n)^2 \to \mathbb{R} \). As with kernel selection, \( K \) is typically not given a-priori but selected from a set of “known” covariance functions (kernels) using heuristics such as max-log-likelihood. Nevertheless the speed of convergence is critically dependent on having a good model for \( f \), which requires selection of an appropriate covariance function.

In this experiment we consider the case where we have access to prior knowledge that is related to - but not generated by - \( f \). Let \( D_0 = \{(x_{oi}, y_{oi}) | x_{oi} \in \mathbb{R}^n, y_{oi} = f_0(x_{oi}) \in \mathbb{Y} \} \). In general \( f_0 \neq f \) and \( \mathbb{Y} \neq \mathbb{R} \), but we assume that both \( f \) and \( f_0 \) are influenced by the same (or very similar) features. In this experiment we use \( D_0 \) to tune our covariance function \( K \) via algorithm 1 to fit \( f_0 \) (and hence \( f \)), giving us a better fit for our covariance function and accelerated convergence. Our algorithm is presented in algorithm 2 which is like a standard BO algorithm except for the covariance function pre-tuning step.

Algorithm 2 Bayesian Optimisation with Kernel re-weighting.

**input** \( D_0, D_q \), free kernel \( K_m \) of order 2.

Generate pre-tuned kernel \( K_2^E \) using algorithm 1.

Modelling \( f \sim \text{GP}(0, K_2^E) \), proceed:

for \( t = 1, 2, \ldots, T \) do

Select test point \( x_t = \arg \max_{x_t} a_t(x) \).

Perform Experiment \( y_t = f(x_t) + \epsilon \).

Update \( D_t := D_{t-1} \cup \{(x_t, y_t)\} \).

end for

As noted previously we model \( f \sim \text{GP}(0, K_2^E) \), allowing us to model the posterior \( f(x) | D_t \sim \mathcal{N}(\mu_t(x), \sigma_t^2(x)) \) at iteration \( t \) with mean \( \mu_t(x) \) and variance \( \sigma_t^2(x) \) in the usual manner [14]. For the acquisition function \( a_t \) we test expected improvement (EI) [8] and GP upper confidence bound (GP-UCB) [19], respectively (alternatives include probability of improvement (PI) [9] and predictive entropy search (PES) [7]).

5.0.1 Short Polymer Fibres

In this experiment we have tested our algorithm on the real-world application of optimizing short polymer fibre (SPF) to achieve a given (median) target length [11]. This process involves the injection of one polymer into another in a special device [20]. The process is controlled by 3 geometric parameters (channel width (mm), constriction angle (degree), device position (mm)) and 2 flow factors (butanol speed (ml/hr), polymer concentration (cm/s)) that parametrise the experiment - see figure 3. Two devices (A and B) were used. Device A is armed by a gear pump and
allows for three butanol speeds (86.42, 67.90 and 43.21). The newer device B has a lobe pump and allows butonal speed 98, 63 and 48. Our goal is to design a new short polymer fibre for Device B that results in a (median) target fibre length of 500 μm.

We write the device parameters as \( x \in \mathbb{R}^5 \) and the result of experiments (median fibre length) on each device as \( d_A(x) \) and \( d_B(x) \), respectively. Device A has been characterised to give a dataset \( D_0 = \{ (x_{0i}, y_{0i}) \mid y_{0i} = d_A(x_{0i}) \} \) of 163 input/output pairs. We aim to minimise: \( f(x) = (d_B(x) - 500)^2 \), noting that \( f \neq d_B \) (the objective \( f \) differs from the function generating \( D_0 \), although both relate to fibre length). Device B has been similarly characterised and this grid forms our search space for Bayesian optimisation.

For this experiment we have used the free RBF kernel \( K_m \). An SVM was trained using \( D_0 \) and this kernel (hyperparameters \( C \) and \( \sigma \) were selected to minimise leave-one-out mean-squared-error (LOO-MSE)) to obtain \( \xi = \{ (x_{0i}, \alpha_{0i}) \} \). The re-weighted kernel \( K^2_2 \) obtained from this was normalised (to ensure good conditioning along the diagonal of \( K_2 \)) and used in Bayesian optimisation as per algorithm 2. All data was normalised to \([0, 1]\) and all experiments were averaged over 40 repetitions.

We have tested both the EI and GP-UCB acquisition functions. Figure 4 shows the convergence of algorithms in terms of minimum squared distance from the set target versus iterations. GP-UCB and EI indicate acquisition function used. MK indicates mixture kernel used. rmK indicates our proposed method.

![Figure 4: Short Polymer Fibre design. Comparison of algorithms in terms of minimum squared distance from the set target versus iterations.](image)

5.0.2 Aluminium Alloy Design using Thermo-Calc

This experiment considers optimising a new hybrid Aluminium alloy for target yield strength. Designing an alloy is an expensive process. Casting an alloy and then measuring its properties usually takes long time. An alloy has certain phase structures that determine its material properties. For example, phases such as C14LAVES and ALSC3 are known to increase yield strength whilst others such as AL3ZR_D023 and ALLI_B32 reduce the yield strength of the alloy. However a precise function relating the phases to yield strength does not exist. The simulation software Thermo-Calc takes a mixture of component elements as input and computes the phase composition of the resulting alloy. We consider 11 elements as potential constituents of the alloy and 24 phases. We use Thermo-Calc for this computation.

A dataset \( D_0 \) of 46 closely related alloys filed as patents was collected. This dataset consists information about the composition of the elements in the alloy and their yield strength. The phase compositions extracted from Thermo-Calc simulations for various alloy compositions were used to understand the positive or negative contribution of phases to the yield strength of the alloy using linear regression. The weights retrieved for these phases were then used formulate a utility function. Figure 5 shows the regression coeffs for the phases contributing to the yield strength.

The kernel selection and tuning procedure was used here as for the short polymer fibre experiment. We have tested both the EI and GP-UCB acquisition functions. Figure 6 shows the convergence of
our proposed algorithm compared to standard Bayesian optimisation (using a standard RBF kernel as our covariance function). Relevant hyperparameters in Bayesian optimisation (ν for our method and kernel mixtures, ν and σ for standard Bayesian optimisation) were selected using max-log-likelihood at each iteration. As can be seen from figure 6 our proposed approach outperforms standard Bayesian optimisation by a significant margin for both EI and GP-UCB.

5.0.3 Simulated Experiment

In this experiment we consider use of kernel re-weighting to incorporate domain knowledge into a kernel design. We aim to minimise the function:

\[ f(\mathbf{x}) = \sin(5\pi \| \mathbf{x} \|_2) \exp \left( -5 \left( \| \mathbf{x} \|_2 - \frac{1}{2} \right)^2 \right) \]

as illustrated in figure 7, where \( \mathbf{x} \in [-1, 1]^2 \). Noting that this function has rotational symmetry we select an additional dataset to exhibit this property, namely: \( D_\diamond = \{(\mathbf{x}_\diamond, y_\diamond) | y_\diamond = \| \mathbf{x}_\diamond \|_2 \} \), of 100 vectors, where \( \mathbf{x}_\diamond \) is selected uniformly randomly. Thus \( D_\diamond \) reflects the rotational symmetry of the target optimisation function \( f \) but not its form. As for previous experiments a free RBF kernel was chosen and re-weighted using algorithm 1 with hyperparameters selected to minimise LOO-MSE. However in this case we have not normalised the reweighted kernel \( K_{E}^2 \) but rather used a composite kernel \( K(\mathbf{x}, \mathbf{x}') = K_{E}^2(\mathbf{x}, \mathbf{x}') \) which implies a 2-layer feature map, the first layer being the re-weighted feature map implied by \( K_{E}^2 \) and the second layer being the standard feature map implied by the RBF kernel. All experiments were averaged over 10 repetitions.

We have tested both the EI and GP-UCB acquisition functions. Figure 7 shows the convergence of our proposed algorithm compared to standard Bayesian optimisation (using a standard RBF kernel) and standard Bayesian optimisation with a kernel mixture model as per our short polymer fibre experiment trained on \( D_\diamond \) used as the covariance function. Curiously in this case, while our method combined with GP-UCB outperforms the alternatives, the results are less clear for our method combined with EI. The precise reason for this will be investigated in future work.

6 Conclusion

In this paper we have presented a novel approach to kernel tuning. We have based our method on \( m \)-kernel techniques from reproducing kernel Banach space theory and \( \ell^p \)-regression. We have defined free kernels families whose implied feature map is independent of \( m \), along with a means of constructing them (with examples), and shown how the properties of these may be utilised to tune them by (implicitly) re-weighting the features in feature space in a principled manner. As an application we have presented an accelerated Bayesian optimisation algorithm that pre-tunes the covariance function on auxiliary data to achieve accelerated convergence, demonstrating the efficacy of our proposal.
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Figure 5: Regression coefficients for 25 phases as determined from patent data.

Figure 6: Aluminium alloy design. Comparison of algorithms in terms of maximum utility score versus iterations. GP-UCB and EI indicate acquisition function used. rmK indicates our proposed method.
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