# À la Carte — Learning Fast Kernels

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## Abstract

Kernel methods have great promise for learning rich statistical representations of large modern datasets. However, compared to neural networks, kernel methods have been perceived as lacking in scalability and flexibility. We introduce a family of fast, flexible, lightly parametrized and general purpose kernel learning methods, derived from Fastfood basis function expansions. We provide mechanisms to learn the properties of groups of spectral frequencies in these expansions, which require only $\mathcal{O}(m \log d)$ time and $\mathcal{O}(m)$ memory, for $m$ basis functions and $d$ input dimensions. We show that the proposed methods can learn a wide class of kernels, outperforming the alternatives in accuracy, speed, and memory consumption.

## 1 Introduction

The generalisation properties of a kernel method are entirely controlled by a kernel function, which represents an inner product of arbitrarily many basis functions. Kernel methods typically face a tradeoff between speed and flexibility. Methods which learn a kernel lead to slow and expensive to compute function classes, whereas many fast function classes are not adaptive. This problem is compounded by the fact that expressive kernel learning methods are most needed on large modern datasets, which provide unprecedented opportunities to automatically learn intricate statistical representations.

For example, the recent spectral kernels proposed by Wilson and Adams (2013) are flexible, but require an arbitrarily large number of basis functions, combined with many free hyperparameters, which can lead to major computational restrictions. Conversely, the recent Random Kitchen Sinks of Rahimi and Recht (2009) and Fastfood (Le et al., 2013) methods offer efficient finite basis function expansions, but only for *known* kernels, a priori hand chosen by the user. These methods do not address the fundamental issue that it is exceptionally difficult to know a priori which kernel might perform well; indeed, an appropriate kernel might not even be available in closed form.

We introduce a family of kernel learning methods which are expressive, scalable, and general purpose. In particular, we introduce flexible kernels, including a novel piecewise radial kernel, and derive Fastfood basis function expansions for these kernels. We observe that the frequencies in these expansions can in fact be adjusted, and provide a mechanism for automatically learning these frequencies via marginal likelihood optimisation. Individually adjusting these frequencies provides the flexibility to learn any translation invariant kernel. However, such a procedure has as many free parameters as basis functions, which can lead to over-fitting, troublesome local optima, and computational limitations. We therefore further introduce algorithms which can control the scales, spread, and locations of *groups* of frequencies. These methods are computationally efficient and flexible, with a minimal number of free parameters requiring training. By controlling groups of spectral frequencies, we can use arbitrarily many basis functions with no risk of over-fitting. Moreover, we do not require that the inputs have special structure, such as regular sampling intervals.

Overall, we introduce four new kernel learning methods with distinct properties, and evaluate these methods on a wide range of real datasets. We show major advantages in accuracy, speed, and memory consumption. We begin by describing related work in more detail in section 2. We then provide additional background on kernel methods, including basic properties and Fastfood approximations, in section 3. In section 4 we introduce new tools for kernel learning. Section 5 contains an evaluation of the proposed techniques. We conclude in section 6.

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## 2 Related Work

Rahimi and Recht (2008) introduced *Random Kitchen Sinks* finite Fourier basis function approximations to *fixed* stationary kernels, using a Monte Carlo sum obtained by sampling from spectral densities. For greater flexibility, one can consider a weighted sum of random kitchen sink expansions of Rahimi and Recht (2009). In this case, the expansions are fixed, corresponding to a priori chosen kernels, but the weighting can be learned from the data. Recently, Lu et al. (2014) have shown how weighted sums of random kitchen sinks can be incorporated into scalable logistic regression models. First, they separately learn the parameters of $L$ logistic regression models, each of which uses a separate random kitchen sinks expansion, enabling parallelization. They then jointly learn the weightings of each expansion. Learning proceeds through stochastic gradient descent. Lu et al. (2014) achieve promising performance on acoustic modelling problems, in some instances outperforming deep neural networks. Alternatively, Lázaro-Gredilla et al. (2010) considered optimizing the locations of all spectral frequencies in Random Kitchen Sinks expansions, as part of a sparse spectrum Gaussian process formalism (SSGPR).

For further gains in scalability, Le et al. (2013) approximate the sampling step in Random Kitchen Sinks by a combination of matrices which enable fast computation. The resulting *Fastfood* expansions perform similarly to Random Kitchen Sinks expansions (Le et al., 2013), but can be computed more efficiently. In particular, the Fastfood expansion requires $\mathcal{O}(m \log d)$ computations and $\mathcal{O}(m)$ memory, for $m$ basis functions and $d$ input dimensions. Recently, the Doubly Stochastic Kernel Machine of Dai et al. (2014) considered generating random features on the fly, allowing Random Kitchen Sink based methods to scale up to datasets with millions of points (such as ImageNet).

To allow for highly flexible kernel learning, Wilson and Adams (2013) proposed spectral mixture kernels, derived by modelling a spectral density by a scale-location mixture of Gaussians. These kernels can be computationally expensive, as they require arbitrarily many basis functions combined with many free hyperparameters. Recently, Wilson et al. (2014) modified spectral mixture kernels for Kronecker structure, and generalised scalable Kronecker (Tensor product) based learning and inference procedures to incomplete grids. Combining these kernels and inference procedures in a method called *GPatt*, Wilson et al. (2014) show how to learn rich statistical representations of large datasets with kernels, naturally enabling extrapolation on problems involving images, video, and spatiotemporal statistics. Indeed the flexibility of spectral mixture kernels makes them ideally suited to large datasets. However, GPatt requires that the input domain of the data has at least partial grid structure in order to see efficiency gains.

In this paper, we consider weighted mixtures of Fastfood expansions, where we propose to learn *both* the weighting of the expansions *and* the properties of the expansions themselves. We propose several approaches under this framework. We consider learning all of the spectral properties of a Fastfood expansion. We also consider learning the properties of groups of spectral frequencies, for lighter parametrisations and useful inductive biases, while retaining flexibility. For this purpose, we show how to incorporate Gaussian spectral mixtures into our framework, and also introduce novel piecewise linear radial kernels. Overall, we show how to perform simultaneously flexible and scalable kernel learning, with interpretable, lightly parametrised and general purpose models, requiring no special structure in the data. We focus on regression for clarity, but our models extend to classication and non-Gaussian likelihoods without additional methodological innovation.

## 3 Kernel Methods

### 3.1 Basic Properties

Denote by $\mathcal{X}$ the domain of covariates and by $\mathcal{Y}$ the domain of labels. Moreover, denote $X := \{x_1, \ldots, x_n\}$ and $Y := \{y_1, \ldots, y_n\}$ data drawn from a joint distribution $p$ over $\mathcal{X} \times \mathcal{Y}$. Finally, let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a symmetric positive semidefinite kernel (Mercer, 1909), such that every matrix $K$ with entries $K_{ij} := k(x_i, x_j)$ satisfies $K \succeq 0$.

The key idea in kernel methods is that they allow one to represent inner products in a high-dimensional feature space implicitly, using

$$k(x, x') = \langle \phi(x), \phi(x') \rangle . \tag{1}$$

While the existence of such a mapping $\phi$ is guaranteed by the theorem of Mercer (1909), manipulation of $\phi$ is not generally desirable since it might be infinite dimensional. Instead, one uses the representer theorem (Kimeldorf and Wahba, 1970; Schölkopf et al., 2001) to show that when solving regularized risk minimization problems, the optimal solution $f(x) = \langle w, \phi(x) \rangle$ can be found as linear combination of kernel functions:

$$\langle w, \phi(x) \rangle = \left\langle \sum_{i=1}^{n} \alpha_i \phi(x_i), \phi(x) \right\rangle = \sum_{i=1}^{n} \alpha_i k(x_i, x).$$

While this expansion is beneficial for small amounts of data, it creates an unreasonable burden when the number of datapoints $n$ is large. This problem can be overcome by computing approximate expansions.

### 3.2 Fastfood

The key idea in accelerating $\langle w, \phi(x) \rangle$ is to find an explicit feature map such that $k(x, x')$ can be approximated by $\sum_{j=1}^{m} \psi_j(x) \psi_j(x')$ in a manner that is both fast and memory efficient. Following the spectral ap-

proach of Rahimi and Recht (2009), we exploit that for translation invariant kernels $k(x, x') = \kappa(x - x')$ we have

$$k(x, x') = \int \rho(\omega) \exp\left(i \langle \omega, x - x' \rangle\right) d\omega \,. \tag{2}$$

Here $\rho(\omega) = \rho(-\omega) \geq 0$ to ensure that the imaginary parts of the integral vanish. Without loss of generality we assume that $\rho(\omega)$ is normalized, e.g. $\|\rho\|_1 = 1$. A similar spectral decomposition holds for inner product kernels $k(x, x') = \kappa(\langle x, x' \rangle)$ (Le et al., 2013; Schoenberg, 1942).

Rahimi and Recht (2009) suggested to sample from the spectral distribution $\rho(\omega)$ for a Monte Carlo approximation to the integral in (2). For example, the Fourier transform of the popular Gaussian kernel is also Gaussian, and thus samples from a normal distribution for $\rho(\omega)$ can be used to approximate a Gaussian (RBF) kernel.

This procedure was refined by Le et al. (2013) by approximating the sampling step with a combination of matrices that admit fast computation. They show that one may compute *Fastfood* approximate kernel expansions via

$$\tilde{k}(x, x') \propto \frac{1}{m} \sum_{j=1}^{m} \phi_j(x) \phi_j^*(x') \tag{3}$$

$$\text{where } \phi_j(x) = \exp\left(i [SHG\Pi HBx]_j\right) .$$

The random matrices $S, H, G, \Pi, B$ are chosen so as to provide a sufficient degree of randomness while also allowing for efficient computation.

$B$ **Binary decorrelation** The entries $B_{ii}$ of this diagonal matrix are drawn uniformly from $\{\pm 1\}$. This ensures that the data have zero mean in expectation over all matrices $B$.

$H$ **Hadamard matrix** It is defined recursively via

$$H_1 := \begin{bmatrix} 1 \end{bmatrix} \text{ and } H_{2d} := \begin{bmatrix} H_d & H_d \\ H_d & -H_d \end{bmatrix}$$

The recursion shows that the dense matrix $H_d$ admits fast multiplication in $O(d \log d)$ time, i.e. as efficiently as the FFT allows.

$\Pi$ **Permutation matrix** This decorrelates the eigensystems of the two Hadamard matrices. Generating such a random permutation (and executing it) can be achieved by reservoir sampling, which amounts to $n$ in-place pairwise swaps.

$G$ **Gaussian matrix** $G$ is a diagonal matrix with Gaussian entries drawn iid via $G_{ii} \sim \mathcal{N}(0, 1)$. The result of using it is that each of the rows of $HG\Pi HB$ consist of iid Gaussian random variables. Note, though, that the rows of this matrix are not quite independent.

$S$ **Scaling matrix** This diagonal matrix encodes the spectral properties of the associated kernel. Consider $\rho(\omega)$ of (2). There we draw $\omega$ from the spherically symmetric distribution defined by $\rho(\omega)$ and use its length to rescale $S_{ii}$ via

$$S_{ii} = \|\omega_i\| \, \|G\|_{\text{Frob}}^{-1}$$

It is straightforward to change kernels, for example, by adjusting $S$. Moreover, all the computational benefits of decomposing terms via (3) remain even after adjusting $S$. Therefore we can customize kernels for the problem at hand rather than applying a generic kernel, without incurring additional computational expenses.

## 4 À la Carte

In keeping with the culinary metaphor of Fastfood, we now introduce a flexible and efficient approach to kernel learning *à la carte*. That is, we will adjust the spectrum of a kernel in such a way as to allow for a wide range of translation-invariant kernels. Note that unlike previous approaches, this can be accomplished without any additional cost since these kernels only differ in terms of their choice of scaling.

In Random Kitchen Sinks and Fastfood, the frequencies $\omega$ are sampled from the spectral density $\rho(\omega)$. One could instead learn the frequencies $\omega$ using a kernel learning objective function. Moreover, with enough spectral frequencies, such an approach could learn any stationary (translation invariant) kernel. This is because each spectral frequency corresponds to a point mass on the spectral density $\rho(\omega)$ in (2), and point masses can model any density function.

However, since there are as many spectral frequencies as there are basis functions, individually optimizing over all the frequencies $\omega$ can still be computationally expensive, and susceptible to over-fitting and many undesirable local optima. In particular, we want to enforce smoothness over the *spectral distribution*. We therefore also propose to learn the scales, spread, and locations of *groups* of spectral frequencies, in a procedure that modifies the expansion (3) for fast kernel learning. This procedure results in efficient, expressive, and lightly parametrized models.

In sections 4.1 and 4.2 we describe a procedure for learning the free parameters of these models, assuming we already have a Fastfood expansion. Next we introduce four new models under this efficient framework – a Gaussian spectral mixture model in section 4.3, a piecewise linear radial model in section 4.4, and models which learn the scaling ($S$), Gaussian ($G$), and binary decorrelation ($B$) matrices in Fastfood in 4.5.

### 4.1 Learning the Kernel

We use a Gaussian process (GP) formalism for kernel learning. For an introduction to Gaussian processes,

see e.g., Rasmussen and Williams (2006). Here we assume we have an efficient Fastfood basis function expansion for kernels of interest; in the next sections we derive such expansions.

A primary goal of this paper is to demonstrate how Fastfood can be extended to learn a kernel, independently of a *specific* kernel learning objective. Note that there are many other choices for kernel learning objectives. For instance, Ong et al. (2003) provide a rather encyclopedic list of alternatives. However, the marginal likelihood of a Gaussian process provides a general purpose probabilistic framework for kernel learning, particularly suited to training highly expressive kernels (Wilson, 2014). For clarity, we focus on regression, but we note our models can be used for classification and non-Gaussian likelihoods without additional methodological innovation.

Denote by $\mathcal{X}$ an index set with $X := \{x_1, \dots x_n\}$ drawn from it. We assume that the observations $y$ are given by

$$y = f + \epsilon\,, \text{ where } \epsilon \sim \mathcal{N}\left(0, \sigma^2\right). \tag{4}$$

Here $f$ is drawn from a Gaussian process $\mathrm{GP}(0, k_\gamma)$. Eq. (4) means that any *finite dimensional realization* $f \in \mathbb{R}^n$ is drawn from a normal distribution $\mathcal{N}(0, K)$, where $K_{ij} = k(x_i, x_j)$ denotes the associated kernel matrix. This also means that $y \sim \mathcal{N}(0, K + \sigma^2 I)$, since the additive noise $\epsilon$ is drawn iid for all $x_i$. For finite-dimensional feature spaces we can equivalently use the representation of Williams (1998):

$$f(x) = \langle w, \phi(x) \rangle \text{ , where } w \sim \mathcal{N}(0, \sigma^2 I)$$

$$\text{hence } f \sim \mathrm{GP}(0, k)\,, \text{ where } k(x, x') = \sigma^2 \left\langle \phi(x), \phi(x') \right\rangle$$

The kernel of the Gaussian process is parametrized by $\gamma$. Learning the kernel therefore involves learning $\gamma$ and $\sigma^2$ from the data, or equivalently, inferring the structure of the feature map $\phi(x)$.

Our working assumption is that $k_\gamma$ corresponds to a $Q$-component mixture model of kernels $k_q$ with associated weights $v_q^2$. Moreover we assume that we have access to a Fastfood expansion $\phi_q(x)$ for each of the components into $m$ terms. This leads to

$$f(x) = \sum_{q=1}^{Q} \sum_{j=1}^{m} w_{qj} \phi_{qj}(x|\theta_q) \text{ where } w_{qj} \sim \mathcal{N}\left(0, m^{-1} v_q^2\right)$$

$$k(x, x') = \sum_{q=1}^{Q} \frac{v_q^2}{m} \sum_{j=1}^{m} \phi_{qj}(x|\theta_q) \phi_{qj}(x'|\theta_q)$$

This kernel is parametrized by $\gamma = \{v_q, \theta_q\}$. Here $v_q$ are mixture weights and $\theta_q$ are parameters of the (nonlinear) basis functions $\phi_{qj}$.

### 4.2 Marginal Likelihood

We can marginalise the Gaussian process governing $f$ by integrating away the $w_{qj}$ variables above to express the marginal likelihood of the data solely in terms of the kernel hyperparameters $v, \theta$ and noise variance $\sigma^2$.

Denote by $\Phi_\theta \in \mathbb{R}^{Qm \times n}$ the design matrix, as parametrized by $\theta$, from evaluating the functions $\phi_{qj}(x|\theta_q)$ on $X$. Moreover, denote by $V \in \mathbb{R}^{Qm \times Qm}$ the diagonal scaling matrix obtained from $v$ via

$$V := m^{-1} \mathrm{diag}(v_1, \dots, v_1, \dots, v_Q, \dots v_Q). \tag{5}$$

Since $\epsilon$ and $f$ are independent, their covariances are additive. For $n$ training datapoints $y$, indexed by $X$, we therefore obtain the marginal likelihood

$$y|X, v, \theta, \sigma^2 \sim \mathcal{N}(0, \Phi_\theta^\top V \Phi_\theta + \sigma^2 I) \tag{6}$$

and hence the negative log marginal likelihood is

$$\begin{aligned} -\log p(y|X, \gamma, \sigma^2) =& \frac{n}{2} \log 2\pi + \frac{1}{2} \log \left| \Phi_\theta^\top V \Phi_\theta + \sigma^2 I \right| \\ &+ \frac{1}{2} y^\top \left[ \Phi_\theta^\top V \Phi_\theta + \sigma^2 I \right]^{-1} y \end{aligned} \tag{7}$$

To learn the kernel $k$ we minimize the negative log marginal likelihood of (7) with respect to $v, \theta$ and $\sigma^2$. Similarly, the predictive distribution at a test input $\bar{x}$ can be evaluated using

$$\begin{aligned} &\bar{y}|\bar{x}, X, y, v, \theta, \sigma^2 \sim \mathcal{N}(\bar{\mu}, \bar{\sigma}^2) \\ &\text{where } \bar{\mu} = k(\bar{x})^\top \left[ \Phi^\top V \Phi + \sigma^2 I \right]^{-1} y \\ &\text{and } \bar{\sigma}^2 = \sigma_n^2 + k(\bar{x})^\top \left[ \Phi^\top V \Phi + \sigma^2 I \right]^{-1} k(\bar{x}). \end{aligned} \tag{8}$$

Here $k(\bar{x}) := (k(\bar{x}, x_1), \dots, k(\bar{x}, x_n))^\top$ denotes the vector of cross covariances between the test point $x$ and and the $n$ training points in $X$. On closer inspection we note that these expressions can be simplified greatly in terms of $\Phi$ and $\phi_{qj}(\bar{x})$ since

$$\begin{aligned} k(\bar{x}) &= \phi(\bar{x})^\top V \Phi \text{ and hence} \\ \bar{\mu} &= \phi(\bar{x})^\top \beta \text{ for } \beta = V \left[ \Phi^\top V \Phi + \sigma^2 I \right]^{-1} y \end{aligned}$$

with an analogous expression for $\bar{\sigma}^2$. More importantly, instead of solving the problem in terms of the kernel matrix we can perform inference in terms of $\beta$ directly. This has immediate benefits:

- Storing the solution only requires $O(Qmn)$ parameters regardless of $X$, provided $\phi(x)$ can be stored and computed efficiently, e.g. by Fastfood.
- Computation of the predictive variance is also efficient: $\Phi^\top V \Phi$ has at most rank $Qm$, hence the evaluation of $\bar{\sigma}^2$ can be accomplished via the Sherman-Morrison-Woodbury formula, thus requiring only $O(Q^2 m^2 n)$ computations. Moreover, randomized low-rank approximations of
$$V^{\frac{1}{2}} \Phi \left[ \Phi^\top V \Phi + \sigma_n^2 I \right]^{-1} \Phi^\top V^{\frac{1}{2}},$$
using e.g. randomized projections (Halko et al., 2009) allow for even more efficient computation.

Overall, standard Gaussian process kernel representations (Rasmussen and Williams, 2006) require $O(n^3)$

computations and $O(n^2)$ memory. Therefore, when using a Gaussian process kernel learning formalism, the expansion in this section, using $\Phi$, is computationally preferable whenever $Qm < n$.

### 4.3 Gaussian Spectral Mixture Models

For the Gaussian Spectral Mixture kernels of Wilson and Adams (2013), translation invariance holds, yet rotation invariance is violated: the kernels satisfy $k(x, x') = k(x + \delta, x' + \delta)$ for all $\delta \in \mathbb{R}^d$; however, in general rotations $U \in \mathrm{SO}(d)$ do not leave $k$ invariant, i.e. $k(x, x') \neq k(Ux, Ux')$. These kernels have the following explicit representation in terms of their Fourier transform $F[k]$

$$F[k](\omega) = \sum_q \frac{v_q^2}{2} \left[\chi\left(\omega, \mu_q, \Sigma_q\right) + \chi\left(-\omega, \mu_q, \Sigma_q\right)\right]$$

$$\text{where } \chi(\omega, \mu, \Sigma) = \frac{e^{-\frac{1}{2}(\mu-\omega)^\top \Sigma^{-1}(\mu-\omega)}}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}}$$

In other words, rather than choosing a spherically symmetric representation $\rho(\omega)$ as typical for (2), Wilson and Adams (2013) pick a mixture of Gaussians with mean frequency $\mu_q$ and variance $\Sigma_q$ that satisfy the symmetry condition $\rho(\omega) = \rho(-\omega)$ but not rotation invariance. By the linearity of the Fourier transform, we can apply the inverse transform $F^{-1}$ componentwise to obtain

$$k(x - x') = \sum_q v_q^2 \frac{|\Sigma_q|^{\frac{1}{2}}}{(2\pi)^{\frac{d}{2}}} \exp\left(-\frac{1}{2}\left\|\Sigma_q^{\frac{1}{2}}(x - x')\right\|^2\right) \cos\left\langle x - x', \mu_q\right\rangle \tag{9}$$

**Lemma 1 (Universal Basis)** *The expansion (9) can approximate any translation-invariant kernel by approximating its spectral density.*

**Proof** This follows since mixtures of Gaussians are universal approximators for densities (Silverman, 1986), and by the Fourier-Plancherel theorem, approximation in the Fourier domain amounts to approximation in the original domain.

Note that the expression in (9) is *not* directly amenable to the fast expansions provided by Fastfood since the distributions are shifted. However, a small modification allows us to efficiently compute kernels of the form of (9). The key insight is that shifts in Fourier space by $\pm\mu_q$ are accomplished by multiplication by $\exp\left(\pm i \left\langle \mu_q, x\right\rangle\right)$. Here the inner product can be precomputed, which costs only $O(d)$ operations. Moreover, multiplications by $\Sigma_q^{-\frac{1}{2}}$ induce multiplication by $\Sigma_q^{\frac{1}{2}}$ in the original domain, which can be accomplished as *preprocessing*. For diagonal $\Sigma_q$ the cost is $O(d)$.

In order to preserve translation invariance we compute a symmetrized set of features. We have the following algorithm (we assume diagonal $\Sigma_q$ — otherwise simply precompute and scale $x$):

**Preprocessing** — **Input** $m, \{(\Sigma_q, \mu_q)\}$
**for each** $q$ generate random matrices $S_q, G_q, B_q, \Pi_q$

Combine group scaling $B_q \leftarrow B_q \Sigma_q^{\frac{1}{2}}$

**Feature Computation** — **Input** $S, G, B, \Pi, \mu, \Sigma$
**for** $q = 1$ **to** $Q$ **do**
  $\zeta \leftarrow \langle \mu_q, x\rangle$ (offset)
  $\xi \leftarrow [S_q H G_q \Pi_q H B_q x]$ (Fastfood product)
  Compute features
    $\phi_{q\cdot 1} \leftarrow \sin(\xi + \zeta)$ and $\phi_{q\cdot 2} \leftarrow \cos(\xi + \zeta)$
    and $\phi_{q\cdot 3} \leftarrow \sin(\xi - \zeta)$ and $\phi_{q\cdot 4} \leftarrow \cos(\xi + \zeta)$
**end for**

To learn the kernel we learn the weights $v_q$, dispersion $\Sigma_q$ and locations $\mu_q$ of spectral frequencies via marginal likelihood optimization, as described in section 4.2. This results in a kernel learning approach which is similar in flexibility to individually learning all $md$ spectral frequencies and is less prone to overfitting and local optima. In practice, this can mean optimizing over about 10 free parameters instead of $10^4$ free parameters, with improved predictive performance and efficiency. See section 5 for more detail.

### 4.4 Piecewise Linear Radial Kernel

In some cases the freedom afforded by a mixture of Gaussians in frequency space may be more than what is needed. In particular, there exist many cases where we *want* to retain invariance under rotations while simultaneously being able to adjust the spectrum according to the data at hand. For this purpose we introduce a novel piecewise linear radial kernel.

Recall (2) governs the regularization properties of $k$. We require $\rho(\omega) = \rho(\|\omega\|) := \rho(r)$ for rotation invariance. For instance, for the Gaussian RBF kernel we have

$$\rho(\|\omega\|_2) \propto \|\omega\|_2^{d-1} \exp\left(-\tfrac{\|\omega\|_2^2}{2}\right). \tag{10}$$

For high dimensional inputs, the RBF kernel suffers from a concentration of measure problem (Le et al., 2013), where samples are tightly concentrated at the maximum of $\rho(r)$, $r = \sqrt{d-1}$. A fix is relatively easy, since we are at liberty to pick any nonnegative $\rho$ in designing kernels. This procedure is flexible but leads to intractable integrals: the Hankel transform of $\rho$, i.e. the radial part of the Fourier transform, needs to be analytic if we want to compute $k$ in closed form.

However, if we remain in the Fourier domain, we can use $\rho(r)$ and sample *directly* from it. This strategy kills two birds with one stone: we do not need to compute the inverse Fourier transform and we have a readily available sampling distribution at our disposal for the Fastfood expansion coefficients $S_{ii}$. All that is needed is to find an efficient parametrization of $\rho(r)$.

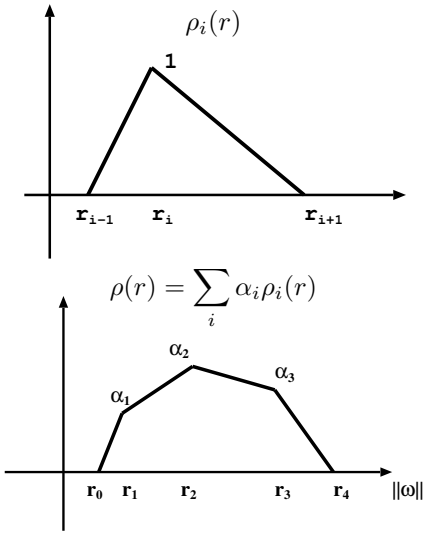



Figure 1: Piecewise linear functions. Top: single basis function. Bottom: linear combination of three functions. Additional degrees of freedom are fixed by $\rho(r_0) = \rho(r_4) = 0$.

We begin by providing an explicit expression for piecewise linear functions $\rho_i$ such that $\rho_i(r_j) = \delta_{ij}$ with discontinuities only at $r_{i-1}, r_i$ and $r_{i+1}$. In other words, $\rho(r)$ is a 'hat' function with its mode at $r_i$ and range $[r_{i-1}, r_{i+1}]$. It is parametrized as

$$\rho_i(r) := \max\left(0, \min\left(1, \frac{r - r_{i-1}}{r_i - r_{i-1}}, \frac{r_i - r}{r_{i+1} - r_i}\right)\right)$$

By construction each basis function is piecewise linear with $\rho_i(r_j) = \delta_{ij}$ and moreover $\rho_i(r) \geq 0$ for all $r$.

**Lemma 2** *Denote by $\{r_0, \ldots, r_n\}$ a sequence of locations with $r_i > r_{i-1}$ and $r_0 = 0$. Moreover, let $\rho(r) := \sum_i \alpha_i \rho_i(r)$. Then $\rho(r) \geq 0$ for all $r$ if and only if $\alpha_i \geq 0$ for all $i$. Moreover, $\rho(r)$ parametrizes all piecewise linear functions with discontinuities at $r_i$.*

Now that we have a parametrization, we only need to discuss how to draw $\omega$ from $\rho(\|\omega\|) = \rho(r)$. We have several strategies at our disposal:

- $\rho(r)$ can be normalized explicitly via
$$\bar{\rho} := \int_0^\infty \rho(r)dr = \sum_i \frac{\alpha_i}{2(r_{i+1} - r_{i-1})}$$
Since each segment $\rho_i$ occurs with probability $\alpha_i/(2\bar{\rho}(r_{i+1} - r_{i-1})$ we first sample the segment and then sample from $\rho_i$ explicitly by inverting the associated cumulative distribution function (it is piecewise quadratic).

- Note that sampling can induce considerable variance in the choice of locations. An alternative is to invert the cumulative distribution function and pick $m$ locations equidistantly at locations $\frac{i}{m} + \xi$ where $\xi \sim U[0, 1/m]$. This approach is commonly used in particle filtering (Doucet et al., 2001). We choose this strategy, since it is efficient yet substantially reduces the variance of sampling.

The basis functions are computed as follows:

**Preprocessing**$(m, \{(\{\alpha_i\}_{i=1}^n, \{r_i\}_{i=0}^{n+1}, \Sigma)\})$
Generate random matrices $G, B, \Pi$
Update scaling $B \leftarrow B\Sigma^{\frac{1}{2}}$
Sample $S$ from $\rho(\|\omega\|)$ as above

**Feature Computation**$(S, G, B, \Pi)$
$\phi_1 \leftarrow \cos([SHG\Pi HBx])$ and $\phi_2 \leftarrow \sin([SHG\Pi HBx])$

The rescaling matrix $\Sigma_q$ is introduced to incorporate automatic relevance determination into the model. Like with the Gaussian spectral mixture model, we can use a mixture of piecewise linear radial kernels to approximate any radial kernel. Supposing there are $Q$ components of the piecewise linear $\rho_q(r)$ function, we can repeat the proposed algorithm $Q$ times to generate all the required basis functions.

### 4.5 Fastfood Kernels

The efficiency of Fastfood is partly obtained by approximating Gaussian random matrices with a product of matrices described in section 3.2. Here we propose several expressive and efficient kernel learning algorithms obtained by optimizing the marginal likelihood of the data in Eq. (7) with respect to these matrices:

**FSARD** The scaling matrix $S$ represents the spectral properties of the associated kernel. For the RBF kernel, $S$ is sampled from a chi-squared distribution. We can simply change the kernel by adjusting $S$. By varying $S$, we can approximate any radial kernel. We learn the diagonal matrix $S$ via marginal likelihood optimization. We combine this procedure with *Automatic Relevance Determination* of Neal (1998) – learning the scale of the input space – to obtain the **FSARD** kernel.

**FSGBARD** We can further generalize **FSARD** by additionally optimizing marginal likelihood with respect to the diagional matrices $G$ and $B$ in Fastfood to represent a wider class of kernels.

In both **FSARD** and **FSGBARD** the Hadamard matrix $H$ is retained, preserving all the computational benefits of Fastfood. That is, we only modify the scaling matrices while keeping the main computational drivers such as the fast matrix multiplication and the Fourier basis unchanged.

## 5 Experiments

We evaluate the proposed kernel learning algorithms on many regression problems from the UCI repository.

We show that the proposed methods are flexible, scalable, and applicable to a large and diverse collection of data, of varying sizes and properties. In particular, we demonstrate scaling to more than 2 million datapoints (in general, Gaussian processes are intractable beyond $10^4$ datapoints); secondly, the proposed algorithms significantly outperform standard exact kernel methods, and with only a few hyperparameters are even competitive with alternative methods that involve training orders of magnitude more hyperparameters.[1] The results are shown in Table 1 in the supplement. All experiments are performed on an Intel Xeon E5620 PC, operating at 2.4GHz with 32GB RAM. Details such as initialization are in the supplement.

**RBF and ARD** On smaller datasets, with fewer than $n = 2000$ training examples, where exact methods are tractable, we use exact Gaussian RBF and ARD kernels with hyperparameters learned via marginal likelihood optimization. ARD kernels use Automatic Relevance Determination (Neal, 1998) to adjust the scale of each input coordinate. Since these exact methods are intractable on larger datasets, we use Fastfood basis function expansions of these kernels for $n > 2000$.

**GM** For Gaussian Mixtures we compute a mixture of Gaussians in frequency domain, as described in section 4.3. As before, optimization is carried out with regard to marginal likelihood.

**PWL** For rotation invariance, we use the novel Piecewise Linear radial kernels described in section 4.4. PWL has a simple spectral parametrization.

**SSGPR** Sparse Spectrum Gaussian Process Regression is a kitchen sinks (RKS) based model which individually optimizes the locations of *all* spectral frequencies (Lázaro-Gredilla et al., 2010). We note that SSGPR is heavily parametrized. Moreover, SSGPR is a special case of the proposed GM model if $Q = m$, and we set all GM bandwidths to 0 and weigh all terms equally.

**FSARD and FSGBARD** See section 4.5.

We use the *same* number of basis functions for all methods. We use $Q$ to denote the number of components in GM and PWL and $m$ to denote the number of basis functions in each component. For all other methods, we use $Qm$ basis functions. For the largest datasets in Table 1 we favoured larger values of $Q$, as the flexibility of having more components $Q$ in GM and PWL becomes more valuable when there are many datapoints; although we attempted to choose sensible $Q$ and $m$ combinations for a particular model and number of datapoints $n$, these parameters were not fine tuned. We choose $Qm$ to be as large as is practical given computational constraints, and SSGPR is allowed a significantly larger parametrization.

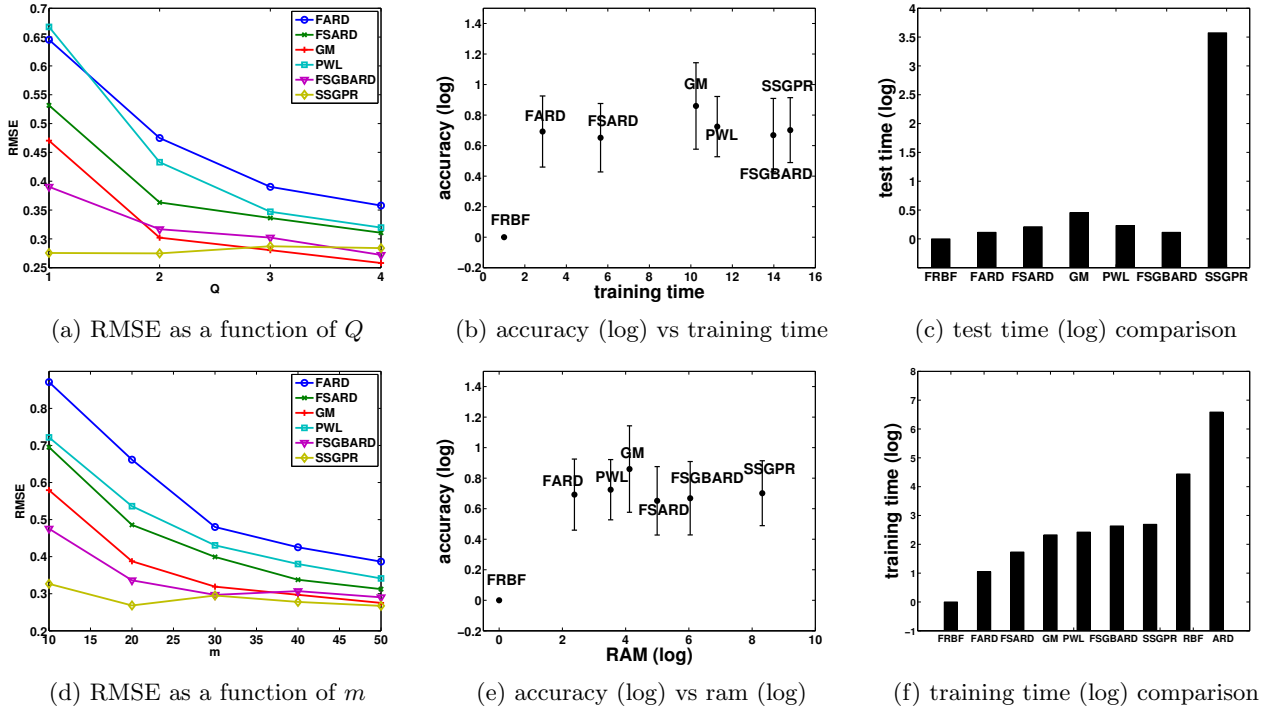
Indeed SSPGR is allowed $Qmd + 2$ free parameters to learn, and we set $Q \ll m$. This setup gives SSGPR a significant advantage over our proposed models. However, we wish to emphasize that the GM, PWL, and FSGBARD models are competitive with SSGPR, even in the adversarial situation when SSGPR has many orders of magnitude more free parameters than GM or PWL. For comparison, the required numbers of hyperpararameters for each model are RBF (3), ARD $(d + 2)$, PWL $(Q(d + 3) + 1)$, GM $(Q(2d + 1) + 1)$, FSARD $(Qm + d + 2)$, and FSGBARD $(3Qm + d + 2)$.

Gaussian processes are most commonly implemented with exact RBF and ARD kernels, which we run on the smaller ($n < 2000$) datasets in Table 1, where the proposed GM and PWL approaches generally perform better than all alternatives. On the larger datasets, exact ARD and RBF kernels are entirely intractable, so we compare to Fastfood expansions. That is, GM and PWL are both more expressive and profoundly more scalable than exact ARD and RBF kernels, far and above the most popular alternative approaches.

In Figures 2a we investigate how RMSE performance changes as we vary $Q$ and $m$. The GM and PWL models continue to increase in performance as more basis functions are used. This trend is not present with SSGPR or FSGBARD, which unlike GM and PWL, becomes more susceptible to over-fitting as we increase the number of basis functions. Indeed, in SSGPR, and in FSGBARD and FSARD to a lesser extent, more basis functions means more parameters to optimize, which is not true with the GM and PWL models.

We further investigate the performance of all seven methods, in terms of average normalised log predictive accuracy, training time, testing time, and memory consumption, shown in Figures 2b and 2c (higher accuracy scores and lower training time, test time, and memory scores, correspond to better performance). Despite the reduced parametrization, GM and PWL outperform all alternatives in accuracy, yet require similar memory and runtime to the much less expressive FARD model, a Fastfood expansion of the ARD kernel. Although SSGPR performs third best in accuracy, it requires more memory, training time, testing runtime (as shown in Fig 2c), than all other models. FSGBARD performs similar in accuracy to SSGPR, but is significantly more time and memory efficient, because it leverages a Fastfood representation. For clarity, we have so far considered log plots. If we view the results

[1] GM, PWL, FSARD, and FSGBARD are novel contributions of this paper, while RBF and ARD are popular alternatives, and SSGPR is a recently proposed state of the art kernel learning approach.




(a) RMSE as a function of $Q$ (b) accuracy (log) vs training time (c) test time (log) comparison

(d) RMSE as a function of $m$ (e) accuracy (log) vs ram (log) (f) training time (log) comparison

Figure 2: Fig. 2a and Fig. 2d illustrate how RMSE changes as we vary $Q$ and $m$ on the *SML* dataset. For variable $Q$, the number of basis functions per group $m$ is fixed to 32. For variable $m$ the number of clusters $Q$ is fixed to 2. FRBF and FARD are Fastfood expansions of RBF and ARD kernels, respectively. Fig. 2b and Fig. 2e compare all methods in terms of accuracy, training time and memory. The accuracy score of a method on a given dataset is computed as $\text{accuracy}_{\text{method}} = \text{RMSE}_{\text{FRBF}}/\text{RMSE}_{\text{method}}$. For runtime and memory we take the reciprocal of the analogous metric, so that a lower score corresponds to better performance. For instance, $\text{time}_{\text{method}} = \text{walltime}_{\text{method}}/\text{walltime}_{\text{FRBF}}$. log denotes an average of the (natural) log scores, across all datasets. Fig. 2c and Fig. 2f compares all methods in terms of log test and training time (Fig. 2f also includes the average log training time for the exact ARD and RBF kernels across the smallest five medium datasets; these methods are intractable on any larger datasets).

without a log transformation, as in Fig 4 (supplement) we see that GM and SSGPR are outliers: on average GM greatly outperforms all other methods in predictive accuracy, and SSGPR requires profoundly more memory than all other methods.

## 6 Discussion

Kernel learning methods are typically intractable on large datasets, even though their flexibility is most valuable on large scale problems. We have introduced a family of flexible, scalable, general purpose and lightly parametrized kernel methods, which learn the properties of groups of spectral frequencies in Fastfood basis function expansions. We find, with a minimal parametrization, that the proposed methods have impressive performance on a large and diverse collection of problems – in terms of predictive accuracy, training and test runtime, and memory consumption. In the future, we expect additional performance and efficiency gains by automatically learning the relative numbers of spectral frequencies to assign to each group.

In short, we have shown we can have simultaneously scalable and expressive kernel methods. We hope this work will help unify efforts in enhancing scalability and flexibility for kernel methods. In a sense, flexibility and scalability are one problem: we want the most expressive methods for the biggest datasets.

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