Chapter 1

Higher-order Additive GPs

In this chapter, we introduce a Gaussian process model of functions which are *additive*. An additive function is one which decomposes into a sum of low-dimensional functions, each depending on only a subset of the input variables. Additive GPs generalize both Generalized Additive Models, and the standard GP models which use squared-exponential kernels. We introduce an expressive but tractable parameterization of the kernel function, which allows efficient evaluation of all input interaction terms, whose number is exponential in the input dimension. The additional structure discoverable by this model results in state-of-the-art predictive power in regression tasks, as well as increased interpretability.

1.1 Introduction

Most statistical regression models in use today are of the form:

$$g(y) = f(x_1) + f(x_2) + \cdots + f(x_D). \tag{1.1}$$

Popular examples include logistic regression, linear regression, and Generalized Linear Models (Nelder and Wedderburn, 1972). This family of functions, known as Generalized Additive Models (GAM) (Hastie and Tibshirani, 1990), are typically easy to fit and interpret. Some extensions of this family, such as smoothing-splines ANOVA (Wahba, 1990), add terms depending on more than one variable. However, such models generally become intractable and difficult to fit as the number of terms increases.

At the other end of the spectrum are kernel-based models, which typically allow the response to depend on all input variables simultaneously. These have the form:

$y = f(x_1, x_2, \ldots, x_D)$. A popular example would be a Gaussian process model using a squared-exponential (or Gaussian) kernel. We denote this model as SE-GP. This model is much more flexible than the GAM, but its flexibility makes it difficult to generalize to new combinations of input variables.

In this paper, we introduce a Gaussian process model that generalizes both GAMs and the SE-GP. This is achieved through a kernel which allow additive interactions of all orders, ranging from first order interactions (as in a GAM) all the way to Dth-order interactions (as in a SE-GP). Although this kernel amounts to a sum over an exponential number of terms, we show how to compute this kernel efficiently, and introduce a parameterization which limits the number of parameters to $\mathcal{O}(D)$. A Gaussian process with this kernel function (an additive GP) constitutes a powerful model that allows one to automatically determine which orders of interaction are important. We show that this model can significantly improve modeling efficacy, and has major advantages for model interpretability.

We can see that a GP with a first-order additive kernel is an example of a GAM: Each function drawn from this model is a sum of orthogonal one-dimensional functions. Compared to functions drawn from the higher-order GP, draws from the first-order GP have more long-range structure.

We can expect many natural functions to depend only on sums of low-order interactions. For example, the price of a house or car will presumably be well approximated by a sum of prices of individual features, such as a sun-roof. Other parts of the price may depend jointly on a small set of features, such as the size and building materials of a house. Capturing these regularities will mean that a model can confidently extrapolate to unseen combinations of features.

1.2   Additive Kernels

We now give a precise definition of additive kernels. We first assign each dimension $i \in \{1 \ldots D\}$ a one-dimensional *base kernel* $k_i(x_i, x_i')$. We then define the first order,

second order and nth order additive kernel as:

$$k_{add_1}(\mathbf{x}, \mathbf{x}') = \sigma_1^2 \sum_{i=1}^{D} k_i(x_i, x_i') \tag{1.2}$$

$$k_{add_2}(\mathbf{x}, \mathbf{x}') = \sigma_2^2 \sum_{i=1}^{D} \sum_{j=i+1}^{D} k_i(x_i, x_i') k_j(x_j, x_j') \tag{1.3}$$

$$k_{add_n}(\mathbf{x}, \mathbf{x}') = \sigma_n^2 \sum_{1 \leq i_1 < i_2 < \ldots < i_n \leq D} \left[\prod_{d=1}^{n} k_{i_d}(x_{i_d}, x_{i_d}') \right] \tag{1.4}$$

$$k_{add_D}(\mathbf{x}, \mathbf{x}') = \sigma_n^2 \sum_{1 \leq i_1 < i_2 < \ldots < i_D \leq D} \left[\prod_{d=1}^{D} k_{i_d}(x_{i_d}, x_{i_d}') \right] = \sigma_D^2 \prod_{d=1}^{D} k_d(x_d, x_d') \tag{1.5}$$

where D is the dimension of our input space, and σ_n^2 is the variance assigned to all nth order interactions. The nth covariance function is a sum of $\binom{D}{n}$ terms. In particular, the Dth order additive covariance function has $\binom{D}{D} = 1$ term, a product of each dimension's covariance function:

$$k_{add_D}(\mathbf{x}, \mathbf{x}') = \sigma_D^2 \prod_{d=1}^{D} k_d(x_d, x_d') \tag{1.6}$$

In the case where each base kernel is a one-dimensional squared-exponential kernel, the Dth-order term corresponds to the multivariate squared-exponential kernel:

$$k_{add_D}(\mathbf{x}, \mathbf{x}') = \sigma_D^2 \prod_{d=1}^{D} k_d(x_d, x_d') = \sigma_D^2 \prod_{d=1}^{D} \exp\left(-\frac{(x_d - x_d')^2}{2l_d^2} \right) = \sigma_D^2 \exp\left(-\sum_{d=1}^{D} \frac{(x_d - x_d')^2}{2l_d^2} \right)$$
$$\tag{1.7}$$

also commonly known as the Gaussian kernel. The full additive kernel is a sum of the additive kernels of all orders.

1.2.1 Parameterization

The only design choice necessary in specifying an additive kernel is the selection of a one-dimensional base kernel for each input dimension. Any parameters (such as length-scales) of the base kernels can be learned as usual by maximizing the marginal likelihood of the training data.

In addition to the parameters of each dimension-wise kernel, additive kernels are equipped with a set of D parameters $\sigma_1^2 \ldots \sigma_D^2$ controlling how much variance we assign to each order of interaction. These "order variance" parameters have a useful interpreta-

tion: the dth order variance hyperparameter controls how much of the target function's variance comes from interactions of the dth order. Table 1.1 shows examples of the variance contributed by the different orders of interaction, learned on real datasets.

Table 1.1 Percentage of variance contributed by each order of the additive model, on different datasets. The maximum order of interaction is set to 10, or smaller if the input dimension less than 10.

Dataset	Order of interaction									
	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
pima	0.1	0.1	0.1	0.3	1.5	**96.4**	1.4	0.0		
liver	0.0	0.2	**99.7**	0.1	0.0	0.0				
heart	**77.6**	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	22.0
concrete	**70.6**	13.3	13.8	2.3	0.0	0.0	0.0	0.0		
pumadyn-8nh	0.0	0.1	0.1	0.1	0.1	0.1	0.1	**99.5**		
servo	**58.7**	27.4	0.0	13.9						
housing	0.1	0.6	**80.6**	1.4	1.8	0.8	0.7	0.8	0.6	12.7

On different datasets, the dominant order of interaction estimated by the additive model varies widely. An additive GP with all of its variance coming from the 1st order is equivalent to a GAM; an additive GP with all its variance coming from the Dth order is equivalent to a SE-GP.

Because the variance parameters can specify which degrees of interaction are important, the additive GP can capture many different types of structure. If the function we are modeling is decomposable into a sum of low-dimensional functions, our model can discover this fact and exploit it. Discovering such structure allows long-range extrapolation, as we saw in **??**. If low-dimensional additive structure is not present, the kernel parameters can specify a suitably flexible model, with interactions between as many variables as necessary.

1.2.2   Efficient Evaluation of Additive Kernels

An additive kernel over D inputs with interactions up to order n has $O(2^n)$ terms. Naïvely summing over these terms quickly becomes intractable. In this section, we show how one can evaluate the sum over all terms in $O(D^2)$.

To efficiently compute the additive kernel, we exploit the fact that the nth order additive kernel corresponds to the nth *elementary symmetric polynomial* (Macdonald,

1998) of the base kernels, which we denote e_n. For example: if $\mathbf{x}$ has 4 input dimensions ($D = 4$), and if we use the shorthand notation $k_d = k_d(x_d, x'_d)$, then

$$k_{\text{add}_0}(\mathbf{x}, \mathbf{x}') = e_0(k_1, k_2, k_3, k_4) = 1 \tag{1.8}$$

$$k_{\text{add}_1}(\mathbf{x}, \mathbf{x}') = e_1(k_1, k_2, k_3, k_4) = k_1 + k_2 + k_3 + k_4 \tag{1.9}$$

$$k_{\text{add}_2}(\mathbf{x}, \mathbf{x}') = e_2(k_1, k_2, k_3, k_4) = k_1 k_2 + k_1 k_3 + k_1 k_4 + k_2 k_3 + k_2 k_4 + k_3 k_4 \tag{1.10}$$

$$k_{\text{add}_3}(\mathbf{x}, \mathbf{x}') = e_3(k_1, k_2, k_3, k_4) = k_1 k_2 k_3 + k_1 k_2 k_4 + k_1 k_3 k_4 + k_2 k_3 k_4 \tag{1.11}$$

$$k_{\text{add}_4}(\mathbf{x}, \mathbf{x}') = e_4(k_1, k_2, k_3, k_4) = k_1 k_2 k_3 k_4 \tag{1.12}$$

The Newton-Girard formulae give an efficient recursive form for computing these polynomials:

$$k_{\text{add}_n}(\mathbf{x}, \mathbf{x}') = e_n(k_1, \ldots, k_D) = \frac{1}{n} \sum_{a=1}^{n} (-1)^{(a-1)} e_{n-a}(k_1, \ldots, k_D) \sum_{i=1}^{D} k_i^a \tag{1.13}$$

The Newton-Girard formulae have time complexity $\mathcal{O}(D^2)$, while computing a sum over an exponential number of terms. Note that the same sum can be computed in time

Conveniently, we can use the same trick to efficiently compute all of the necessary derivatives of the additive kernel with respect to the base kernels. We merely need to remove the kernel of interest from each term of the polynomials:

$$\frac{\partial k_{add_n}}{\partial k_j} = e_{n-1}(k_1, \ldots, k_{j-1}, k_{j+1}, \ldots k_D) \tag{1.14}$$

This trick allows us to optimize the base kernel parameters with respect to the marginal likelihood.

1.2.3 Computational Cost

The computational cost of evaluating the Gram matrix of a product kernel (such as the SE kernel) is $\mathcal{O}(N^2 D)$, while the cost of evaluating the Gram matrix of the additive kernel is $\mathcal{O}(N^2 D R)$, where R is the maximum degree of interaction allowed (up to D). In higher dimensions, this can be a significant cost, even relative to the fixed $\mathcal{O}(N^3)$ cost of inverting the Gram matrix. However, as our experiments show, typically only the first few orders of interaction are important for modeling a given function; hence if one is computationally limited, one can simply limit the maximum degree of interaction without losing much accuracy.

1.3   Non-local Interactions

By far the most popular kernels for regression and classification tasks on continuous data are the SE kernel, and the Matérn kernels. These kernels depend only on the scaled Euclidean distance between two points, both having the form:

$$k(\mathbf{x}, \mathbf{x}') = g\left(\sum_{d=1}^{D} \left(\frac{x_d - x_d'}{l_d} \right)^2 \right) \qquad (1.15)$$

Bengio et al. (2006) argue that models based on squared-exponential kernels are particularly susceptible to the *curse of dimensionality*. They emphasize that the locality of the kernels means that these models cannot capture non-local structure. They argue that many functions that we care about have such structure. Methods based solely on local kernels will require training examples at all combinations of relevant inputs.

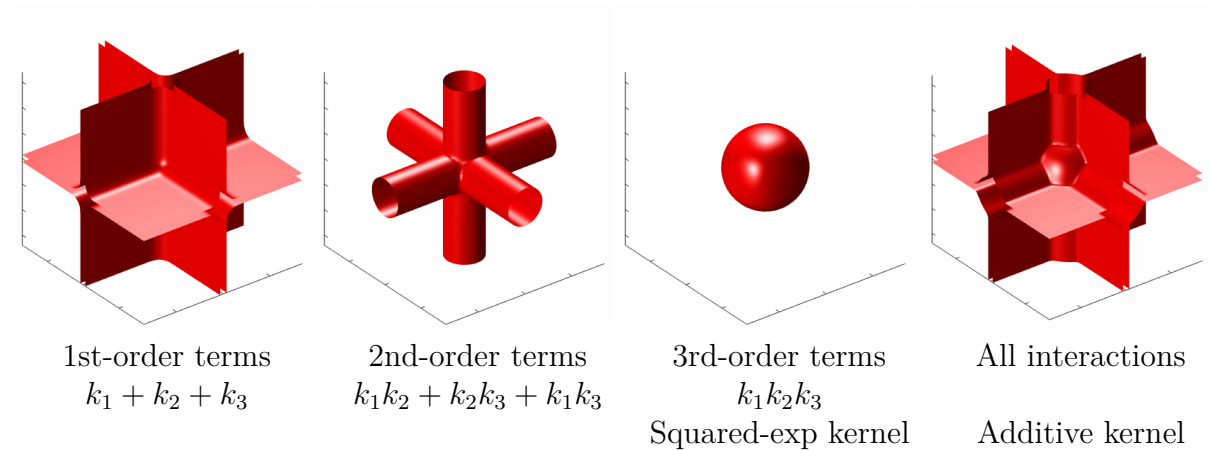| 1st-order terms	2nd-order terms	3rd-order terms	All interactions
$k_1 + k_2 + k_3$	$k_1 k_2 + k_2 k_3 + k_1 k_3$	$k_1 k_2 k_3$	
		Squared-exp kernel	Additive kernel

Fig. 1.1 Isocontours of additive kernels in 3 dimensions. The third-order kernel only considers nearby points relevant, while the lower-order kernels allow the output to depend on distant points, as long as they share one or more input value.

Additive kernels have a much more complex structure, and allow extrapolation based on distant parts of the input space, without spreading the mass of the kernel over the whole space. For example, additive kernels of the second order allow strong non-local interactions between any points which are similar in any two input dimensions. Figure 1.1 provides a geometric comparison between squared-exponential kernels and additive kernels in 3 dimensions.

## 1.4	Dropout in Gaussian Processes

Dropout is a method for regularizing neural networks (Hinton et al., 2012; Srivastava, 2013). Training with dropout entails randomly and independently "dropping" (setting to zero) some proportion p of features or inputs, in order to improve the robustness of the resulting network by reducing co-dependence between neurons. To maintain similar overall activation levels, weights are multiplied by $1/p$ at test time. Alternatively, feature activations are multiplied by $1/p$ during training. At test time, the set of models defined by all possible ways of dropping-out neurons is averaged over, usually in an approximate way.

Baldi and Sadowski (2013) and Wang and Manning (2013) analyzed dropout in terms of the effective prior induced by this procedure in several models, such as linear and logistic regression. In this section, we examine the priors on functions that result from performing dropout in the one-hidden-layer neural network implicitly defined by a GP (equation (**??**)).

### 1.4.1	Dropout on Feature Activations

First, we examine the prior that results from randomly dropping features from $\mathbf{h}(\mathbf{x})$ with probability p. If these features have a weight distribution with finite moments $\mathbb{E}[\alpha_i] = \mu, \mathbb{V}[\alpha_i] = \sigma^2$, then the distribution of weights after each one has been dropped out with probability p is:

$$r_i \overset{\text{iid}}{\sim} \text{Ber}(p) \qquad \mathbb{E}[r_i \alpha_i] = p\mu, \quad \mathbb{V}[r_i \alpha_i] = p^2 \sigma^2 . \tag{1.16}$$

However, after we increase the remaining activations to maintain the same expected activation by multiplying them by $1/p$, the resulting moments are again:

$$\mathbb{E}\left[\frac{1}{p}r_i \alpha_i\right] = \frac{p}{p}\mu = \mu, \quad \mathbb{V}\left[\frac{1}{p}r_i \alpha_i\right] = \frac{p^2}{p^2}\sigma^2 = \sigma^2 . \tag{1.17}$$

Thus, dropping out features of an infinitely-wide MLP does not change the model at all, since no individual feature can have more than infinitesimal contribution to the network output.

1.4.2   Dropping Out Inputs

In a GP with kernel $k(\mathbf{x}, \mathbf{x}') = \prod_{d=1}^{D} k_d(x_d, x_d')$, exact averaging over all possible ways of dropping out inputs with probability $1/2$ results in a mixture of GPs, each depending on only a subset of the inputs:

$$p\left(f(\mathbf{x})\right) = \frac{1}{2^D} \sum_{\mathbf{r} \in \{0,1\}^D} \mathrm{GP}\left(0, \prod_{d=1}^{D} k_d(x_d, x_d')^{r_d}\right) \tag{1.18}$$

We present two results ways to gain intuition about this model.

First, if the kernel on each dimension has the form $k_d(x_d, x_d') = g\left(\frac{x_d - x_d'}{w_d}\right)$, as does the SE kernel, then any input dimension can be dropped out by setting its lengthscale w_d to ∞. Thus, dropout on the inputs of a GP corresponds to a spike-and-slab prior on lengthscales, with each dimension independently having $w_d = \infty$ with probability $1/2$.

Another way to understand the resulting prior is to note that the dropout mixture (1.18) has the same covariance as

$$f(\mathbf{x}) \sim \mathrm{GP}\left(0, \frac{1}{2^{-2D}} \sum_{\mathbf{r} \in \{0,1\}^D} \prod_{d=1}^{D} k_d(x_d, x_d')^{r_d}\right) \tag{1.19}$$

A GP whose covariance is a sum of kernels corresponds to a sum of functions, each distributed according to a GP. Therefore, (1.19) describes a sum of 2^D functions, each depending on a different subset of the inputs.

1.5   Related Work

Since the non-local structure capturable by additive kernels is necessarily axis-aligned, we can naturally consider that an initial transformation of the input space might allow us to recover non-axis aligned additivity in functions. This avenue was explored by Gilboa et al. (2013), who developed a linearly-transformed first-order additive GP model, called projection-pursuit GP regression. They further showed that inference in this model was possible in $\mathcal{O}(N)$ time.

Plate (1999) constructed an additive GP using only the first-order and Dth-order terms. This model is motivated by the desire to trade off the interpretability of first-order models with the flexibility of full-order models. Our experiments show that often, the intermediate degrees of interaction contribute most of the variance.

A related functional ANOVA GP model (Kaufman and Sain, 2010) decomposes the

mean function into a weighted sum of GPs. However, the effect of a particular degree of interaction cannot be quantified by that approach. Also, computationally, the Gibbs sampling approach used in (Kaufman and Sain, 2010) is disadvantageous.

Christoudias et al. (2009) previously showed how mixtures of kernels can be learnt by gradient descent in the Gaussian process framework. They call this *Bayesian localized multiple kernel learning*. However, their approach learns a mixture over a small, fixed set of kernels, while our method learns a mixture over all possible products of those kernels.

1.5.1   Hierarchical Kernel Learning

A similar model class has been recently explored by Bach (2009) called Hierarchical Kernel Learning (HKL). HKL uses a regularized optimization framework to learn a weighted sum over an exponential number of kernels which can be computed in polynomial time. This method chooses among *hull* of kernels, defined as a subset of all terms such that if $\prod_{j \in J} k_j(\mathbf{x}, \mathbf{x}')$ is included in the subset, then so are all terms $\prod_{j \in J/i} k_j(\mathbf{x}, \mathbf{x}')$, for all $i \in J$. HKL computes the sum over all orders in $\mathcal{O}(D)$ time by the formula:

$$k_a(\mathbf{x}, \mathbf{x}') = v^2 \prod_{d=1}^{D} \left(1 + \alpha k_d(x_d, x_d')\right) \tag{1.20}$$

which forces the weight of all nth order terms to be weighted by α^n.

Figure 1.2 contrasts the HKL model class with the additive GP model. Neither method is strictly more flexibile than the other. The main difficulty with the approach of Bach (2009) is that the kernel parameters are hard to set, other than by cross-validation.

1.5.2   ANOVA Procedures

Vapnik (1998) introduced the support vector ANOVA decomposition, which has the same form as our additive kernel. They recommend approximating the sum over all D orders with only one term "of appropriate order", presumably because of the difficulty of setting the parameters of an SVM. Stitson et al. (1999) performed experiments which favourably compared the predictive accuracy of the support vector ANOVA decomposition against polynomial and spline kernels. They too allowed only one order to be active, and set parameters by cross-validation.

A closely related procedure from Wahba (1990) is smoothing-splines ANOVA (SS-ANOVA). An SS-ANOVA model is a weighted sum of splines along each dimension, plus a sum of
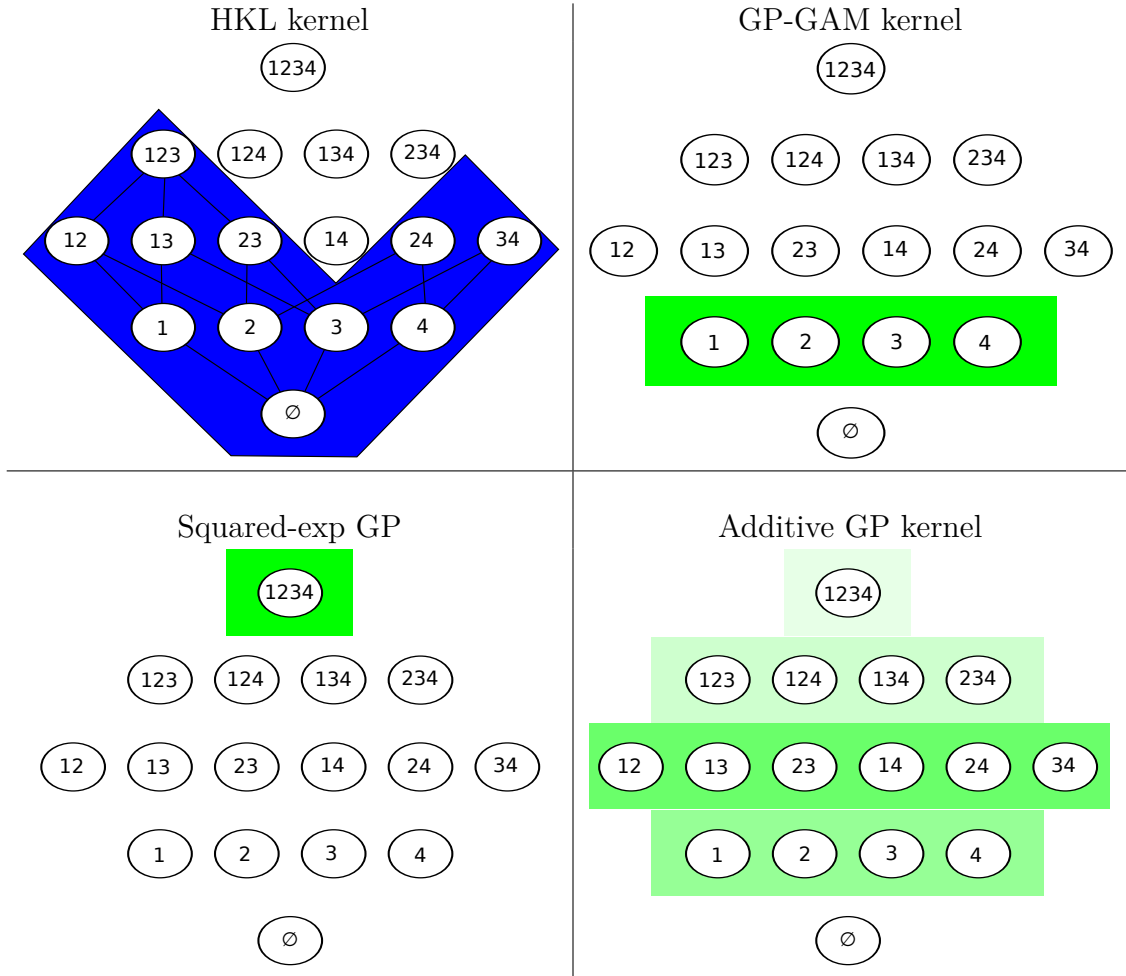
Fig. 1.2 A comparison of different additive model classes. Nodes represent different interaction terms, ranging from first-order to fourth-order interactions. Far left: HKL can select a hull of interaction terms, but must use a pre-determined weighting over those terms. Far right: the additive GP model can weight each order of interaction seperately. Neither HKL nor the additive model dominate one another in terms of flexibility, however the GP-GAM and the SE-GP are special cases of additive GPs.

splines over all pairs of dimensions, all triplets, etc, with each individual interaction term having a separate weighting parameter. Because the number of terms to consider grows exponentially in the order, in practice, only terms of first and second order are usually considered. Learning in SS-ANOVA is usually done via penalized-maximum likelihood with a fixed sparsity hyperparameter.

In contrast to these procedures, our method can easily include all D orders of interaction, each weighted by a separate hyperparameter. As well, we can learn kernel parameters individually per input dimension, allowing automatic relevance determina-

tion to operate.

1.6   Experiments

Overfitting and Parameterization

A D-dimensional SE-ARD kernel has D lengthscale parameters and the output variance. An first-order additive SE model has $2 \times D$ parameters. A fully-parametrized model including all orders of interaction, with a seperate output variance for each scale will have $3 \times D$ parameters. Because each additional parameter increases the tendency to overfit, we recommend allowing only one kernel parameter per input dimension. In our experiments, we parametrized each one-dimensional kernel with only the lengthscale, fixing the output variance to be 1.

On a diverse collection of datasets, we compared five different models. In the results tables below, GP Additive refers to a GP using the additive kernel with squared-exp base kernels. For speed, we limited the maximum order of interaction in the additive kernels to 10. GP-GAM denotes an additive GP model with only first-order interactions. GP Squared-Exp is a GP model with a squared-exponential ARD kernel. HKL was run using the all-subsets kernel, which corresponds to the same set of kernels as considered by the additive GP with a squared-exp base kernel.

For all GP models, we fit kernel parameters by the standard method of maximizing training-set marginal likelihood, using L-BFGS (Nocedal, 1980) for 500 iterations, allowing five random restarts. In addition to learning kernel parameters, we fit a constant mean function to the data. In the classification experiments, approximate GP inference was done using Expectation Propagation (Minka, 2001).

Bach Synthetic Dataset

In addition to standard UCI repository datasets, we generated a synthetic dataset following the same recipe as Bach (2009). This dataset was designed by Bach (2009) to demonstrate the advantages of HKL over GP-ARD. It is generated by passing correlated Gaussian-distributed inputs $x_1, x_2, \ldots, x_8$ through the quadratic function

$$f(\mathbf{x}) = \sum_{i=1}^{4} \sum_{j=1+1}^{4} x_i x_j + \epsilon \qquad \epsilon \sim \mathcal{N}(0, \sigma_\epsilon) \tag{1.21}$$

This dataset is well-modeled by an additive kernel which includes all two-way interactions over the first 4 variables, but does not depend on the extra 4 irrelevant inputs.

If the dataset is large enough, HKL can construct a hull around only those subsets of cross terms that are optimal for predicting the output. GP-ARD, in contrast, can learn to ignore the noisy copy variables, but cannot learn to ignore the higher-term interactions between the predictive variables. However, a GP with an additive kernel can learn both to ignore irrelevant variables, and to ignore missing orders of interaction. With enough data, the marginal likelihood will favour hyperparameters specifying such a model.

1.6.1 Results

Tables 1.2, 1.3, 1.4 and 1.5 show mean performance across 10 train-test splits. Because HKL does not specify a noise model, it could not be included in the likelihood comparisons.

Table 1.2 Regression Mean Squared Error

Method	bach	concrete	pumadyn-8nh	servo	housing
Linear Regression	1.031	0.404	0.641	0.523	0.289
GP GAM	1.259	0.149	0.598	0.281	0.161
HKL	**0.199**	0.147	0.346	0.199	0.151
GP Squared-exp	**0.045**	0.157	**0.317**	**0.126**	**0.092**
GP Additive	**0.045**	**0.089**	**0.316**	**0.110**	**0.102**

Table 1.3 Regression Negative Log Likelihood

Method	bach	concrete	pumadyn-8nh	servo	housing
Linear Regression	2.430	1.403	1.881	1.678	1.052
GP GAM	1.708	0.467	1.195	0.800	0.457
GP Squared-exp	-0.131	0.398	**0.843**	0.429	**0.207**
GP Additive	-0.131	**0.114**	**0.841**	**0.309**	0.194

The model with best performance on each dataset is in bold, along with all other models that were not significantly different under a paired t-test. The additive model

Table 1.4 Classification percent error

Method	breast	pima	sonar	ionosphere	liver	heart
Logistic Regression	7.611	24.392	26.786	16.810	45.060	**16.082**
GP GAM	**5.189**	**22.419**	**15.786**	**8.524**	**29.842**	16.839
HKL	**5.377**	24.261	**21.000**	9.119	**27.270**	18.975
GP Squared-exp	**4.734**	**23.722**	**16.357**	**6.833**	31.237	20.642
GP Additive	**5.566**	**23.076**	**15.714**	**7.976**	30.060	18.496

Table 1.5 Classification negative log-likelihood

Method	breast	pima	sonar	ionosphere	liver	heart
Logistic Regression	0.247	0.560	4.609	0.878	0.864	0.575
GP GAM	**0.163**	**0.461**	**0.377**	**0.312**	**0.569**	**0.393**
GP Squared-exp	**0.146**	0.478	**0.425**	**0.236**	0.601	0.480
GP Additive	**0.150**	**0.466**	**0.409**	**0.295**	**0.588**	**0.415**

never performs significantly worse than any other model, and sometimes performs significantly better than all other models. The difference between all methods is larger in the case of regression experiments. The performance of HKL is consistent with the results in (Bach, 2009), performing competitively but slightly worse than SE-GP.

The additive GP performed best on datasets well-explained by low orders of interaction, and approximately as well as the SE-GP model on datasets which were well explained by high orders of interaction (see table 1.1). Because the additive GP is a superset of both the GP-GAM model and the SE-GP model, instances where the additive GP performs slightly worse are presumably due to over-fitting, or due to the hyperparameter optimization becoming stuck in a local maximum. Performance ccould be expected to benefit from integrating over the kernel parameters.

1.6.2 Source Code

Additive Gaussian processes are particularly appealing in practice because their use requires only the specification of the base kernel; all other aspects of GP inference remain the same. Note that we are free to choose a different covariance function along each dimension.

All of the experiments in this chapter were performed using the standard GPML

toolbox, available at `http://www.gaussianprocess.org/gpml/code/`. Code to perform all experiments is available at `http://github.com/duvenaud/dropout-gps`

1.7   Conclusion

We present additive Gaussian processes: a simple family of models which generalizes two widely-used classes of models. Additive GPs also introduce a tractable new type of structure into the GP framework. Our experiments indicate that such additive structure is present in real datasets, allowing our model to perform better than standard GP models. In the case where no such structure exists, our model can recover arbitrarily flexible models, as well.

In addition to improving modeling efficacy, the additive GP also improves model interpretability: the variance parameters on each order of intercation indicate which sorts of structure are present in our model.

Compared to HKL, which is the only other tractable procedure able to capture the same types of structure, our method benefits from being able to learn individual kernel parameters, as well as the weightings of different orders of interaction. Our experiments show that additive GPs are a state-of-the-art regression model.

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