Evolution of Covariance Functions for Gaussian Process Regression using Genetic Programming

Gabriel Kronberger and Michael Kommenda

School of Informatics, Communications and Media,
University of Applied Sciences Upper Austria,
Softwarepark 11, 4232, Hagenberg
{gabriel.kronberger,michael.kommenda}@fh-hagenberg.at

Abstract. In this contribution we describe an approach to evolve composite covariance functions for Gaussian processes using genetic programming. A critical aspect of Gaussian processes and similar kernel-based models such as SVM is, that the covariance function should be adapted to the modeled data. Frequently, the squared exponential covariance function is used as a default. However, this can lead to a misspecified model, which does not fit the data well.

In the proposed approach we use a grammar for the composition of covariance functions and genetic programming to search over the space of sentences that can be derived from the grammar.

We tested the proposed approach on synthetic data from two-dimensional test functions, and on the Mauna Loa CO_2 time series. The results show, that our approach is feasible, finding covariance functions that perform much better than a default covariance function. For the CO_2 data set a composite covariance function is found, that matches the performance of a hand-tuned covariance function.

Keywords: Gaussian Process, Genetic Programming, Structure Identification

1 Introduction

The composition of covariance functions is a non-trivial task and has been described as a black art [2]. On the one hand, it is critical to tune the covariance function to the data set, that should be modeled, because this is the primary option to integrate prior knowledge into the learning process [10]; on the other hand a lot of experience and knowledge about the modeled system is required to do this correctly. Frequently, and especially for multi-dimensional data sets it is far from obvious how the covariance function should be structured.

In this work we discuss the composition of covariance functions for Gaussian processes, that can be used for nonparametric machine learning tasks e.g., for regression or classification [10]. In this context a Gaussian process is used as a Bayesian prior over functions, relating the input variables to the target variable. Gaussian process regression allows modeling of non-linear functional dependencies through different covariance functions, and produces posterior probability distribution estimates for the target values instead of point estimates only.

1.1 Our Contribution

The aim of this paper is to describe the idea of using a grammar for covariance functions and genetic programming to search for a good covariance function for a given data set. We also describe our prototype implementation using grammarguided tree-based GP, and finally, present results as a proof-of concept. We have not yet evaluated the difficulty of this problem for genetic programming, and in particular, if GP suited well for this kind of problem. The results of our experiments indicate that the idea is feasible, producing good covariance functions for low-dimensional data sets.

1.2 Previous Work

In a very recent contribution, the problem of structure identification for covariance functions has been approached using a grammar, or rather a set of rewriting rules, as a basis for searching over composite covariance functions for Gaussian processes [2]. This approach is actually very similar to our work; the main difference is, that in our work we use genetic programming to search over the set of possible structures, while Duvenaud et al. enumerate over composite functions, starting with standard functions.

Another recent contribution discusses more flexible families of covariance functions, instead of composing covariance functions from simple terms [12]. Also related is earlier work that describes additive Gaussian processes [3], which are equivalent to a weighted additive composition of base kernels, but can be calculated efficiently.

Genetic programming has been used previously to evolve kernel functions for SVMs with mixed results [4], [6]. The latest contribution found that genetic programming was able to "rediscover multiple standard kernels, but no significant improvements over standard kernels were obtained" [7]. These results can, however, not be transferred directly to Gaussian processes because of several major differences between Gaussian processes and SVMs. In particular, in the case of Gaussian processes hyper-parameters are optimized using a ML-II approach, in contrast to SVMs, where hyper-parameter values are usually tuned using cross-validation and grid-search. Additionally, in contrast to all other previous work, simple embeddings of covariance functions by masking dimensions are supported.

2 Gaussian Processes

A Gaussian process is a non-parametric model that produces predictions solely from the specified mean and covariance functions and the available training data [10]. The inference of function values f^* for observed input values X^* based on observations of g and g involves the calculation of the covariance matrices g(X,X) and g(X,X) and inference from the multi-dimensional Gaussian shown in Equation 1.

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}^* \end{bmatrix} \sim N \left(\begin{bmatrix} m(X) \\ m(X^*) \end{bmatrix}, \begin{bmatrix} K(X,X) + \sigma^2 I & K(X,X^*) \\ K(X^*,X) & K(X^*,X^*) \end{bmatrix} \right)$$
(1)

The term $\sigma^2 I$ is necessary to account for Gaussian distributed noise with variance σ^2 . From this definition it follows that the posterior for f^* is again a multi-dimensional Gaussian. For model selection and hyper-parameter learning the marginal likelihood p(y|X) must be calculated. The model is a multi-dimensional Gaussian so an analytical form of the likelihood can be derived.

Calculation of the marginal likelihood requires a matrix inversion and, thus, has asymptotic complexity $O(n^3)$. Usually, the covariance function K(x,x') has hyper-parameters that must optimized. This is often accomplished in a simple ML-II fashion, optimizing the hyper-parameters w.r.t. the likelihood using a quasi-Newton method (e.g., BFGS). Since the gradients of the marginal likelihood for the hyper-parameters can be determined with an additional computational complexity of $O(n^2)$ for each hyper-parameter, it is feasible to use gradient-based methods. The drawback is that the likelihood is typically multimodal, and especially for covariances with many hyper-parameters (e.g., ARD) the optimizer can converge to a local optimum. Thus, it is typically suggested to execute several random restarts. A better solution would be to include priors on the hyper-parameters and optimizing w.r.t. posterior distribution (MAP). However, this can only be accomplished using a MCMC approach which is computationally expensive.

Frequently used covariance functions for Gaussian processes include the linear, polynomial, squared exponential (SE), rational quadratic (RQ) and the Matérn function. Covariance functions can be combined to more complex covariance functions, for instance as products or sums of different covariance functions [10].

3 Genetic Programming

Genetic programming generally refers to the automatic creation of computer programs using genetic algorithms [8]. The basic principle is to evolve variable-length structures, frequently symbolic expression trees, which represent potential solutions to the problem. One of the most prominent applications of genetic programming is symbolic regression, the synthesis of regression models without a predetermined structure. Genetic programming makes it possible to optimize the structure of solutions in combination with their parameters. Thus, it should also be possible to synthesize composite covariance functions with genetic programming. In the following, we use a grammar-guided genetic programming system to make sure that only valid covariance functions are produced. A good survey of grammar-guided genetic programming is given in [9].

4 Grammar for Covariance Functions

The grammar for covariance functions has been derived from the rules for the composition of kernels as e.g., discussed in [10]. It should be noted that the grammar shown below is not complete, meaning that several constructions that would

lead to a valid covariance function are not possible¹. The following represents the grammar G(Cov) for covariance functions in EBNF notation²:

The functions Prod and Sum produce the product and sum of multiple covariance functions, which can again be composite covariance functions. The scale operator can be used to add a scaling factor to any covariance function. The Mask operator selects a potentially empty subset of input variables from all possible input variables. The non-terminal symbol BitVector can be derived to a list of zeros and ones. The bit vector is used to mask selected dimensions in the data set, effectively reducing the dimensionality. The length of the bit mask has to match the total number of dimensions; this is checked when the resulting covariance function is evaluated.

Finally, the non-terminal symbol TerminalCov can be derived to a range of default covariance functions. Currently, we only included isometric covariance functions, but other covariance functions can be added to the grammar easily. The grammar does not include the hyper-parameters, because they are not optimized by genetic programming. Instead, hyper-parameters are optimized for each potential solution, using a gradient-descent technique.

5 Experiments

For the experiments we implemented Gaussian processes, a set of commonly used covariance functions, and the grammar for covariance functions in HeuristicLab³ [11] which already provides an implementation of grammar-guided tree-based genetic programming.

The aim of the experiments presented in this contribution is mainly to test the feasibility of the idea. Two different types of data sets are used for the experiments, and the forecasts of the synthesized covariance functions are compared to a set of default covariance functions and also to hand-tuned covariance functions. The first data set is the univariate Mauna Loa atmospheric CO_2 time series. This data set has been chosen, because a hand-tuned covariance function for this data set is presented in [10]. For the second experiment we created several synthetic data sets sampled randomly from two-dimensional Gaussian process priors shown in Equation 2. The data generated from these functions are difficult to model with a single isometric covariance function. Multiple covariance functions have to be combined and the correct dimension masking vectors have

One example is vertical scaling of covariance functions: K'(x, x') = a(x)K(x, x')a(x')

² The grammar is largely based on the capabilities of the GPML package by Rasmussen and Nickisch, http://gaussianprocess.org/gpml/code.

³ HeuristicLab version 3.3.8 is available from http://dev.heuristiclab.com/

to be identified. Each data set contains 882 samples of the function on a regular two-dimensional grid.

$$SE+RQ(\boldsymbol{x}, \boldsymbol{x'}) = SE(x_0, x'_0) + RQ(x_1, x'_1)$$

$$SE+Matérn(\boldsymbol{x}, \boldsymbol{x'}) = SE(x_0, x'_0) + Matérn1(x_1, x'_1)$$

$$SE+Periodic(\boldsymbol{x}, \boldsymbol{x'}) = SE(x_0, x'_0) + RQ(x_1, x'_1)$$

$$(2)$$

5.1 Genetic Programming Parameter Settings

Training of Gaussian processes is computationally expensive, and because it is necessary to optimize the hyper-parameters for each evaluated covariance function the run time of the genetic programming algorithm grows quickly. Therefore, we used very restrictive parameter settings, in particular a small population size of only 50 individuals. All other parameter settings are shown in Table 1.

Table 1. Genetic programming parameter settings for all experiments.

Parameter	Value
Population size	50
Max. length / height	25 / 7
Initialization	PTC2
Parent selection	gender-specific (proportional $+$ random)
Mutation rate	15%
ML-II iterations	50
Offspring selection [1]	strict (success ratio $= 1$, comparison factor $= 1$)
Max. selection pressure	100
Max. generations	20

5.2 Results on Mauna Loa CO_2 Data Set

The results for the CO_2 time series are positive. The algorithm was able to consistently find covariance functions that fit well in the training period (1958 – 2004), accurate forecasts over the testing period (2004 – 2012). The structures of two exemplary solutions are shown in Equation 3. The first solution (K1) is actually very similar to the hand-tuned covariance solution proposed in [10]. The second covariance function is more complex and has only a slightly better likelihood. Unfortunately, genetic programming often leads to overly complex solutions which is a critical drawback of our approach. Both solutions have been found after only 800 evaluated solution candidates and achieve a negative log-likelihood of 129.8 and 116, respectively. The correlation coefficients for the forecasts in the test partition are above 0.99. Figure 1 shows the output of the first model.

$$K1(x,x') = \operatorname{SE}(x,x') + \operatorname{Periodic}(x,x') + \operatorname{Mat\acute{e}rn1}(x,x') + \\ \operatorname{SE}(x,x') + \operatorname{Mat\acute{e}rn5}(x,x') + \operatorname{Const}$$

$$K2(x,x') = \operatorname{Mat\acute{e}rn3}(x,x') * \operatorname{Perioric}(x,x') * \operatorname{RQ}(x,x') * \\ (\operatorname{Mat\acute{e}rn1}(x,x') + \operatorname{Mat\acute{e}rn3}(x,x') + \operatorname{Mat\acute{e}rn5}(x,x') + \\ \operatorname{Perioric}(x,x') + \operatorname{Linear}(x,x')) * \\ (\operatorname{Mat\acute{e}rn1}(x,x') + \operatorname{Mat\acute{e}rn3}(x,x') + \operatorname{RQ}(x,x'))$$

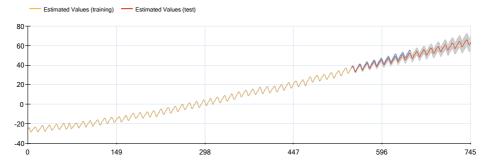


Fig. 1. The output and forecast for the Mauna Loa CO_2 time series of a Gaussian process using the first evolved covariance function (K1) shown in Equation 3.

5.3 Results on Synthetic Data Sets

The results for the synthetic two-dimensional data set are shown in Table 2. In this experiment we trained multiple Gaussian process models using several frequently used covariance functions. We trained many models using random restarts for each data set and covariance function, and report the best negative log-likelihood for each pair. As expected, the models with the isometric covariance functions do not fit well. In contrast, the composite covariance functions produced by genetic programming fit much better. For comparison, we also report the negative log-likelihood, that can be achieved with the optimal covariance function for each data set. In these experiments, the exact structure of the covariance could not be rediscovered, thus, the evolved functions are worse than the optimal solution.

6 Summary and Discussion

In this contribution we described an approach for the synthesis of composite covariance function for Gaussian processes using grammar-guided genetic programming. In the proposed approach a set of commonly used covariance functions is

Table 2. Best negative log-likelihood achieved for the three synthetic two-dimensional test functions, with default covariance functions and with evolved composite covariance functions.

		Problem instance				
		SE+RQ	SE+Matérn	SE+Periodic		
variance	SE	-204	-492	440		
	RQ	-272	-492	103		
	Periodic Matérn	-221	-492	479		
	Matérn	-27	31	304		
	Evolved	-803	-760	-640		
	Optimal	-2180	-2187	-2131		

used to compose more complex covariance functions, using sums or products of several covariance functions. The set of valid covariance functions is defined via a grammar and genetic programming is used to search the space of possible derivations from this grammar. The hyper-parameters of covariance functions are not subject to the evolutionary search, but are optimized w.r.t. the likelihood using a standard gradient-descent optimizer (i.e., LBFGS).

The proposed approach was tested on two types of low-dimensional problems as a proof of concept. We found, that for the univariate Mauna Loa CO_2 time series it is possible to consistently find good covariance functions with genetic programming. The identified solutions perform as well as a hand-tuned covariance function for this problem. The results for our two-dimensional synthetic functions show that it is possible to find composite covariance functions, which perform much better than default covariance functions on these data sets.

In contrast to previous work by the genetic programming community [7], which focused mainly on kernel synthesis for SVMs, this contribution discusses kernel synthesis for Gaussian processes, which are non-parametric fully Bayesian models. For Gaussian process models the hyper-parameters can be optimized with a standard gradient-descent approach, and it is not strictly necessary to execute cross-validation [10]. Previous work either used grid-search and cross-validation to tune hyper-parameters, which is very computationally expensive, or did not consider hyper-parameter optimization at all. Additionally, we are using a grammar to compose covariance functions from simple covariance functions instead of evolving the full function.

In the statistics community, a very recent contribution has also discussed the usage of grammars for the composition of covariance functions [2]. The main difference to this work is that here genetic programming is used to search over the derivations of the grammar. Another relevant difference is that the grammar in this contribution also supports simple embeddings through the masking function. It should be noted, that we have not yet analyzed if genetic programming is well suited for this task, and in particular we did not compare the approach to simple enumeration or random search.

One question that remains for future work is whether composed covariance functions also work well for data sets with more variables. We have observed that simple covariance functions often work very well, and tuned covariance functions do not have a strong beneficial effect for these data sets.

Another interesting topic for future research is to look at alternative ways for searching over the space of covariance functions defined by a grammar. Recently, an interesting approach has been described that uses variational methods for Bayesian learning of probabilistic context free grammars for this task [5]. This idea could be especially useful for Bayesian models such as Gaussian processes.

Acknowledgments The authors would like to thank Jeffrey Emanuel for the initial idea leading to this contribution. This work has been supported by the Austrian Research Promotion Agency (FFG), on behalf of the Austrian Federal Ministry of Economy, Family and Youth (BMWFJ), within the program "Josef Ressel-Centers".

References

- Affenzeller, M., Winkler, S., Wagner, S., Beham, A.: Genetic Algorithms and Genetic Programming: Modern Concepts and Practical Applications. Numerical Insights, CRC Press, Singapore (2009)
- Duvenaud, D., Lloyd, J.R., Grosse, R., Tenenbaum, J.B., Ghahramani, Z.: Structure Discovery in Nonparametric Regression through Compositional Kernel Search. ArXiv e-prints (Feb 2013)
- 3. Duvenaud, D., Nickisch, H., Rasmussen, C.E.: Additive Gaussian processes. arXiv preprint arXiv:1112.4394 (2011)
- Gagne, C., Schoenauer, M., Sebag, M., Tomassini, M.: Genetic programming for kernel-based learning with co-evolving subsets selection. In: Proc. of PPSN IX. LNCS, vol. 4193, pp. 1008–1017. Springer-Verlag (2006)
- 5. Hasegawa, Y., Iba, H.: Latent variable model for estimation of distribution algorithm based on a probabilistic context-free grammar. IEEE Transactions on Evolutionary Computation 13(4), 858–878 (Aug 2009)
- Howley, T., Madden, M.G.: An evolutionary approach to automatic kernel construction. In: Proc. of ICANN 2006. LNCS, vol. 4132, pp. 417–426. Springer-Verlag (2006)
- 7. Koch, P., Bischl, B., Flasch, O., Beielstein, T., Weihs, C., Konen, W.: Tuning and evolution of support vector kernels. Evolutionary Intelligence 5, 153–170 (2012)
- 8. Koza, J.R.: Genetic programming: on the programming of computers by means of natural selection. MIT Press, Cambridge, MA, USA (1992)
- 9. McKay, R.I., Hoai, N.X., Whigham, P.A., Shan, Y., O'Neill, M.: Grammar-based genetic programming: a survey. Genetic Programming and Evolvable Machines 11(3/4), 365–396 (Sep 2010)
- Rasmussen, C.E., Williams, C.K.: Gaussian Processes for Machine Learning. MIT Press (2006)
- 11. Wagner, S.: Heuristic optimization software systems Modeling of heuristic optimization algorithms in the HeuristicLab software environment. Ph.D. thesis, Institute for Formal Models and Verification, Johannes Kepler University, Linz (2009)
- 12. Wilson, A.G., Prescott Adams, R.: Gaussian Process Covariance Kernels for Pattern Discovery and Extrapolation. ArXiv e-prints (Feb 2013)