

## Preface

Over the last decade there has been an explosion of work in the “kernel machines” area of machine learning. Probably the best known example of this is work on support vector machines, but during this period there has also been much activity concerning the application of Gaussian process models to machine learning tasks. The goal of this book is to provide a systematic and unified treatment of this area. Gaussian processes provide a principled, practical, probabilistic approach to learning in kernel machines. This gives advantages with respect to the interpretation of model predictions and provides a well-founded framework for learning and model selection. Theoretical and practical developments of over the last decade have made Gaussian processes a serious competitor for real supervised learning applications.

kernel machines

Roughly speaking a stochastic *process* is a generalization of a probability distribution (which describes a finite-dimensional random variable) to *functions*. By focussing on processes which are *Gaussian*, it turns out that the computations required for inference and learning become relatively easy. Thus, the supervised learning problems in machine learning which can be thought of as learning a function from examples can be cast directly into the Gaussian process framework.

Gaussian process

Our interest in Gaussian process (GP) models in the context of machine learning was aroused in 1994, while we were both graduate students in Geoff Hinton’s Neural Networks lab at the University of Toronto. This was a time when the field of neural networks was becoming mature and the many connections to statistical physics, probabilistic models and statistics became well known, and the first kernel-based learning algorithms were becoming popular. In retrospect it is clear that the time was ripe for the application of Gaussian processes to machine learning problems.

Gaussian processes  
in machine learning

Many researchers were realizing that neural networks were not so easy to apply in practice, due to the many decisions which needed to be made: what architecture, what activation functions, what learning rate, etc., and the lack of a principled framework to answer these questions. The probabilistic framework was pursued using approximations by MacKay [1992b] and using Markov chain Monte Carlo (MCMC) methods by Neal [1996]. Neal was also a graduate student in the same lab, and in his thesis he sought to demonstrate that using the Bayesian formalism, one does not necessarily have problems with “overfitting” when the models get large, and one should pursue the limit of large models. While his own work was focused on sophisticated Markov chain methods for inference in large finite networks, he did point out that some of his networks became Gaussian processes in the limit of infinite size, and “there may be simpler ways to do inference in this case.”

neural networks

large neural networks  
≡ Gaussian processes

It is perhaps interesting to mention a slightly wider historical perspective. The main reason why neural networks became popular was that they allowed the use of *adaptive* basis functions, as opposed to the well known linear models. The adaptive basis functions, or hidden units, could “learn” hidden features

adaptive basis functions

many fixed basis  
functions

useful for the modelling problem at hand. However, this adaptivity came at the cost of a lot of practical problems. Later, with the advancement of the “kernel era”, it was realized that the limitation of fixed basis functions is not a big restriction if only one has enough of them, i.e. typically infinitely many, and one is careful to control problems of overfitting by using priors or regularization. The resulting models are much easier to handle than the adaptive basis function models, but have similar expressive power.

useful representations

Thus, one could claim that (as far as machine learning is concerned) the adaptive basis functions were merely a decade-long digression, and we are now back to where we came from. This view is perhaps reasonable if we think of models for solving practical learning problems, although MacKay [2003, ch. 45], for example, raises concerns by asking “did we throw out the baby with the bath water?”, as the kernel view does not give us any hidden representations, telling us what the useful features are for solving a particular problem. As we will argue in the book, one answer may be to learn more sophisticated covariance functions, and the “hidden” properties of the problem are to be found here. An important area of future developments for GP models is the use of more expressive covariance functions.

supervised learning  
in statistics

Supervised learning problems have been studied for more than a century in statistics, and a large body of well-established theory has been developed. More recently, with the advance of affordable, fast computation, the machine learning community has addressed increasingly large and complex problems.

statistics and  
machine learning

Much of the basic theory and many algorithms are shared between the statistics and machine learning community. The primary differences are perhaps the types of the problems attacked, and the goal of learning. At the risk of oversimplification, one could say that in statistics a prime focus is often in understanding the *data* and relationships in terms of *models* giving approximate summaries such as linear relations or independencies. In contrast, the goals in machine learning are primarily to make predictions as accurately as possible and to understand the behaviour of learning *algorithms*. These differing objectives have led to different developments in the two fields: for example, neural network algorithms have been used extensively as black-box function approximators in machine learning, but to many statisticians they are less than satisfactory, because of the difficulties in interpreting such models.

data and models

algorithms and  
predictions

bridging the gap

Gaussian process models in some sense bring together work in the two communities. As we will see, Gaussian processes are mathematically equivalent to many well known models, including Bayesian linear models, spline models, large neural networks (under suitable conditions), and are closely related to others, such as support vector machines. Under the Gaussian process viewpoint, the models may be easier to handle and interpret than their conventional counterparts, such as e.g. neural networks. In the statistics community Gaussian processes have also been discussed many times, although it would probably be excessive to claim that their use is widespread except for certain specific applications such as spatial models in meteorology and geology, and the analysis of computer experiments. A rich theory also exists for Gaussian process models

in the time series analysis literature; some pointers to this literature are given in Appendix B.

The book is primarily intended for graduate students and researchers in machine learning at departments of Computer Science, Statistics and Applied Mathematics. As prerequisites we require a good basic grounding in calculus, linear algebra and probability theory as would be obtained by graduates in numerate disciplines such as electrical engineering, physics and computer science. For preparation in calculus and linear algebra any good university-level textbook on mathematics for physics or engineering such as Arfken [1985] would be fine. For probability theory some familiarity with multivariate distributions (especially the Gaussian) and conditional probability is required. Some background mathematical material is also provided in Appendix A.

intended audience

The main focus of the book is to present clearly and concisely an overview of the main ideas of Gaussian processes in a machine learning context. We have also covered a wide range of connections to existing models in the literature, and cover approximate inference for faster practical algorithms. We have presented detailed algorithms for many methods to aid the practitioner. Software implementations are available from the website for the book, see Appendix C. We have also included a small set of exercises in each chapter; we hope these will help in gaining a deeper understanding of the material.

focus

In order limit the size of the volume, we have had to omit some topics, such as, for example, Markov chain Monte Carlo methods for inference. One of the most difficult things to decide when writing a book is what sections not to write. Within sections, we have often chosen to describe one algorithm in particular in depth, and mention related work only in passing. Although this causes the omission of some material, we feel it is the best approach for a monograph, and hope that the reader will gain a general understanding so as to be able to push further into the growing literature of GP models.

scope

The book has a natural split into two parts, with the chapters up to and including chapter 5 covering core material, and the remaining sections covering the connections to other methods, fast approximations, and more specialized properties. Some sections are marked by an asterisk. These sections may be omitted on a first reading, and are not pre-requisites for later (un-starred) material.

book organization

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errata

Despite our best efforts it is inevitable that some errors will make it through to the printed version of the book. Errata will be made available via the book's website at

<http://www.GaussianProcess.org/gpml>

We have found the joint writing of this book an excellent experience. Although hard at times, we are confident that the end result is much better than either one of us could have written alone.

looking ahead

Now, ten years after their first introduction into the machine learning community, Gaussian processes are receiving growing attention. Although GPs have been known for a long time in the statistics and geostatistics fields, and their use can perhaps be traced back as far as the end of the 19th century, their application to real problems is still in its early phases. This contrasts somewhat the application of the non-probabilistic analogue of the GP, the support vector machine, which was taken up more quickly by practitioners. Perhaps this has to do with the probabilistic mind-set needed to understand GPs, which is not so generally appreciated. Perhaps it is due to the need for computational short-cuts to implement inference for large datasets. Or it could be due to the lack of a self-contained introduction to this exciting field—with this volume, we hope to contribute to the momentum gained by Gaussian processes in machine learning.

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