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Automatic Graph Tracking in Dynamic Probabilistic Programs via Source Transformations

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Affidavit

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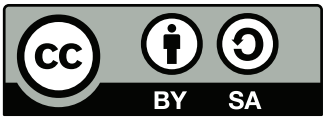

The LaTeX source of this document is available at
https://github.com/phipsgabler/master-thesis
or upon request from the author.[1]

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Abstract

This thesis presents a novel approach for the implementation of a tracking system to facilitate program analysis, based on program transformations. The system is then applied to a specific problem in the field of probabilistic programming.

The main contribution is a general system for the extraction of rich computation graphs in the Julia programming language, based on a transformation of the intermediate representation (IR) used by the compiler. These graphs contain the whole recursive structure of any Julia program in terms of executed IR instructions. The system is flexible enough to be used for multiple purposes that require dynamic program analysis or abstract interpretation, such as automatic differentiation or dependency analysis.

The second part of the thesis describes the application of this graph tracking system to probabilistic programs written for Turing, a probabilistic programming system implemented as an embedded language within Julia. Through this, an executed Turing model can be analyzed, and the dependency structure of involved random variables be extracted from it. Given this structure, analytical Gibbs conditionals can be calculated and passed to Turing's inference mechanism, where they are used in Markov-Chain Monte Carlo samplers approximating the modelled distribution.

Contents

Notation

$\mathbb{P}[\Theta \in A \mid X = x]$	Random variables and their realizations will usually be denoted with upper and lower case letters, respectively (with some exceptions for Greek variable names). Sets are written with uppercase letters.
$\mathbb{E}[X]$, $\mathbb{V}_X[Y]$	Expectation and variance; if necessary, the variable with respect to which the moment is taken is indicated.
$f(x)$, $\phi_Z(x)$	Density function are named using letters commonly used for functions, with an optional subscript indicating the random variable they belong to.
$p(x, y \mid z)$	The usual abuse of notation with the letter "p" standing for any density indicated by the names of the variables given to it is used as well (in this case, $f_{X,Y\mid Z}$ is implied).
$\int p(x)\,\mathrm{d}x = 1$	Integrals over the whole domain of a density are written as indefinite integrals, where the usage is clear.

1 Introduction

1.1 Problem Description

1.2 Related Work

2 Background

This section provides the background for the concepts used later in chapters 3 and 4. Initially, it gives a quick overview of Baysian inference and probabilistic programming in general, necessary to understand the requirements and usual approaches of probabilitic programming systems.

Consequently, the machinery and language used to develop the graph tracking system forming the main part of the work are described. This consists firstly of a short introduction to graph tracking and source-to-source automatic differentiation, which contain many ideas and terminology that will be used later, and often provided inspiration. Secondly, the basic notions and techniques of the Julia compilation process as well as the language's metaprogramming capabilities are described, which form the basis of the implementation.

2.1 Bayesian Inference and Probabilistic Programming

Probabilistic modelling is a technique for modelling phenomena based on the assumption that observables can be fully described through some stochastic process. When we assume this process to belong to a specified family of processes, the estimation of the "best" process is a form of learning: if we have a good description of how obserations are generated, we can make summary statements about the whole population (descriptive statistics) or predictions about new observations. When observations come in pairs of independent and dependent variables, learning the conditional model of one given the other solves a regression or classification problem.

Within a Baysian statistical framework, we assume that the family of processes used is specified by a joint distribution of random variables related through conditional distributions with densities, which describe how the observables would be generated: some *latent variables* are generated from *prior distributions*, and the observed *data* are generated conditionally on the latent variables. The goal is to learn the *posterior distribution* of the parameters given the observations, which is the inverse of how the problem is specified.

As an example, consider image classification: if we assume that certain percentages of an image data set picture cats and dogs, recpectively, the distribution of these labels forms the prior. Given the information which animal is depicted on it, an image can then be generated as a matrix of pixels based on a distribution of images

conditioned on labels. The posterior distribution is then the "inverse" distribution of the label given an image. When we have this information, we can, for example, build a Baysian classifier, by returning for a newly observed image that label which has the higher probability under the posterior.

This kind of learning is called Bayesian inference since, in the form of densities, the form of the model can be expressed using Bayes' theorem:

$$p(\theta \mid x) = \frac{p(x \mid \theta)\, p(\theta)}{p(x)}, \tag{2.1}$$

where x is the vector of observed data, and θ are the parameters.[1] (In practice, not all of the latent variables have to parameters we are actually interested in; these can be integrated out).

Going beyond simple applications like the classifier mentioned above, using the posterior gets difficult, though. Simply evaluating the posterior density $\theta \mapsto p(\theta|x)$ at single points is not enough for usages such as parameter estimation with continuous parameters, or even simple probability evaluation; and even for discrete variables, combinatorial explosion limits the usability of the simple summation approach to calculate probabilities. The reason is that almost all of the relevant quantities depend on some sort of expectation over the posterior density, which is an integral:

$$\mathbb{E}[f(\Theta) \mid X = x] = \int f(\theta) p(\theta \mid x)\, \mathrm{d}\theta, \tag{2.2}$$

with the base measure depending on the type of Θ. When the distributions involved form a sufficiently "nice" combination, e.g., when they form a conjugate pair , the integrals can be calculated analytically since the posterior density has a closed form for a certain known distribution, or at least is a known integral. In general, however, this is not possible, and approximation have to be made, for which different approaches are available: for example, expectation maximization for models with latent variables or message passing and variational methods for general graphical models.

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The applications described in this thesis fall into another framework for approximating posterior information: Monte Carlo methods, which derive from a specified density a procedure that provides a sample of random variables for which a law of large numbers (LLN) holds:

$$\frac{1}{n} \sum_{i=1}^{n} f(\Theta_i) \to \mathbb{E}[f(\Theta) \mid X = x], \quad \text{as} \quad n \to \infty \tag{2.3}$$

in some appropriate stochastic convergence (usually convergence in probability is enough). When $\Theta_i \sim p(\cdot \mid x)$ can be sampled exactly, and the Θ_i are thus i.i.d., the LLN holds trivially; such samplers exist, but might also be difficult to derive or not possess good enough convergence properties. Another large class of samplers is

[1] Note the abuse of notation with $p()$ and the integral; see page xi on notation.

formed by *Markov Chain Monte Carlo* (MCMC) methods, which, instead of sampling exactly from the density, provide a Markov chain whose stationary distribution is the target density. The advantage of MCMC methods is that they mostly treat the density as a black box, without requiring any more formal manipulations on it.

The general scheme of MCMC methods consists of the definition of a transition kernel by means of two helper fuctions: a proposal distribution with density q, and an acceptance rate α, both depending on the old value in the chain:

1. Start from an arbitrary $\Theta_1 = \theta_1$.
2. For each $i \geq 1$:
    1. Propose $\hat{\Theta}_i \sim q(\cdot \mid \Theta_{i-1})$.
    2. With probability $\alpha(\hat{\Theta}_i, \Theta_{i-1})$, set $\Theta_i = \hat{\Theta}_i$; else, keep $\Theta_i = \Theta_{i-1}$.

2.1.1 Probabilistic Programming

Probabilistic programming is a means of describing probabilistic models through the syntax of a programming language. Probabilistic programms distinguish themselves from normal programs by the possibility of being sampled from conditionally, with some of the internal variables fixed to observed values. While probabilistic programming systems are often implemented as separate, domain-specific languages, they can also be embedded into "host" programming languages with sufficient syntactic flexibility. The latter is advantageous if one wants to use regular general-purpose programming constructs or interact with other functionalities of the host language.

2.2 Computation Graphs and Automatic Differentiation

2.3 Metaprogramming and Compilation in Julia

3 Implementation of Dynamic Graph Tracking in Julia

3.1 Automatic Graph Tracking and Extended Wengert Lists

4 Graph Tracking in Probabilistic Models

5 Discussion

5.1 Future Work

Colophon

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