How to Train Your Program: a Probabilistic Programming Pattern for Bayesian Learning From Data

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1 Introduction

The ultimate Bayesian approach to learning from data is embodied by hierarchical models (Gelman et al., 2013; Goodman et al., 2016; McElreath, 2020). In a hierarchical generative model, the distribution of each observation $y_{ij}$ from the $i$th group of observations depends on group parameter $\theta_i$, and the distribution of each $\theta_i$ depends on hyperparameter $\tau$:

$$
\tau \sim H \\
\theta_i|\tau \sim D(\tau) \\
y_{ij}|\theta_i \sim F(\theta_i)
$$

(1)

A hierarchical model can be thought of as a way of inferring, or ‘learning’, the prior of $\theta_i$ from all observations in the data set. Consider the following example problem: multiple boxes are randomly filled by $K$ marbles from a bag containing a mixture of blue and white marbles. We are presented with a few draws with replacement from each of the boxes, $y_{ij}$ being the $j$th draw from the $i$th box; our goal is to infer the number of blue marbles $\theta_i$ in each box. Intuitively, since the boxes are filled from the same bag, the posterior distribution of $\theta_i$ should account both for draws from the $i$th box and, indirectly, for draws from all other boxes. This is formalized by the following hierarchical model:

$$
\tau \sim \text{Beta}(1, 1) \\
\theta_i|\tau \sim \text{Beta}(K \tau, K (1 - \tau)) \\
y_{ij}|\theta_i \sim \text{Bernoulli}(\theta_i)
$$

(2)

Model (2) learns from the data in the sense that inference for each box is influenced by draws from all boxes. However, learning from training data to improve inference on future data with a hierarchical model is computationally inefficient — if a new box is presented, one has to add observations of the new box to the previously available data and re-run inference on the extended data set. Inference performance can be improved by employing data subsampling (Korattikara et al., 2014; Bardenet et al., 2014, 2017; Maclaurin and Adams, 2014; Quiroz et al., 2018), but the whole training data set still needs to be kept and made accessible to the inference algorithm. A hierarchical model cannot ‘compress’, or summarize, training data for efficient inference on future observations.

An alternative approach, known as empirical Bayes (Robbins, 1951; Casella, 1985; Robbins, 1992), consists in adjusting the hyperprior based on the training data; e.g. by fixing $\tau$ at a likely value, or by replacing $H$ in (1) with a suitable approximation of the posterior distribution of $\tau$. However, empirical Bayes is not Bayesian. While practical efficiency of empirical Bayes was demonstrated in a number of settings (Robbins, 1992), in other settings empirical Bayes may result in a critically misspecified model and overconfident or biased inference outcomes.

In this work, we propose an approach to learning from data in probabilistic programs which is both Bayesian in nature and computationally efficient. First, we state the problem of learning from data in the context of Bayesian generative models (Section 2). Then, we introduce the approach and discuss its implementation (Section 3). For evaluation, we apply the approach to inference in synthetic and real-world problems (Section 5). Finally, we conclude with a overview of related work and discussion (Sections 6 and 7).

2 Problem: Learning from Data

The challenge we tackle here is re-using inference outcomes on the training data set for inference on new data. Formally, population $\mathcal{Y}$ is a set of sets $y_i \in \mathcal{Y}$ of observations $y_{ij} \in y_i$. Members of each $y_i$ are assumed to be drawn from a known distribution $F$ with unobserved parameter $\theta_i$, $y_{ij} \sim F(\theta_i)$. $\theta_i$ are assumed to be drawn from a common distribution $H$. Our goal is to devise a scheme that, given a subset $Y \subset \mathcal{Y}$, the training set, infers the posterior distribution of $\theta_k|Y, y_k$ for any $y_k \in \mathcal{Y}$ in a shorter amortized time than running in-
In quest of devising such a scheme, we make two observations which eventually help us arrive at a satisfactory solution:

1. In Bayesian modelling, information about data is usually conveyed through conditioning of the model on various aspects of the data.

2. In a hierarchical model, influence of the $i$th group of observations on the hyperparameters $\tau$ and, consequently, on other groups, passes exclusively through the group parameters $\theta_i$.

If, instead of conditioning on training data $y_i$, we could condition on parameters $\theta_i$ corresponding to the training data, then we could perform inference on new data item $y_k$ at a lower time and space complexity. Continuing the well known analogy between a hierarchical model and a tree, with the hyperparameter $\tau$ at the root and observations $y_{ij}$ in the leaves, we can liken a model which receives all $\theta_i$ of the training data and new data item $y_k$ to a stump — the hierarchical model with the trunk cut off just after the hyperparameters — and a fungus growing on the stump — the new data item. The problem is, of course, that we infer distributions, rather than fixed values, of $\theta_i$, and the model must be, somewhat unconventionally, conditioned on the distributions of $\theta_i$.

However, a recently introduced notion of stochastic conditioning (Tolpin et al., 2021) makes conditioning on distributions of $\theta_i$ possible, both theoretically and in the practical case when the posteriors of $\theta_i$ are approximated using Monte Carlo samples. Stochastic conditioning (Tolpin et al., 2021) extends deterministic conditioning $p(x|y = y_0)$, i.e. conditioning on some random variable $y$ taking on a particular value $y_0$, to conditioning $p(x|y \sim D_0)$ on $y$ having the marginal distribution $D_0$. A probabilistic model with stochastic conditioning is a tuple $(p(x, y), D)$ where $p(x, y)$ is the joint probability density of random variable $x$ and observation $y$ and $D$ is the distribution of observation $y$, with density $q(y)$. To infer $p(x|y \sim D)$, one must be able to compute $p(x, y \sim D) = p(x)p(y \sim D|x)$. $p(y \sim D|x)$ has the following unnormalized density:

$$p(y \sim D|x) = \exp \left( \int_Y (\log p(y|x)) \, q(y)dy \right) \quad (3)$$

Conditioning the model both stochastically on the posterior distributions of $\theta_i$ on training data and deterministically on new data $y_k$ would yield the same posterior distribution of $\theta_i$ as inference on the full hierarchical model. However, that would also mean that the inference algorithm can sample from the posterior distribution of $\theta_i$ to infer $y_k$. To achieve the objective of ‘compression’ of the training set for faster inference on new data, the parameter posterior can be approximated by a weighted finite set of samples. This is related to Bayesian coresets (Huggins et al., 2016; Zhang et al., 2021), although with essential differences, discussed in Section 6. Based on this, we propose the ‘stump-and-fungus’ pattern for learning from data in probabilistic programs:

1. Training is accomplished through inference on a hierarchical model, in the usual way.

2. The parameter posterior is approximated by a set of $M$ weighted samples $(\tilde{\theta}, w)$.

   - $\tilde{\theta}$ are drawn from the mixture of parameter posteriors of all groups. The set size $M$ is chosen as a compromise between approximation accuracy and inference performance.
   - The weights are selected to minimize approximation error of the hyperparameter posterior, as detailed in Section 4.

3. For inference on new data $y$, a stump-and-fungus model is employed:

   $$\tau \sim H$$

   $$(\tilde{\theta}, w)|\tau \sim D(\tau) \quad \text{— stochastic conditioning}$$

   $$y|\theta \sim F(\theta) \quad (4)$$

The unnormalized conditional log probability of $(\tilde{\theta}, w)$ given $\tau$ is computed as (5), following Tolpin et al. (2021):

$$\log p((\tilde{\theta}, w)|\tau) = \sum_{j=1}^{M} w_j \log p(\tilde{\theta}_j|\tau) \quad (5)$$

A gain in time and space complexity follows from replacing the dataset $Y$ with a weighted sample set $(\tilde{\theta}, w)$ of size $M$. Many inference algorithms scale at least linearly with the size of the data, hence the corresponding complexity term decreases from $O(|Y|)$ to $O(M)$. In addition, the likelihood of a weighted sample skips the lowest level of the hierarchy and is thus cheaper to compute than of an observation, though the exact gain depends on the particular model.

Although two models — hierarchical and stump-and-fungus — are involved in the pattern, the models are in fact two roles fulfilled by the same generative model, combining stochastic conditioning on training data and deterministic conditioning on new data (consisting potentially of multiple data items). This preserves a common practice in machine learning in which the same model is used for both training and inference.
4 Weighted Sample Set Approximation of Parameter Posterior

In Section 3, we suggested to stochastically condition the model on the posterior distributions of \( \theta_i \) of the training data. We further suggested that, to ‘compress’ the training set, the distribution be approximated by a finite weighted sample set \((\theta, w)\) of size \( M \). Let us assume that the sample set \((\theta)\) is drawn and fixed, and show how the weights \( w \) are computed.

Our objective is to approximate the posterior of the hyperparameter \( \tau \) given the training set \( Y \), by conditioning \( \tau \) on \((\theta, w)\). We can achieve this by selecting weights \( w \) such that the KL divergence between \( p(\tau|Y) \) and \( p(\tau|\theta, w) \) is minimized. Since \( p(\tau|Y) \) does not depend on \( w \), minimizing \( KL[p(\tau|Y)||p(\tau|\theta, w)] \) is equivalent to the following maximization problem:

\[
\mathbf{w} = \arg \max_{\mathbf{w}} S(\mathbf{w})
\]

\[
S(\mathbf{w}) = \int_{\tau \in T} p(\tau|Y) \log p(\tau|\theta, w))d\tau
\]

where, from (5)

\[
p(\tau|\theta, w) = \frac{p(\tau) \exp \left( \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau) \right)}{\int_{\tau' \in T} p(\tau') \exp \left( \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau') \right)d\tau'}
\]

In the context of Bayesian inference in hierarchical generative models, the posterior is commonly approximated by a set of Monte Carlo samples. Assuming that \( \tau|Y \) is approximated by a (large) set of \( N \) samples \( \tau_1...\tau_N \), \( S(\mathbf{w}) \) can be estimated as

\[
\hat{S}(\mathbf{w}) = \sum_{i=1}^{N} \log \frac{p(\tau_i) \exp \left( \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_i) \right)}{\sum_{k=1}^{M} p(\tau_k) \exp \left( \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_k) \right)}
\]

\[
= \sum_{i=1}^{N} \left( \log p(\tau_i) + \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_i) \right)
\]

\[
- N \log \sum_{i=1}^{N} \exp \left( \log p(\tau_i) + \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_i) \right)
\]

When it is feasible to impose a uniform improper prior \( p(\tau) = C \) on the hyperparameter, such as in the case of a sufficiently large number of groups in the hierarchy, (7) simplifies to (8):

\[
\hat{S}(\mathbf{w}) = \sum_{i=1}^{N} \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_i)
\]

\[
- N \log \sum_{i=1}^{N} \exp \left( \sum_{j=1}^{M} w_j \log p(\hat{\theta}_j|\tau_i) \right)
\]

\[
\nabla_w \hat{S}(\mathbf{w}) \text{ is readily obtainable, either analytically or algorithmically, and (6) can be solved using gradient ascent. Although } S(\mathbf{w}) \text{ is not concave in general, there is an obvious initial guess } \mathbf{w} = \mathbf{1} \text{ in proximity of the global maximum; the larger } M, \text{ the closer is the guess to the maximum.}
\]

Let us illustrate the computation on a toy example. We use model (9)

\[
p(\mu, \log \sigma) \propto 1
\]

\[
y_j | \mu, \sigma \sim \text{Normal}(\mu, \sigma)
\]

to infer the parameters of a single-dimensional normal distribution given observations \( y = \{-1.33, -0.61, -0.20, 0.34, 0.71, 1.23, 1.45, 1.47, 1.83, 2.05\} \). The posterior is shown in blue in Figure 1b. Then, we draw 10 samples from the predictive posterior, and condition (9) on the samples. The new posterior is likely to be different, with the standard deviation of the mean \( \approx 0.33 \). For \( y = \{-2.77, -1.80, -0.71, -0.62, 0.31, 0.38, 0.43, 0.70, 1.66, 2.6\} \), the posterior is shown in green in Figure 1b. We then compute, according to (6) and (8), the weights (Figure 1a), and condition model (9) on the weighted sample, resulting in the posterior (orange in Figure 1b) almost coinciding with the original posterior. In a hierarchical model, hyperparameters \( \tau \) would correspond to \( \mu \) and \( \sigma \), and group parameters \( \theta \) to \( y \).

5 Case Studies

We evaluate the stump-and-fungus pattern on three case studies. We begin with a basic synthetic case study “Boxes With Marbles” (Section 5.1), which, while does not pose computational challenges, allows us to show most aspects of application of the pattern to a hierarchical model. We then continue to a didactic study “Tumor Incidence in Rats” (Section 5.2) which involves a large number of groups in the hierarchy. Finally, we apply the pattern to “Educational Attainment in Secondary Schools” (Section 5.3), an elaborated cross-classified model based on data used in a real-world sociological research. We implemented in the studies in Inference (Tolpin, 2019) and fit models using HMC (Neal, 2011) or NUTS (Hoffman and Gelman, 2011). We used gradient ascent with momentum for computation of sample weights.
The data and source code for the case studies are provided in the supplementary material.

### 5.1 Boxes With Marbles

This case study is inspired by an introductory example in McElreath (2020). Boxes are filled with marbles from a bag with a mix of blue and white marbles. There are 6 boxes, with 4 marbles in each box. Marbles are drawn from the boxes, with replacement, and observed. The number of blue marbles in each box are to be inferred. The problem is formalized by model (10):

\[
\begin{align*}
p_0 & \sim \text{Uniform}(0, 1) \\
p_i | p_0 & \sim \text{Beta}(4p_0, 4(1 - p_0)) \\
y_{ij} | p_{b_j} & \sim \text{Bernoulli}(p_{b_j})
\end{align*}
\]

where \( p_0 \) is the proportion of blue marbles in the bag, \( p_i \) — in the \( i \)th box, \( y_{ij} \) is 1 if the \( j \)th drawn marble was blue, 0 otherwise, and \( b_j \) is the box from which the \( j \)th marble was drawn.

We fit
- the hierarchical model;
- the empirical Bayes model in which \( p_0 \) is fixed to the posterior mean of \( p_0 \) in the hierarchical model;
- 6 stump-and-fungus models, with each box as the fungus, in turn, using 10 samples from the parameter posterior for the stump.

Figure 2 compares the posteriors. Figure 2a shows the posterior distributions of \( p_i \) from the hierarchical model (white) and each of the stump-fungus models (light blue), overlaid. Similarly, Figure 2b compares the posteriors of the hierarchical and the empirical Bayes models. One can observe that stump-and-fungus results in a better approximation of the posterior than empirical Bayes. Figure 2c visualizes discrepancy between the posteriors with the distribution of Kolmogorov-Smirnov statistics of \( p_{\text{stump}} \) over boxes, confirming the advantage of stump-and-fungus.

### 5.2 Tumor Incidence in Rats

In this case study, based on Tarone (1982) and discussed in Gelman et al. (2013, Chapter 5), data on tumor incidence in rats in \( N = 70 \) laboratory experiments is used to infer tumor incidence based on outcomes of yet another experiment. A different number of rats \( n_i \) was involved in each experiment, and the number of tumor cases \( y_i \) was reported. An application of the stump-and-fungus pattern in this case would be to replace the original data set of size \( N \times 2 \) with a ‘stump’ of a smaller size \( M \times 2 \) for assessment of outcomes of future experiments. The problem is formalized by model (11):

\[
\begin{align*}
\alpha, \beta & \sim \text{Prior} \\
p_i | \alpha, \beta & \sim \text{Beta}(\alpha, \beta) \\
y_i | p_i & \sim \text{Binomial}(n_i, p_i)
\end{align*}
\]

where the non-informative prior distribution is set such that \( p(\alpha, \beta) \propto (\alpha + \beta)^{-5/2} \) (Gelman et al., 2013, Section 5.3). In addition, each group can be fit an ‘unpooled’ Beta-Binomial model (12):

\[
\begin{align*}
p_i & \sim \text{Beta}(1, 1) \\
y_i | p_i & \sim \text{Binomial}(n_i, p_i)
\end{align*}
\]

We fit
- a separate ‘unpooled’ model for each experiment;
- the hierarchical model;
- 71 stump-and-fungus models, with each experiment as the fungus, in turn, using 10 samples from the parameter posterior for the stump.

Since Gelman et al. (2013, Section 5.3) give a detailed account of empirical Bayes vs. hierarchical model, we omit this comparison here.

Inference on model (11) can be performed efficiently thanks to summarization of \( n \) observations from \( \text{Bernoulli}(p) \) as a single observation from \( \text{Binomial}(n, p) \). In general however, the use of a hierarchical model would require carrying all observations of all previous experiments for learned inference on findings of a new experiment.

Figure 3 shows the posterior distributions for \( p \) inferred on 71 unpooled models (Figure 3a), on the hierarchical model (Figure 3b) and through 71 applications of stump-and-fungus (Figure 3c). One can observe that the posteriors obtained on both hierarchical and stump-and-fungus models appear to be the same, except for small discrepancies apparently caused by finite sample size approximation. Compared to the unpooled posteriors, significant shrinkage takes place. Table 1 shows the inference times for each of the models. Inference on a single group with the stump-and-fungus model takes less than 10% of time on the hierarchical model.
Hierarchical model

Separate

Weights

2.1

Empirical

Bayes

Hierarchical

Stump & Fungus

Hierarchical

Stump & Fungus

Weights

20

93

860

224

Empirical

Bayes

Hierarchical

20

7.2

236

Stump & Fungus

Hierarchical

Stump & Fungus

490

10

15

Weights

(b) Hierarchical model

(c) Stump-and-fungus models

Figure 3: Tumor incidence in rats. The posteriors are the same in hierarchical and stump-and-fungus model, except for small discrepancies apparently caused by finite sample size approximation. Colorful lines are posterior distributions of \( p \) for each of 71 experiments. Black lines are posterior distributions of \( p \) for a future experiment.

Table 1: Tumor incidence in rats: inference times for 1000 burn-in and 5000 posterior samples, 10 stump samples.

| Model          | Hierarchical | Separate | Stump & Fungus | Weights |
|----------------|--------------|----------|----------------|---------|
| Time, sec      | 93           | 2.1      | 7.2            | 15±1.1  |

5.3 Educational Attainment in Secondary Schools

This study is based on Paterson (1991) and explores educational attainment of children in Scotland. There are two real-valued predictors: social class scale \( CC \) and verbal reasoning score \( VRQ \) on entry to the secondary school, three hierarchies: by secondary school (\( SID \)), by gender (\( SEX \)), and by primary school (\( PID \)), and a real valued target — attainment score \( ATTAIN \) at the age of 16. There are 3,435 children, 148 primary schools, and 19 secondary schools in the data set. An application of stump-and-fungus problem would be to provide a new secondary school with a small ‘stump’, instead of the full data set, for attainment assessment. The problem can be formalized as model (13), a cross-classified hierarchical linear regression model:

\[
\begin{align*}
\mu_{\beta_h}, \log \sigma_{\beta_h}, \mu_\sigma, & \log \sigma_\sigma \sim \text{Uniform}(-\infty, \infty) \\
\beta | \mu_{\beta_h}, \sigma_{\beta_h} & \sim \text{Normal}(\mu_{\beta_h}, \sigma_{\beta_h}) \\
\log \sigma | \mu_\sigma, \sigma_\sigma & \sim \text{Normal}(\mu_\sigma, \sigma_\sigma) \\
\end{align*}
\]

\[
p(y_i | \beta, \sigma) = \prod_h \text{Normal}(y_i | \beta_{gh_h}, \sigma_{gh_h}, x_i)
\]

Here, \( h \) is the hierarchy index, \( x_i \) and \( y_i \) are the predictors and the target of the \( ih \) pupil, \( gh_h \) is the group index of the \( ih \) pupil in the \( h \)th hierarchy. \( \mu_{\beta_h}, \log \sigma_{\beta_h}, \mu_\sigma, \log \sigma_\sigma \) are the hyperparameters of the model, and \( \beta, \sigma \) are the group parameters; in total, the model has 700 real-valued parameters, of which 18 are hyperparameters.

We fit

- the empirical Bayes model in which the hyperparameters are fixed to their posterior means in the hierarchical model;
- 19 stump-and-fungus models, with each secondary school as the fungus, in turn, using 10 and 20 samples from the parameter posterior for the stump. Since parameters in each hierarchy are mutually independent given hyperparameters, a separate weight is assigned to each component of a sample, rather than to the sample as a whole.

Figure 4 compares the posteriors. Figures 4a and 4b show the posterior distributions of \( p_i \) from the hierarchical model (white) and each of the stump-fungus models (light blue) for 10 and 20 samples, correspondingly. Similarly, Figure 4c compares the posteriors of the hierarchical and the empirical Bayes models. One can observe that stump-and-fungus results in a better approximation of the posterior than empirical Bayes. Figure 4d visualizes discrepancy between the posteriors with the distribution of Kolmogorov-Smirnov statistics of the group parameters over the secondary schools, confirming the advantage of stump-and-fungus. Table 2 shows the inference times for each of the models. Inference on a single group with the stump-and-fungus model takes less than 25% of time on the hierarchical model.

Table 2: Educational attainment: inference times for 1000 burn-in and 5000 posterior samples, 10 and 20 stump samples.

| Model          | Hierarchical | Empirical | Stump & Fungus | Weights |
|----------------|--------------|-----------|----------------|---------|
| Time, sec      | 908          | 860       | 180±12         | ±224±15 |

6 Related Work

The importance of learning from data is well appreciated in probabilistic programming. Along with empirical Bayes, applicable to probabilistic programming as well as to Bayesian generative models in general, probabilistic-programming specific approaches were proposed. One possibility is to induce a probabilistic program suited for a particular data set (Liang et al., 2010; Perov and Wood, 2014; Perov, 2018; Hwang et al., 2011). A related but different research direction is inference compilation (Le et al., 2017; Baydin et al., 2019), where the cost of inference is amortized through learning proposal distributions from data. Another line of research is concerned by speeding up inference algorithms by tuning them based on training data (Eslami et al., 2014; Mansinghka et al., 2018). Our approach to learning from data in probabilistic programs is different in that it does not require any particular implementation of probabilistic programming to be used, nor introspection into the structure of probabilistic programs or infer-
ence algorithms. Instead, the approach uses inference in ubiquitously adopted hierarchical models for training, and conditioning on observations for incorporation of training outcomes in inference.

Approximation of a large sample set by a small weighted subset bears similarity to Bayesian coresets (Huggins et al., 2016; Campbell and Beronov, 2019; Manousakas et al., 2020; Zhang et al., 2021) — a family of approaches aiming at speeding up inference with large datasets. A Bayesian coreset is a small weighted subset of the original large dataset, with the promise that inference on the coreset yields the same or approximately the same posterior. However, there are significant differences between Bayesian coresets and the setting in this work. First, in Bayesian coresets, the posterior is unknown when the coreset is constructed. In the stump-and-fungus pattern, the posterior distribution of the hyperparameter is known (as a Monte Carlo approximation) before the samples are selected and the weights are computed. In particular, Campbell and Beronov (2019) minimize the KL divergence between the approximate and the exact posterior, while in this work minimizes the complementary KL divergence between the exact posterior and its stump-and-fungus approximation. This facilitates a simpler formulation of divergence minimization. Second, careful selection of samples to be included in the coreset is necessitated by high dimensionality of data in the dataset (Manousakas et al., 2020). However, even in elaborated hierarchical Bayesian models the group parameters are low-dimensional, and interdependencies between multiple hierarchies in cross-classified models are assumed to be negligible. Because of that, a random draw from the parameter posterior suffices for stump-and-fungus even if it might not work in a higher-dimensional setting.

7 Discussion

We presented a probabilistic programming pattern for Bayesian learning from data. The stump-and-fungus pattern is easy to understand and simple to implement. When applied to hierarchical generative models, the pattern allows to realize learning from data within the Bayesian paradigm, and results in significant improvement in inference performance on new groups. Even if certain aspects of the pattern can be improved, the pattern is applicable in its current form to real-world statistical studies.

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