MODELWIZARD: TOWARD INTERACTIVE MODEL CONSTRUCTION

by

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ABSTRACT

Data scientists engage in model construction to discover machine learning models that well explain a dataset, in terms of predictiveness, understandability and generalization across domains. Questions such as “what if we model common cause Z” and “what if Y’s dependence on X reverses” inspire many candidate models to consider and compare, yet current tools emphasize constructing a final model all at once.

To more naturally reflect exploration when debating numerous models, we propose an interactive model construction framework grounded in composable operations. Primitive operations capture core steps refining data and model that, when verified, form an inductive basis to prove model validity. Derived, composite operations enable advanced model families, both generic and specialized, abstracted away from low-level details.

We prototype our envisioned framework in MODELWIZARD, a domain-specific language embedded in F# to construct Tabular models. We enumerate language design and demonstrate its use through several applications, emphasizing how language may facilitate creation of complex models. To future engineers designing data science languages and tools, we offer MODELWIZARD’s design as a new model construction paradigm, speeding discovery of our universe’s structure.

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To Andy Gordon, from our internship enterprise and beyond,

    May we open our office whiteboards, nay, the whiteboards of our minds,
    so timidly advertised yet so richly energized and ripe to publicize.
    Our whims combined will change the world one puzzle piece at a time.
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Chapter 1
Introduction

In his 2013 visionary article, Dr. Chris Mattmann issued a call for data scientists: “To get the most out of big data, funding agencies should develop shared tools for optimizing discovery and train a new breed of researchers” [Mat13]. This thesis is an answer to Dr. Mattmann’s call, laying groundwork for new tools to help data scientists gain insight faster.

1.1 Data Science as Model Construction

We address three scientific goals:

- **Prediction** of unseen states.\(^1\)
  
  E.g., an apple dropped from a tall building will fall about 122 meters in 5 seconds.

- **Understanding** of the structure that naturally generates states.
  
  E.g., the force of gravity decreases apple elevation quadratically with time. Equivalently, gravity linearly decreases a hidden variable, apple velocity, which in turn linearly decreases apple elevation with time.

- **Generalization** of common structure to other problems and domains.
  
  E.g., quadratic regression generalizes to polynomial regression, a relationship we may apply to light dispersion, roller coasters and plenty other datasets.

---

\(^1\) *State* is a domain-specific term whose definition is clear in the context of a problem. A chemical engineer working on oil refinery design may use *state* to refer to the chemical composition of fluid in a reactor; a statistical physicist to refer to a specific configuration of a thermodynamic system; a computer architect to refer to the contents of each register on a CPU; a stockbroker to refer to the price of equities at a given time. More examples abound.
In the context of data science, we address these goals by analyzing datasets: predicting unseen data values, understanding the structure that generates data, and generalizing that structure to other datasets. We apply these principles to the apple freefall example by imagining a dataset of apple elevations over time in the form of Table 1.1. Each row consisting of a (time, elevation) pair is a data point. We aim to predict unseen rows with missing time or elevation, to understand the structure that generates these pairs, and to generalize that structure to other contexts.

By structure we refer to some mechanism that generates data points. Assuming the standpoint of epistemic uncertainty, there exists a true mechanism that generates data points in reality that we do not fully know. We call the unknown true mechanism true structure, and we call a guess at the true structure a candidate structure, shortened to structure for brevity. We also refer to structure as a model.

We use the language of probability to describe uncertain knowledge of true structure. True structure includes everything up to recording a data point. Including how we collect data points in models can therefore be helpful, in addition to how “nature” generates data points. In the Apple Freefall data for example, if we know our method of recording elevation is particularly inaccurate or imprecise, we ought to reflect

| Time (s) | Elevation (m) |
|----------|---------------|
| 0        | 200           |
| 1        | 196           |
| 2        | 179           |
| 3        | 155.1         |
| 6.5      | 0             |

Table 1.1: Apple in Freefall dataset

\(^2\text{In contrast to aleatory uncertainty, which holds that no true structure may ever be known due to intrinsic randomness. Distinguishing the two types of uncertainty may be useful for determining what uncertainty is reducible by further data collection [KD09], but for our purposes we consider true structure completely discoverable in the limit of infinite data.}\)
that knowledge in our model.\textsuperscript{3} We may also introduce noise to account for model imprecision: that a model may partly account for the true structure mechanism. The magnitude of noise reflects how well that model accounts.

Models represent a (joint) probability distribution over data points. Impossible data points that a model cannot generate have zero probability mass. Possible data points receive probability mass proportional to likelihood that the model will generate them. We create candidate models using the subset of possible data points present in a dataset’s non-missing values.

We are specifically interested in structure taking the form of machine learning models. These are models with a computable sampling procedure to output a data point. Sampling algorithms such as rejection sampling compute samples that satisfy conditions. Inference algorithms solve the reverse problem: computing the probability that the model will generate a data point.

Some models are able to sample and infer data point probabilities for every column in their dataset. We call those models generative, since they specify a distribution that can be used to generate samples over any column. We may also consider discriminative models that do not define distributions over every column.\textsuperscript{4} We cannot sample or infer data point probabilities of “unmodeled” columns in a discriminative model, instead using them as known inputs to sample or infer other columns. Data scientists may find discriminative models relieving because they do not have to specify distributions behind unmodeled columns, saving work required to justify why a certain distribution makes sense for a column.

Define model construction as the process of creating machine learning models for a dataset. A well-built model solves all three goals: predicting unseen states

\textsuperscript{3}See how the Apple Freefall model noise term reflects data imprecision in Figure 1.1a and 1.1b.
\textsuperscript{4}See [BBB\textsuperscript{+}07] for an overview of generative and discriminative models.
by (conditional) sampling, understanding structure by examining model components, and generalizing structure by applying components to machine learning models for other datasets. Prediction is a key link, because high predictive power on unseen data indicates that a machine learning model is close to the true structure generating data. Simplicity is another guide that increases understanding and generalizability; see [Fre14] for further reading on scoring machine learning models for comprehensibility.

In constructing our final model we may consider alternative models, comparing them as we imagine them and choosing models that are simpler and fit our dataset better. We call this process *model exploration*.

The goal of the ModelWizard project is to develop a tool that supports the model exploration workflow. We aim to facilitate creativity, increase interactivity, introduce safety and support abstraction when writing a ModelWizard script that ultimately constructs a Tabular machine learning model.

1.2 Prelude Example: Freefall in ModelWizard

We now introduce ModelWizard’s exploration workflow through a small example, focusing on how a user guides exploration through questions and fitness metrics. Subsections address issues to consider before basing judgements on ModelWizard’s output, and then on the underlying Bayesian mathematics.

Assume the perspective of a data scientist, unaware of gravity, presented with the apple-in-freefall data of Table 1.1, collected on a windy day or by an imprecise instrument to add non-determinism. We may ask several questions: where is the apple at 4 or 5 seconds? What happens past 6 seconds when we observe the apple at elevation zero? At what time does the apple reach an elevation of 50m? We incorporate our questions into the dataset in Table 1.2.
Time (s) | Elevation (m)  
---|---
0   | 200  
1   | 196  
2   | 179  
3   | 155.1
4   |      
5   |      
6.5 | 0    
7   | 50   

Table 1.2: Apple in Freefall dataset, with “missing value” rows

An initial model we may posit for this dataset is a linear relationship between time and apple elevation. To create this model, we use the ModelWizard operations

\[
\text{LinReg} \ "Elevation" \ "Time" \quad (1.1)
\]

\[
\text{Model} \ "tmain" \ "Time" \quad (1.2)
\]

Operation 1.1 places a noisy linear regression model on elevation with explanatory variable time. Operation 1.2 places an uninformative Gaussian distribution on time.

Figure 1.1a shows the resulting linear model. The rows in the bottom table labelled ‘tmain’ list the name, type and model of corresponding columns in the original dataset of Table 1.2. The giant \texttt{LinReg} function block implements linear regression in Tabular syntax such that the Elevation column model may call linear regression as a macro. Detail-oriented readers may skip to Chapter 2 for deeper Tabular syntax and semantics, but for now we recommend accepting linear regression as is, focusing instead on ModelWizard’s workflow. The linear function block’s one addition to usual regression is the noise term, a probabilistic analogue to what statisticians call regression error. Larger inferred noise precision (equivalently, smaller inferred noise variance) tends to indicate less error and greater model fit, though we should take
caution to avoid too high precision which is prone to overfit.

Operation 1.2 converts the model from discriminative to generative. Because the last row of our dataset in Table 1.2 contains a missing value for time, we must use a generative model in order to have a way to predict time. A generative model also allows us to answer questions such as “what is the apple elevation” without specifying time, equivalent to using the posterior distribution (see Section 1.2.2) on time to determine a distribution over elevation. Alternatively, if we omit the last row of Table 1.2 and only care about predicting elevation given time, then we could omit Operation 1.2, leaving time as an input and disallowing missing time values in our dataset. The advantage of the alternative discriminative model is not needing to specify and justify a distribution on time, which we questionably list as a Gaussian distribution. In summary, ModelWizard may construct both generative and discriminative versions of the linear model, and both have advantages in different situations.

Figure 1.1c shows results of inference\(^5\) on the linear model. Inference consists of training a given model on observed (non-missing) values in the input dataset to form a posterior model, outputting posterior model parameters in the left of Figure 1.1c, and outputting marginal distributions from the posterior model on missing values, each conditioned on the observed values in the same row, in the right of Figure 1.1c. Grey-background “PointMass” distributions correspond to observed values in the original dataset of Table 1.2, whereas green-background cells are more meaningful posterior distributions for missing values in the dataset.

It seems suspicious that the linear model predicts positive elevation at 7 seconds, one second after the apple is known to reach 0m elevation. To better evaluate the linear model’s performance using a method less prone to overfitting, we use leave-one-out cross-validation on the known rows of Table 1.1 with the operation\(^5\)We use the Expectation Propagation inference algorithm throughout the Apple Freefall example.
Figure 1.1: Apple Freefall Linear and Quadratic Regression
Green cells are posterior distributions on Table 1.2’s missing values.
CrossValidate_kFold_RMSE "tmain" "Elevation" 5 and similarly for Time. Resulting root mean square errors (not shown in Figure 1.1c) are 14.996m for elevation and 1.046s for time. Viewing these numbers alone, we do not know whether the linear model is optimal or whether other models could deliver lower error.

Could a more complicated model like quadratic regression between time and apple elevation add enough predictive power to merit its increase in model complexity? An answer to this question in either direction—whether quadratic regression is a viable or ill-suited model—is an important clue to understanding the dataset’s structure. Ruling out a model family like the family of quadratic models can be just as informative to a data scientist as showing a model’s plausibility.

We build the quadratic regression model shown in Figure 1.1b by replacing Operation 1.1 with

```
QuadReg "Elevation" "Time"
```

Figure 1.1d tables inference results.

It is heartening to see that the quadratic model predicts negative elevation at 7 seconds and that it has higher noise precision. Running the same cross-validation operation returns root mean square errors of 13.546m for elevation and 0.759s for time, both lower than the linear model. Comparing cross-validation numbers, we see evidence that a quadratic relationship more likely governs the structure behind our dataset than a linear relationship.

Of course, bringing in knowledge of gravity, the quadratic model parameters make more sense than those of the linear model; the inferred parameter $a = -8.625$ is reasonably close to Earth’s $-9.8m/s^2$ true force of gravity. The error is a result of the noisy data set, as the skeptical reader may verify by calculating elevation $= 200 - \frac{9.8 \cdot t^2}{2}$ for observed times $t$ in Table 1.1 and comparing them to the means of the quadratic
model’s posterior distributions.

Model evidence, the probability of observing the dataset under a model, does not function as well as cross-validation for evaluating model fitness, as seen from the quadratic model evidence in Figure 1.1d being lower than the linear model evidence in Figure 1.1c. We demonstrate inference using model evidence in Section 3.1 and then switch to (5-fold, i.e. leave-n/5-out) cross-validation for other applications.

1.2.1 Model Selection Matters: Overfitting and Consistency

Overfit models perform well on training datasets but do not perform well on other datasets generated from the same true structure. Formally, we say a model overfits if it performs better on a training set of data but worse on the distribution of all possible data sets than an alternative model [Mit97]. The Apple Freefall models, for example, would clearly overfit if their noise precisions are excessively high. They would predict tight distributions accurately on their training set that do not predict well on non-training set data.\(^6\)

Model comparison methods can be another source of overfitting. We strive to compare models in a way that does not favor specialized, overfit models. Luckily for the Apple Freefall example, model comparison by leave-one-out cross-validation is equivalent to model comparison by the Akaike information criterion (AIC) [Sto77], which has a desirable model complexity penalty [Boz87] that penalizes models with larger degrees of freedom. The complexity penalty enables realistic comparison between the simpler linear model and the more adaptive and thereby more likely to overfit quadratic model.

We also strive to compare models consistently, that is, to compare models

\(^{6}\)We ignore the case of modeling a perfectly deterministic true structure, in which case a (zero variance) Dirac delta distribution may perfectly capture a deterministic relationship between columns.
with a guarantee that the probability of choosing the “correct” model closer to the
true structure converges to 1 as the number of data points approaches infinity. Un-
fortunately AIC is an inconsistent model comparison method [Sha93], which means
that AIC may not choose the best model even after training on infinite data ob-
servations. We employ leave-one-out cross-validation anyway for convenience in the
Apple Freefall example. Consistent model comparison methods include leave-$n_v$-out
cross-validation, Bayesian information criterion (BIC) and Bayes factors for mod-
els with a finite number of parameters, and consistent methods exist for comparing
nonparametric models too [JWC+10].

1.2.2 Bayesian Inference

We obtain cross-validation scores used to compare models via inference, characterized
by its use of Bayes’ Rule. Beginning with a prior predictive model\footnote{Vocabulary note: a (prior or posterior) predictive model specifies a distribution over a row of data, whereas a (prior or posterior) model specifies a distribution over model parameters. We refer to the latter as parameter models to disambiguate. See [GvD07] for examples of each.} that specifies $\Pr(row)$ for any row of data, we use Bayes’ Rule to iteratively condition on each
observed row of a dataset and form a posterior predictive distribution:

$$
\Pr(row | obsRow) := \alpha \frac{\Pr(obsRow | row)}{\Pr(row)}
$$

where $obsRow$ is a row of observed (non-missing) data points and $row$ is a row of data
for which we wish to calculate its probability via a model that incorporates the data
evidence in $obsRow$. For example, $obsRow$ may be (time = 1, elevation = 196) and
$row$ may be (time = 2, elevation = 0). We hope our model assigns $\Pr(row | obsRow)$
infinitesimal probability.

$\alpha$ is a normalizing constant that ensures the posterior predictive model is a
valid probability distribution, i.e., that $\int \Pr(\text{row}) \, d\text{row} = 1$, integrating over all possible rows:

$$\alpha = \frac{1}{\Pr(\text{obsRow})} = \frac{1}{\sum_{\text{row}} \Pr(\text{obsRow}, \text{row})} = \frac{1}{\sum_{\text{row}} \Pr(\text{obsRow} \mid \text{row}) \Pr(\text{row})}$$

The reasoning is that if $\Pr(\text{obsRow} \mid \text{row}) > \Pr(\text{obsRow})$, then $\text{row}$ increases $\text{obsRow}$'s likelihood, which indicates we should raise $\Pr(\text{row} \mid \text{obsRow})$ since $\text{obsRow}$ is in fact observed. The ‘$<$’ version similarly decreases $\Pr(\text{row} \mid \text{obsRow})$.

In the context of the apple freefall example, we tune our model from prior to posterior by adjusting the value of regression coefficients—free parameters in the model for which we specify (usually uninformative) prior distributions:

$$\Pr(\text{param} \mid \text{obsRow}) := \alpha \Pr(\text{obsRow} \mid \text{param}) \Pr(\text{param})$$

We use parameters in our model to determine a distribution over possible rows of data by $\Pr(\text{row}) = \Pr(\text{row} \mid \text{param}) \Pr(\text{param})$.

The inference algorithms we use in Tabular and ModelWizard are forms of variational inference,\(^8\) a process that fits an easier-to-analyze probability distribution as close as possible to an arbitrary probability distribution like the one our apple freefall model represents. In exchange for approximation error in using the easier-to-analyze distribution in place of the original distribution, we gain computational speedup in estimating the posterior distribution. Other forms of inference are exact inference,\(^9\) explicitly calculating an exact posterior distribution, and sampling-based inference,\(^10\) sampling from a posterior distribution without explicitly calculating it.

---

\(^8\)e.g., variational message passing, expectation propagation, ...

\(^9\)e.g., variable elimination, junction tree, conjugate distributions, ...

\(^10\)e.g., rejection sampling, likelihood weighting, MCMC and its variants, ...
Cross-validation calls inference as a subroutine by using the resulting probability distribution from inference to make predictions on held out data. Well-performing models recover held out data accurately as indicated by low cross-validation error. Cross-validation performs inference in several rounds, holding out different sets of data randomly at each round. Thus, a model with high cross-validation score generally maintains performance when trained on different subsets of data, which is an excellent guard against overfitting as discussed in Section 1.2.

It is useful to imagine comparing models by cross-validation (or other model scoring measures such as model evidence) as an extension of Bayes’ Rule where we select the best fitting model at the same time as the best fitting parameters for each model:

\[
\Pr(model, param | obsRow) := \alpha \Pr(obsRow | param) \Pr(param | model) \Pr(model)
\]

We select model and its parameters with highest probability. Using the cross-validation method, this is the model (with parameters set by usual inference) that scores the least prediction error. Using the model evidence method, this is the model with greatest likelihood. Methods such as BIC, Bayes’ factors and others discussed in Section 1.2 follow the Bayes’ rule pattern similarly. The extension of the distribution over possible rows of data is \(\Pr(row) = \Pr(row | param) \Pr(param | model) \Pr(model)\), though after selection \(\Pr(model)\) is a point mass distribution on the selected model.

An alternative to model selection is model mixing: taking a sum over possible models weighted by likelihood, instead of selecting one “mode” model with highest likelihood. Model mixing has more robustness to change in data when two models both explain the data well, since a small shift in data could change a selected model abruptly while a small shift in data will smoothly change a mixture of models.
We use the model selection approach because understanding is one of our goals. It is easier to interpret a single model than a mixture of models, especially when we use our model as a proxy for true structure in nature.

There is a potential vocabulary conflict with statisticians, who define inference as “the process of deducing properties of an underlying distribution by analysis of data” [UC08]. Recalling that true structure is a probability distribution over possible data, there is no conflict; true structure is the underlying distribution, whose properties we capture in models we create through model construction. “Structure learning” is also equivalent, as seen from the similar breakdown of a model into “structure” and “form” in [KT08].

In this thesis, “model construction” refers to the entire process of finding a model close to true structure, “inference” refers to Bayesian inference procedures to answer queries and calculate posterior distributions by conditioning on data using Bayes’ rule, and “model exploration” refers to determining model family/form, using the term “learning” whenever a choice is guided by dataset predictive power.

1.2.3 Interactive Model Construction

In Section 1.2 we build our quadratic regression model interactively, creating other models like linear regression and comparing them as we naturally posit them through questions about the apple dataset. In this manner, model construction naturally fits into the scientific method. To illustrate the benefits of interactivity, imagine two other extremes of model construction: manual and automated.

Scientists adopting a *manual* model construction strategy take years to study a scenario well enough to become expert and build a good model. The approach works but at high labor cost, whose fruits tend to be one-off, special purpose models applicable to a single problem.
Scientists adopting an *automated* exploration strategy, using algorithms that output good families, face tractability problems trying to search through the space of all models. For example, [CG01a] has $O(n^5)$ complexity searching within the family of discrete Bayesian networks, a small subspace of all possible models. Further, many automated algorithms such as multilayer neural network training generate “black box” models, which predict accurately but offer no insight into why the models work.

Interactivity delivers a happy medium between the two extremes. Data scientists will work hand-in-hand with computers to navigate the space of models, leveraging scientists’ creative insight to guide model search and computers’ automation to present statistics, model performance results and model suggestions as feedback. Scientist and computer together will craft understandable models on multiple data sources faster than either can alone.

### 1.3 Probabilistic Programming

In probabilistic programming, machine learning models take the form of programs. Users write code that samples data points, effectively defining a probability distribution over possible data points. The model specified as a program gains power from programming language constructs, such as functional abstraction and control flow by iteration and conditionals. Compilers use top level probabilistic program code to synthesize inference code. See [GHNR14], [DRK13] and [Goo13] for different flavors of introduction to probabilistic programming.

One success story demonstrating potential benefits for probabilistic programming is on creating a seismic monitoring model to help detect nuclear tests for the UN Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty (CTBTO). One of the CTBTO’s models has on the order of 28,000 lines of code in C [Fis13].
That model was rewritten in the probabilistic programming language BLOG, delivering similar accuracy at 25 lines of code [Rus14]. Reduction in development time and expertise barriers added considerable value.

1.3.1 Tabular and Infer.NET

Tabular is a probabilistic programming language where models consist of probabilistic annotations on database schemas written inside spreadsheets [GGR+14, GRS+15]. Tabular’s motivation is the idea that data scientists would find it easier and more intuitive to specify their model by marking up the schema of their dataset, as opposed to specifying their model in a standalone language separate from their dataset. Data scientists do need an understanding of Tabular’s primitives, which are designed to be easily readable given background knowledge in statistics and probability.

The Tabular compiler compiles Tabular models into Infer.NET probabilistic programs [MWGK12], which can then be run in an Infer.NET inference engine to infer posterior distributions and answer queries. Infer.NET supports variational message passing, expectation propagation, and Gibbs sampling, all of which are accessible from Tabular.

1.4 ModelWizard: Interactive Model Construction for Tabular

ModelWizard is a domain-specific language, embedded in F#, for interactively constructing Tabular models. Users write scripts in ModelWizard that incrementally construct Tabular models, progressing from an initial “do-nothing” Tabular model toward an inference-ready Tabular model, one operation at a time.

ModelWizard is inspired by the difficulty of writing Tabular models, just as Tabular is inspired by the difficulty of writing Infer.NET models. ModelWizard’s goal
is to reduce the time it takes users to build a Tabular model from scratch. We are especially interested in the case where the user does not know what the final model is and is still exploring the space of models.

In this thesis we present the design and implementation of ModelWizard as an embedded DSL, together with case studies in ModelWizard’s use. The following subsections highlight key features in ModelWizard’s design:

1.4.1 Concurrently Refining Data and Model

ModelWizard’s operations modify both a dataset’s machine learning model under construction and the dataset itself. This is different than the traditional “pre-processing phase” approach in machine learning and data mining literature, to perform all dataset-modifying operations prior to constructing a model.

Operations in ModelWizard that traditionally occur during pre-processing are changing types of columns, creating new tables of unique values, remapping values to point to another table with a foreign key relationship, and capturing functional dependencies by moving data between tables, a key step in table normalization. Other operations we imagine as extensions are numeric transformations like taking square roots, full table normalization, data compression by taking principal components and outlier detection and cleaning, to name a few. We also imagine post-processing extensions such as model validation and visualization.

While refining data and model at the same time adds flexibility to the model construction process, we are not yet certain whether it is always helpful. Data scientists may find performing pre-processing activities prior to modeling conceptually easier. User case studies will help illuminate an answer.
1.4.2 Composable Model Primitives

Rather than construct complicated machine learning models all at once, we construct models incrementally via sequences of primitive operations. Think of primitives as bricks and F# code as glue. Composing primitives and F# together cements higher-level, derived operations we think of as pillars and walls. The beauty of derived operations is that we may abstract them, treating them as a reusable single piece by forgetting the bricks and glue that compose them. We construct the mightiest models, machine learning castles indeed, composing all available operations in the blueprint of F#.

We find ModelWizard’s primitive operations naturally capture common machine learning paradigms that when composed into derived models, offer easy access to many model families, such as clustering and Naive Bayes. Creating models as compositions lends understanding into how the models work, since we can “open the box” of a derived operation and inspect its component operations and code to see how it works. At the same time, abstraction allows analysts to consider derived models without worrying about their low-level details by using the models as “closed black boxes.”

For example, operations 1.1 and 1.2 that construct the Apple Freefall model are derived operations, abstracting details of regression and automating choice of model by deducing that time is a real-valued variable. Users who want to ”dig in,” understanding and modifying the derived operations, may do so by inspecting their source code.
1.4.3 Safety in Model Construction

Tabular has typing rules in terms of the domains of data columns and distributions to ensure a schema’s probabilistic annotations make sense and that data actually conforms to the annotated schema. A state, consisting of a dataset plus a Tabular model, is \textit{valid} provided it contains no naming conflicts, is well-typed, that its schema and data satisfy asserted relational properties like primary/foreign key, and that no cyclic references are present.

Users developing models directly can easily construct invalid states. In contrast, ModelWizard ensures only valid states are constructable, throwing exceptions when an operation cannot construct a valid state.

1.5 Thesis Outline

Chapter 2 introduces ModelWizard language syntax and design. We cover core types and OpMonad, ModelWizard’s operation builder, followed by a walk through operations grouped by topic. See Appendix B for a concise ModelWizard operation API.

Chapter 3 opens with simple model construction on small datasets and progresses to advanced model construction on real-world data. We cover Bayesian networks, Naive Bayes classifiers, a hybrid model with functional dependencies and clustering for collaborative filtering. Readers seeking further intuition may skip Chapter 2 to view Chapter 3’s examples.

Chapter 4 concludes by presenting desirable extensions and discussing ModelWizard’s fit in the data science world.
Chapter 2
ModelWizard Language

We illustrate in this chapter the language syntax and design of ModelWizard, a domain-specific language embedded in F#. We cover core types, detail how to build operations safely with OpMonad, survey our current API of operations and show how to use them in model construction. Readers unfamiliar with F# syntax may find [SGC12] a useful reference.

2.1 Types: State, Operation and Safety

ModelWizard’s core data type is \texttt{State}: a pair consisting of a dataset and a Tabular model annotating that dataset. We call the dataset \texttt{Data} and the Tabular model \texttt{Schema}.

\begin{verbatim}
type TableName = string
type ColumnName = string
type DataTable =
  { tablename: TableName;
    colnames: ColumnName[];
    data: System.IComparable[,]}
type Data = DataTable list
type Schema = //...
type State = Schema * Data

type StateOp<'R> = (State -> 'R * State)
\end{verbatim}

\texttt{Data} is a relatively thin wrapper around an in-memory array of tables. A table has a name, an ordered array of column names and a two-dimensional data array,\footnote{The \texttt{System.IComparable[,] type on \texttt{Data} indicates \texttt{Data} values have a total order. Do not think deeply into the total ordering; it is a pragmatic requirement that makes working with F# libraries easier. The total order may be unrelated to the actual meaning of data values. For example, string values are compared lexicographically such that ‘blue’ “is less than” ‘red.’ For modeling purposes we may still treat color as a nominal column, that is, one whose data values have no semantic total order.} of...}
which the first dimension indicates row number and the second dimension indicates column. Missing values have value null.

**Schema** is analogous to the Tabular Schema type [GGR+14]. Its first component is a representation of a classical relational database schema, composed of a list of named tables, each of which has a list of named and typed columns. Its second component is annotations on columns with probabilistic model expressions that define distributions over the data entries corresponding to the schema columns. The Tabular compiler compiles Schemas into code in a probabilistic programming language, with which we run inference using the language’s inference engine. Thus, by manipulating Schema in ModelWizard, we manipulate the machine learning model that we use in inference.

**StateOp<'R>** is an operation on State, returning a new State plus additional information of type 'R. 'R could include information about the new state such as outlier data points or oddly fitting model components, information on other States worth considering, or anything else the user writes in the StateOp function. The new State may be the same as the original State.

### 2.1.1 Defining “Valid” States

The State type by itself offers no guarantee that a State is valid. Before we may provide any notion of validity, let alone the safe construction of valid states, we must define what we mean by “valid” and “safe.”

We call a State valid when its component Schema is valid on its own and when the component Schema conforms to the State’s component Data in the categories listed below. Safety refers to a process of constructing a state that preserves state validity, or informally, that “valid states in yield valid states out; garbage states in and can be semantically compared only for equality.
yield garbage.”

The following categories outline the main kinds of Schema validity and Schema-Data conformance that we check in the ModelWizard implementation:

1. Naming conflicts. Table names must be unique, column names must be unique within each table, and table and column names present in a Schema must correspond to tables and columns in the Data it is paired with. ModelWizard always checks for naming conflicts, especially when parsing arguments that create an operation and executing operations that create new columns or tables.

2. Type checking. Modeled columns in a Schema (that is, columns with Tabular model expressions) must have a type that can be generated by the model on that column. It would not make sense, for example, that a column with a real type have a Discrete model expression. Data values must in turn match column types in the Schema they are paired with. ModelWizard performs type checking at runtime when there is a chance that data may not match a new type, explained further in Section 2.4.

3. Primary and foreign key correctness. ModelWizard guarantees columns with the annotation ‘pk’ are unmodeled and have no duplicate values, such that each value in a primary key column is unique. Further, (foreign key) columns whose domain is that of another (primary key) column may only assume values that are a subset of those in the primary key domain. Section 2.4 and 3.3.1 introduce the primitive operations CreateTableUniques, Link and Exact that carefully check these requirements.

4. Cyclic dependencies. Tabular requires that columns and tables only refer to previously declared columns and tables. We enforce this requirement in Section 2.5.3
via Schema-reordering operations.

Checking state validity at runtime ensures that states are actually valid, at the sacrifice of scalability to big data or big models. While unimplemented, we lower barriers to scalability by running checks only when necessary, running checks lazily in background threads or using other techniques discussed in Section 4.1.

The following notions of state validity are outside the scope of ModelWizard:

1. Detecting data valid according to type and syntax but questionable according to data likelihood. For example, an int-type column with values \{1, 3, 1, 1, 2, 4, 1, 9001, 2, 3, 1\} is valid syntactically and type-wise, but the value 9001 is a huge outlier worth questioning. However, it would be straightforward to write an operation that returns unlikely data values.

2. Suggesting corrections to data values with syntax or type errors. For example, suppose we have the data value ‘15B’. If present in a column containing with many other integers, we could propose that the ‘B’ is a typo, accidentally inserted. We may also interpret the value as hexadecimal and propose replacing ‘15B’ with the decimal ‘347’. With supporting evidence from other columns, a third plausible alternative is that ‘15B’ is the concatenation of two columns, such as an airline seat reservation with row number 15 and seat position B for “aisle.”

We refrain from heroically suggesting remedies for invalid states. More extensive data cleaning is the subject of active research, as seen in the DataTamer [SBI+13] and Potter’s Wheel [RH01] systems among others. We would welcome integrating data cleaning techniques with ModelWizard in order to create a better end-to-end data analytics and model construction platform.

3. Detecting models valid according to type and syntax but questionable according
to data likelihood. For example, nothing in our system prevents a user from placing a Gaussian distribution with mean 10,000 and variance 1 on a column with values \{1, 5, 2, 2\}. However, we do provide features that make model scoring and comparison easier, such as running inference, computing data likelihood scores and running cross-validation. We welcome contributions that perform model scoring in the background, alerting the user if he performs an operation that leads to a very unlikely model.

4. Guaranteeing models are inferable by a particular back-end inference engine. See Section 4.2 for a discussion on model inferability.

Defining and enforcing validity as outlined above allows us to make the guarantee that every model constructed by ModelWizard has a valid Tabular counterpart and will pass Tabular’s type checking, a strong enough guarantee to be useful in practice but not so strong as to result in intractable model checking.

2.1.2 ValidState and ValidOp Types

We use the ValidState type, presented below, to indicate a State ModelWizard guarantees valid. The below code is part of an F# signature file, whose purpose is to declare the types an F# library implementation file exports. Because ValidState’s constructor is missing from the signature file, there is no direct way to construct ValidStates except through other methods that handle ValidStates in a controlled manner, to guarantee preservation of State validity. The function unwrapVS enables de-construction: retrieving encapsulated State from a ValidState.

```fsharptype ValidState  // Constructor hidden!!val unwrapVS : ValidState -> Stateval UNSAFE_VeridState : Schema * Data -> ValidState```
For development convenience and expert users, we include an extra function `UNSAFE_ValidState` which escapes `ValidState`’s safety guarantee and allows direct construction of `ValidStates`. Writing `UNSAFE` in all capitals flags users to be especially careful to only construct truly valid `ValidStates` when calling this function.

`ValidOp` is a type, presented below, for a `StateOp` guaranteed to preserve state validity. In fact, `ValidOps` throw exceptions when run in a way that would create an invalid state and possibly corrupt the user’s data. The user may run `ValidOps` on `ValidStates` by `runValidOp` and on plain old `States` by `unwrapVOP`. `UNSAFE_ValidOp` is similar to `UNSAFE_ValidState`.

```fsharp
type ValidOp<'R> // Constructor hidden!!
val runValidOp : ValidOp<'R> -> ValidState -> 'R * ValidState
val unwrapVOP : ValidOp<'R> -> StateOp<'R>
val UNSAFE_ValidOp : StateOp<'R> -> ValidOp<'R>
```

ModelWizard’s principal workflow is to load a `ValidState` from an original `Data` source (such as an Excel workbook) with a default “do-nothing” `Schema`, perform a series of `ValidOps` that refine `ValidState` incrementally, and end with a final `ValidState` guaranteed valid. We expect users will create many intermediary ModelWizard scripts before settling on a final script that creates a final model. Intermediary scripts may return extra information `'R`, such as inference performance or the names of columns in the range of a functional dependency. See Section 4.3 for a sketch of how we envision users editing scripts interactively.

### 2.1.3 OpMonad: ValidOp Computation Expression

`OpMonad` is an F# computation expression class to create an intuitive syntax for chaining together `ValidOps` into a compound, derived `ValidOp`. As required of a proper monad, `OpMonad` respects the monad laws of left and right identity and associativity [Wad92, Section 2.10]. Code Listing 2.1 lists selected type signatures
type OpMonad =
    member Bind:  ValidOp<'R> * ('R -> ValidOp<'N>) -> ValidOp<'N>
    member Return:  'R -> ValidOp<'R>
    member Zero:  unit -> ValidOp<unit>
    member Combine:  ValidOp<unit> * ValidOp<'R> -> ValidOp<'R>
    member Delay:  (unit -> ValidOp<'R>) -> ValidOp<'R>
    member For:  seq<'a> * ('a -> ValidOp<unit>) -> ValidOp<unit>

val OPM : OpMonad  // shorthand for an OpMonad instance

// Implementation:
member __.Bind(vop, f) = VOP <| fun s ->
    let res, newst = (unwrapVOP vop) s
    in unwrapVOP (f res) newst
member __.Zero() = VOP <| fun s -> (() ,s)
member __.Return(x) = VOP <| fun s -> (x,s)
member __.ReturnFrom(x) = x
member this.Combine(vop1, vop2) = this.Bind(vop1, fun () -> vop2)
member this.Delay(f) = this.Bind(this.Return (), f)

Code Listing 2.1: Selected OpMonad type signatures and implementations

and implementations.

The key notion to understand OpMonad is how let! statements translate to monadic bind. The following guidelines, in which vop is a placeholder for any ValidOp, outline the translation:

- let! r = vop translates to let r,nextState = vop curState
- do! vop is a synonym for let! () = vop for a ValidOp encapsulating StateOp<unit>.
- return x creates a ValidOp that returns x without modifying state.
- return! vop evaluates a ValidOp directly.
- |> and <| are F# operators for function application.

Please see [PS12] for a deeper review of monads as F# computation expressions.
Refer also to Appendix A for an example translation of an OpMonad expression into an F# quotation calling OpMonad’s computation expression components.

2.2 Escape to F#: GetState

GetState links ModelWizard operations to F# code by returning a copy of an executing operation’s current schema and data, exposing them to F# code. Operations may subsequently inspect column names, types and models as well as their underlying data. Nearly every derived operation includes a call to GetState.

There is no corresponding WriteState operation except via UNSAFE operations. Including one would allow a user writing derived operations to easily create an invalid operation, destroying OpMonad’s guarantees. Thus, user code may inspect state but not alter state, except through ModelWizard’s suite of primitive operations.

2.3 Machine Learning Base Models

ModelWizard includes two base machine learning models: Gaussian and Discrete\(^2\) distributions. Both have conjugate priors: Gamma on the precision of a Gaussian, another Gaussian on the mean of a Gaussian, and Dirichlet on the probability vector of a Discrete. Conjugate priors allow inference of a Gaussian and Discrete distribution’s parameters.

Tabular represents Gaussian and Discrete conjugate distributions by the column markup CGaussian and CDiscrete. Figure 2.1 presents the markup’s meaning as a procedure to draw from their represented probability distributions. \(N\) and Mean-Prec are hyperparameters that may be specified in the Tabular model referencing

\(^2\)Throughout this thesis, “Discrete” refers to a Categorical distribution, also known as a generalized Bernoulli distribution. The range of a Discrete distribution are the integers 1 to \(N\) for fixed distribution parameter \(N\). An integer is sampled from a Discrete distribution with probability determined by an \(N\)-dimensional probability vector, stored as a distribution parameter.
CDiscrete(N=\_):

1. Draw table-level $\vec{p}$ from an $N$-dimensional Dirichlet distribution with concentration $\vec{\alpha} = \vec{1}$.
2. For each row, draw from a discrete distribution with probability vector $\vec{p}$.

CGaussian(MeanPrec=\_):

1. Draw table-level $\mu$ from a Gaussian distribution with mean 0 and precision (inverse of variance) MeanPrec.
2. Draw table-level $\tau$ from a Gamma distribution with shape and scale 1.0.
3. For each row, draw from a Gaussian distribution with mean $\mu$ and precision $\tau$.

Figure 2.1: Tabular Conjugate Distributions

the conjugate models, which affect the prior distribution from which conjugate prior distribution itself is drawn. We typically assign uninformative priors to reduce bias by choice of prior in inference, though one can assign informative priors just as easily. CGaussian has in fact, another hyperparameter MeanMean that is the table-level $\mu$ in Figure 2.1 which comes into play when MeanPrec is sufficiently large.

We create these distributions on a column, independent of all other columns, in ModelWizard by the primitive operations **ModelDiscrete** and **ModelGaussian**. **ModelDiscrete** may be performed on any column of type upto(N) or link(T). Link(T) columns are essentially upto columns with N set to the number of rows in table T. **ModelGaussian** may be performed on columns of type real or int, converting the column to type real in the int case. We enforce type constraints by throwing an exception if one operates on a mismatching type.

To make it easier to independently model a column, we use the derived operation **Model** to place a “default” distribution appropriate for the column’s type by means of a call to **ModelDiscrete** or **ModelGaussian**. Columns of type string, the raw text type, are handled by a **TypeNominal** operation described in the next section.

Future work may extend the “two-level” Gaussian and Discrete conjugate distributions to higher levels of hierarchical models. This can be done partially for the
prior on the mean of a Gaussian distribution, since the prior is itself another Gaussian distribution. A Gaussian distribution’s precision (alternatively, variance) is more tricky. As for the Dirichlet distribution, the prior of a Discrete distribution, placing a prior on a Dirichlet requires the nonparametric Dirichlet process [Teh10], which is historically hard to perform variational inference on because the number of variational parameters is nonconstant. Recent work has had more success [BJ04].

We also leave integrating other base distributions into ModelWizard as future work. Good candidates are Gamma, Wishart, Poisson and Binomial, as these distributions all have existing representations in Tabular. Multivariate Gaussian is a particularly excellent candidate as it creates a new way to couple continuous columns alongside polynomial regression. We do not include the Beta and Bernoulli distributions as they are special cases of the Dirichlet and Discrete distributions, respectively. It may also be worth investigating other prior distributions; for example, Gelman argues that a Gaussian distribution truncated to only place probability mass on positive values tends to perform better as a prior on the variance of a Gaussian than the inverse-Gamma we use in CGaussian [Gel06].

A challenge to additional base distributions is their level of inference support in Infer.Net. Using other back-end inference engines such as Stan [Sta14] or R2 [NHRS14] may add diversity to other base distributions’ level of inference support.

2.4 Typing Data, Tables as Nominal Column Domains

Columns in Tabular can have type int, real, link(T), upto(N) and string. The domain of upto(N) is the integers [0, N − 1]. One can imagine a bool type as upto(2). The domain of link(T) is all rows of table T.

We change column types by the operations TypeUpto, TypeReal and
**TypeNominal.** These operations are checked such that they will not place an improper type on a column, and they are only allowed to act on unmodeled input columns. For example, **TypeReal** will check the data to ensure that the target column’s data really are real-valued when there is a chance the data may not be, say when converting from type string as opposed to type int. **TypeUpto** and **TypeLink** act similarly. **TypeInt** is also implemented but not discussed here or in the API as no machine learning models use the int type, taking upto or real in its place.

String types have special handling. One could use the former three type operations to convert a string column that contains numeric data, but it is more common that a string column has **nominal** data, that is, data whose values are only comparable by equality like \{red, blue, red, green\}.

We handle a nominal column C in table T with the primitive operation **CreateTableUniques** T [C]. It creates a new Tabular table (call it NT) whose rows contain the unique values of column C. Thus, NT’s rows form the domain of C. We bind the domain of C in T to NT by the operation **Link** NT [C,C] T C, which changes column C to type link. Read the **Link** operation as “map column C in foreign table T to column C in primary table NT and store the corresponding row matches in foreign table T’s column C.”

Composing **CreateTableUniques** with **Link** forms the derived operation **TypeNominal**, an operation that effectively types a string column as a nominal column. It is also possible to run **TypeNominal** on int and real columns, effectively treating the numbers in those columns as nominal labels instead of numeric values. Running **TypeNominal** on an upto column is redundant and disallowed.

A promising future direction is handling ordinal columns. Ordinal data have ranking in addition to equality comparison, like the data \{first, second, third\}. One way to represent ordinal data is by logistic regression, supposing that ordinal values
are delineated by continuous thresholds and then more easily inferring a continuous number and seeing which “bucket” between thresholds the continuous number lies in. “Indicator” columns perform the logistic regression in Tabular to indicate when a column is “greater than” its threshold value. While we have built this model in Tabular, we have not yet represented it as an operation due to inference troubles related to algorithm support in Infer.NET.

2.4.1 Type Inference

Having access to the data at the time of modeling and interleaving F# code with operations enables typing automation. We can create TypeInfer, a derived operation that infers the type of a column from its data.

We design TypeInfer to first apply a heuristic that columns with less than 5% unique values are likely to be nominal columns, because they contain significantly high redundancy. For example the data {1, 1, 1, 0, 1, 0, 0} is more likely nominal than continuous, with 0 and 1 indicating presence or absence of some label or property. Users may call TypeReal to override this heuristic.

If a column contains greater than 5% unique values, then TypeInfer attempts to type as an int, then to type as a real if the data contains a non-integer, then to type as a nominal as a last resort.

We extend TypeInfer to automatically type all of a table’s input columns by the derived operation TypeInferTable. We show a simplified version of TypeInferTable’s implementation in the OpMonad expression of Appendix A.
2.5 Coupling Columns

The previous two sections introduce how to type columns and place base machine learning models on a column independent of all other columns. We now consider coupling models of columns such that one column depends on another.

2.5.1 Continuous Coupling: Noisy Regression

Our prelude apple freefall example in Section 1.2 introduces LinReg and QuadReg as two operations to couple continuous columns by polynomial regression. The user specifies the domain and the range of the regression as input to the operations. Polynomial regression is a generic, “default” way to couple continuous columns without special knowledge of the structure of a dataset.

We add noise to polynomial regression in order to place a non-point-mass distribution over the range column when the domain column is deterministic (e.g., when the domain column is unmodeled with markup input). The noise has fixed mean 0 so that we may infer the constant term properly (‘b’ in linear regression, ‘c’ in quadratic), or else the noise and constant term would conflict in explaining regression bias. Inferred noise variance corresponds to regression error magnitude.

LinReg and QuadReg rely on the function tables in Figure 1.1a and Figure 1.1b defined above the main tables to implement regression in an abstracted manner. Function tables use a special syntax in Tabular to implement a generic function that involves table-level inputs with default parameters (“hyper” columns), additional table-level columns determined by the inputs (“param” columns), concrete row-level inputs from a table (“input” columns), additional row-level columns that depend on the inputs (“latent” columns), and a row-level “output” column that returns a function’s result to the table that calls it. “Table-level” refers to columns that have
the same value for every row in a table, whereas “row-level” refers to columns whose value may differ for each row of data. Tabular’s compiler inserts function tables inline into the non-function tables that call them, a process similar to macro expansion. The insertion should occur in a way that does not conflict with names in the calling table.

Unfortunately, Tabular syntax forbids function tables that reference other function tables, recursively or not. If we had the ability to conduct recursive calls, then we could implement polynomial regression in a recursive, more concise manner. Imagine the operation \texttt{PolyReg N rngcol domcol} to do \(N\)-ary polynomial regression between domain column \texttt{domcol} and range column \texttt{rngcol}. We may implement \texttt{PolyReg N} by adding an \(N\)\textsuperscript{th} degree term in the function and then recursively calling \texttt{PolyReg (N-1)} for the rest of the regression, down to \texttt{PolyReg 0} base case. Even without the recursive implementation, it is possible to implement \texttt{PolyReg N} without individually using the operations \texttt{LinReg}, \texttt{QuadReg}, and so on by using a symbolic algebra algorithm to create an \(N\)\textsuperscript{th} degree regression as a function table in F# code, though we have not presently implemented this in ModelWizard.

The regression operations place a distribution over the range column determined by the domain column, effectively meaning that the domain column value determines the range column. If the domain column is modeled (i.e., has a probability distribution as opposed to an input column), then the regression on the range column distribution is a function of the domain column distribution.

\subsection{Discrete Coupling: Index}

Indexed models are a natural way to couple Discrete machine learning models. We \texttt{Index a} (discrete or continuous) modeled range column’s distribution by a discrete (modeled or unmodeled) dimension \(D\) domain column by creating an array of copies of the range column’s distribution, one for each of the \(D\) domain values, and selecting the
copy according to the domain column’s corresponding value. The copy distributions are identical to the original range column distribution, except that the copies have their own parameters.

The indexed range column may have any model. We use the notation \texttt{Model[DomCol]} to indicate indexing the range column’s model by discrete domain column \texttt{DomCol}. Section 3.1 and 3.2 show models where a Discrete and Gaussian distribution, respectively, are indexed by a discrete variable. It is also possible to index a \texttt{LinReg} or \texttt{QuadReg} model by a discrete variable. Such an indexing would make sense in the context of Section 1.2’s apple freefall example if we had data for apples on different planets (each with their own force of gravity). We could index the regression on apple elevation by the planet the apple is on.

Figure 2.2a graphically depicts one of the indexed distributions from Section 3.1’s Bayesian network in terms of gates [MW09] and plates [Bun94]. \texttt{PVec} is the probability vector governing sampled outcomes of rain on each row. Alpha is the
concentration vector for the Dirichlet distribution used as the prior for the Discrete
distribution. Alpha is a vector of 1s when left unspecified. \( N=2 \) sets the dimension
of the vectors at 2, which is equal to the number of states of rain (a boolean-valued
column, typed as \( \text{upto}(2) \)).

The dashed box is a plate, which means that its contents are replicated; there is
a distinct PVec for every value of cloudy (also of type \( \text{upto}(2) \), though the dimension
of the domain column need not equal the dimension of the range column in general).
Inputs to the plate (Alpha) are sent to each replicated PVec. The square inside a box
is a gate, which determines the output of the plate (rain) by the indexing variable
cloudy. Figure 2.2b shows the “unfolded” version of the gate and plate.

A helpful way to think about the notation is that there are distinct PVec
parameters for the Discrete distribution governing rain. The distribution of cloudy
determines the weights with which we use each parameter. Thus, we say that cloudy
determines the distribution over rain.

In terms of operations, Index is a simple primitive operation. Index verifies
that the domain column is discrete and the range column is modeled, throwing an
exception if either condition does not hold, and replaces the range column’s distribu-
tion by an indexed version. Syntactically, however, Index is more complicated due
to the occasional need to index distributions across table links. The user may specify
a list of table links to traverse. See Figure 3.9 in the Applications chapter for an
example where movie ratings are indexed across a table link to a cluster column in a
user table and a title table.

Index and LinReg/QuadReg offer venues for a discrete column to determine
a discrete column, for a discrete column to determine a continuous column, and for
a continuous column to determine a continuous column. We do not have a way for
a continuous column to determine a discrete column. As mentioned in Section 2.4
above, we may create a way in the future by implementing a logistic regression operation. With that future addition, we would have “default” ways to couple columns of any type, a valuable ability for users experimenting with dependencies in a dataset.

2.5.3 Bookkeeping: Reordering Tables and Columns

With the power of the coupling operations \texttt{LinReg}, \texttt{QuadReg} and \texttt{Index} to create dependencies between columns, we run the risk of creating cyclic dependencies: one column depending on another that transitively depends on the first. Cyclic dependencies are inexpressible in Tabular; columns may only refer to columns declared above them in a Tabular model. In other words, the overall model must fit into a directed acyclic graph.

We guard against cyclic dependencies by checking the set of columns that a column depends on at operation-runtime. There are three scenarios. If a dependency can be created without changing column order, it is done. If a dependency can be created that requires changing column order, then a \texttt{ReorderColumns} operation is invoked internally. If a dependency cannot be created due to cyclic dependencies (sometimes involving many columns), then an exception is thrown.

The same caution applies to tables. The \texttt{Link} operation, for example, creates a table dependence that may require reordering tables. Cyclic table references are not allowed.

2.6 Latent Columns

A common modeling paradigm is to create latent columns not present in the original dataset in addition to the concrete columns present with data values. Derived from concrete columns, latent columns expose intermediary states of probabilistic modeling
to the user, often increasing model understandability. For example, latent columns inside the function tables of LinReg and QuadReg increase their interpretability by delineating the addition of noise from the regression.

**NewColumn** is an operation that may create an UptoColumn or a LinkColumn. Section 3.4 demonstrates UptoColumn by creating new cluster columns for tables. The number of clusters is given as an argument to UptoColumn. We see these columns as output in Figure 3.9, since we can treat new columns as concrete columns with all missing data. Section 3.3 demonstrates LinkColumn in the ExactInfer operation, where links are created from tables with range columns to tables with domain columns that exactly determine the range columns.

### 2.7 Excel, Inference and Advanced Operations

Operations interfacing with Excel are essential to every application so that we can load and save data and models. ModelWizard reads data from an Excel workbook data model using bindings in the .NET framework API. Luckily, Excel’s data model holds types on columns that are enforced by Excel’s processing model. ModelWizard therefore trusts the type of a column indicated by Excel by using an UNSAFE_ValidState operation when constructing a state directly from an Excel workbook. Writing data is similar, except that data is first written to a user-named Excel spreadsheet and then added to the containing workbook’s data model. Tabular models are read from and written to spreadsheets directly.

Inference operations call the Tabular compiler. We implement them by calling GetState, converting ModelWizard Data and Schema into Tabular Data and Schema and executing the Tabular compiler to create an Infer.NET probabilistic program. The Infer.NET engine returns inference results, which we parse and return to the
caller.

More advanced machine learning operations including NaiveBayes, Exact, ExactInfer and Inferno are described in the next chapter: Applications.
Chapter 3
Applications

In this chapter we illustrate the model construction process with ModelWizard through progressively more complex examples.

3.1 Small Model Search: Discrete Bayesian Networks

In this section we demonstrate how one constructs an acyclic discrete Bayesian network in ModelWizard, and how to search over and select different models using inference to score them. Our model search example is small, selecting between two Bayesian networks that differ in one arrow. One may extend it to larger search spaces bearing in mind computational feasibility.

Suppose we want to model Figure 3.1’s Bayesian network, modified from [Mur01] adding uncertainty in the arrow between wet grass and rain. Does wet grass determine rain’s distribution, rain determine wet grass’s distribution, or are wet grass and rain independent? We answer by building and comparing each candidate model, using data likelihood as selection criterion.

We begin with a default all-input model and dataset that performs no predic-

(a) “No-predict” default State: Data and Schema. ‘upto(2)’ is equivalent to ‘bool’.

Figure 3.1: Uncertain Bayesian Network
A natural first step is to model each column independently, in this case using \textit{ModelDiscrete} since all columns are nominal. \textit{ModelDiscrete} allows inference of each nominal value’s probability (see Section 2.3 for details) and prediction of missing values, as with rain’s missing value in Figure 3.1a. Recall that Tabular inference consists of training a given model on observed (non-missing) values in the input dataset to form a posterior model, outputting posterior model parameters that in this case form conditional probability tables, and outputting marginal distributions from the posterior model on each missing value, conditioned on the observed values in the same row of that missing value.

\textit{Index} correlates two columns. Taking \texttt{Index "tmain" "rain" "cloudy"} (read “Index the distribution of rain by cloudy”), for example, \textit{Index} creates separate distributions on rain for each value of cloudy, effectively creating a conditional probability table where rain depends on cloudy. Rain’s Tabular model suffix ‘[cloudy]’ indicates the new dependence.
let s0 = readValidState inputFile

let le1,s1 = 
  s0 |> runValidOp (OPM {
    do! ModelDiscrete "tmain" "cloudy"
    do! ModelDiscrete "tmain" "rain"
    do! ModelDiscrete "tmain" "sprinkler"
    do! ModelDiscrete "tmain" "wetGrass"
    do! Index "tmain" "rain" "cloudy" []
    do! Index "tmain" "sprinkler" "cloudy" []
    do! Index "tmain" "wetGrass" "sprinkler" []
    return! ScoreLogEvidence}) //Ok: -2286.50

let le2,s2 = 
  s1 |> runValidOp (OPM {
    do! Index "tmain" "rain" "wetGrass" []
    return! ScoreLogEvidence}) //Better: -2128.71

let le3,s3 = 
  s1 |> runValidOp (OPM {
    do! Index "tmain" "wetGrass" "rain" []
    return! ScoreLogEvidence}) //Best: -1963.57

let candidates= List.zip [le1;le2;le3] [s1;s2;s3]

let bestle,bestmodel = List.maxBy fst candidates

Code Listing 3.1: Script to build and select Figure 3.1’s most likely model
Model candidates $s_1$, $s_2$ and $s_3$ follow from further indexing. Rain and wetGrass are independent in model $s_1$, rain indexes the distribution of wetGrass in model $s_2$, and wetGrass indexes the distribution of rain in model $s_3$. We use the ScoreLogEvidence procedure to compile the current Tabular model into Infer.NET inference code, execute inference and return model log evidence scores under 1000 rows of input data, storing scores in $le_1$ through $le_3$.

An unusual paradigm in the example is the reuse of State $s_1$ in the construction of $s_2$ and $s_3$. Many monads are “single-track” in the sense that they disallow storing and reusing internal state because it could lead to undesirable operations, such as saving a pointer to a file, then deleting the file, then attempting to access the file through the pointer. This kind of behavior is also disallowed in OpMonad since OpMonad expressions evaluate to a single ValidState. We had to jump outside the OpMonad construct into general F# let bindings in order to save state $s_1$ and use it in the construction of two different states bound at the top level. We retain “single-track” enforcement in OpMonad for efficiency, since copying State in the current implementation entails copying Data within that State eagerly. Section 4.1 discusses delayed approaches to updating Data.

We find model $s_3$ is most likely because $le_3$ is greatest, fulfilling our intuition that rain more likely causes wet grass (assuming conditions necessary for causal interpretation; see [KTHO05]). We also recover the same conditional probability tables (not shown) from Tabular inference as the Infer.NET program, proof that Tabular succeeded in learning the true model for this simple scenario. In fact, we generated the 1000 rows of input data from an Infer.NET probabilistic program with model $s_3$ as ground truth and fixed conditional probability tables,\(^1\) and so model $s_3$ is the true

---

\(^1\)Adapted from http://research.microsoft.com/en-us/um/cambridge/projects/infernet/docs/discrete%20bayesian%20network.aspx
model.

We call our procedure interactive model search because the user specifies the search space through scripts like Figure 3.1. The user may initiate a larger search, perhaps over the space of all Bayesian networks as an automated search algorithm would, by searching over the presence and direction of every arrow. See [CG01b] for a survey of learning algorithms on several variants of Bayesian networks. In short, ModelWizard opens a design space in which the user insightfully scripts ad hoc searches through model subspaces, writing in automated selection or prioritization as needed to search spaces large enough to be useful without resorting to infeasible, exhaustive search.

Model selection by data likelihood is prone to overfitting. In remaining examples we switch to the cross-validation inference scoring method: holding out a test set of data and measuring test set predictive accuracy according to a user-defined error function, such as the 0-1 loss function on predicting rain.

3.2 Derived Model Family: Naive Bayes

We now illustrate data-transforming and derived operations. Suppose we want to construct a Naive Bayes model to classify gender given height, weight and footsize as features, for a dataset taken from [Wik14]. Naive Bayes is a machine learning family of classifiers where a class column determines the distribution behind feature columns, and the features are assumed independent given class.

Figure 3.3 shows our beginning all-input state. A new difficulty is that our data source has string type for gender, a type which Tabular cannot perform inference over. CreateTableUniques and Link in Code Listing 3.2 overcome this difficulty, the former by creating a new table of gender’s unique values called T_gender, and the
Figure 3.3: Initial State: Data and Schema before Naive Bayes

| ID | gender | height | weight | footsize |
|----|--------|--------|--------|----------|
| 0  | Male   | 6      | 180    | 12       |
| 1  | Male   | 5.92   | 190    | 11       |
| 2  | Male   | 5.58   | 170    | 12       |
| 3  | Female | 5.92   | 165    | 10       |
| 4  | Female | 5      | 100    | 6        |
| 5  | Female | 5.5    | 150    | 8        |
| 6  | Female | 5.42   | 130    | 7        |
| 7  | Female | 5.75   | 150    | 9        |

| ID | int | input |
|----|-----|-------|
| gender | string | input |
| footsize | real | input |
| height | real | input |
| weight | real | input |

```
let! tn = CreateTableUniques "tmain" ["gender"]
do! Link tn ["gender","gender"] "tmain"["gender"

do! ModelDiscrete "tmain" "gender"
do! ModelGaussian "tmain" "height"
do! ModelGaussian "tmain" "weight"
do! ModelGaussian "tmain" "footsize"
do! Index "tmain" "height" "gender" []
do! Index "tmain" "weight" "gender" []
do! Index "tmain" "footsize" "gender" []
```

Code Listing 3.2: Naive Bayes script expressed in primitives

latter by changing tmain’s data such that gender is an integer link to the appropriate ID column of T_gender. The annotation ‘pk’ in the gender column of T_gender enforces that every row of T_gender must have a unique value. Because T_gender has two rows, Gender’s new ‘link(T_gender)’ type is synonymous with ‘upto(2).’

Figure 3.4 shows the final Naive Bayes model after running the rest of Code Listing 3.2. ModelGaussian is similar to ModelDiscrete in that it allows inference

Figure 3.4: Naive Bayes result state after Code Listing 3.2 runs on Figure 3.3
NaiveBayes tn classname = OPM {
    do! TypeNominal tn classname
    do! ModelDiscrete tn classname
    let! schema, _ = GetState
    let table = getSchemaTableByName schema tn
    let classcol = getColumnByName table classname
    let rngColList = // collect feature columns
        table.columns |> List.filter (fun col ->
            match (col, classcol) with
            | a,b when a.name = b.name -> false
            | {name=n},_ when n="ID" -> false
            | IndependentOf -> true
            | _ -> false)
    // Model & Index features by classcol
    for col in rngColList do
        if col.markup = Input
            then do! Model tn col.name
            do! Index tn col.name classname []
}

Code Listing 3.3: NaiveBayes derived operation

of mean and precision for a Gaussian distribution generating a column.

Naive Bayes is a common pattern in machine learning, and as [LBFPPB13] concurs, probabilistic programming languages naturally express Naive Bayes. The derived operation in Code Listing 3.3 provides one such expression to facilitate its construction on future datasets. It offers abstraction in that we no longer need worry about its component operations or F# code and can treat it as a black box. Alternatively, we gain understanding into how Naive Bayes works by looking at its code. The derived operation simplifies Code Listing 3.2 to the one-liner do! NaiveBayes "tmain" "gender".

We anticipate users use derived operations in two ways. On a basic level, users may record a list of operations on a dataset, initially taken ad-hoc, for replay on a similar dataset. After recognizing that a list of operations is an instance of a more
common modeling pattern, as in the case of Naive Bayes, a user can abstract and
generalize the derived operation to apply more widely. These operations include both
transformations on the dataset, like the conversion of string gender values to links in
a new table, and construction of a Tabular model.

### 3.3 Hybrid Model: Internet Plant Sales

We now turn to a real world example: modeling Internet plant sales. We use more
advanced pre-processing, capturing functional dependencies, in combination with the
previous section’s Naive Bayes model.

Figure 3.5 shows a few rows from a dataset, acquired from staff at the Royal
Botanic Gardens in Kew UK who are interested in predicting Wild Propagate: whether
a sale is of a wild plant or a propagate plant grown in a greenhouse. Predicting
whether a plant is wild or propagate is a key step in identifying illegal plant sales.
Perhaps more important than prediction, it is important to understand how strongly
other columns impact Wild Propagate, including sale price, country of sale, plant con-
servation priority, and status on the CITES list of endangered plant species [CIT73].

In database literature [Dat90], a functional dependence (FD) between domain
columns and a range column hold when domain column values uniquely determine
range column value. FDs may hold for continuous domains (as in the relationship
\( y = x^2 \) where \( x \) functionally determines \( y \)), but in this thesis we restrict FDs to
only use discrete domains. We sometimes refer to an FD as an “exact” dependence,
Figure 3.6: EFD-augmented Naive Bayes model classifying Wild_Propagate
Tables of unique values for nominal variables omitted.

because the domain of an FD exactly determines the value of its range. The Internet
plant sales dataset has two FDs: that Genus and Species determine conservation
priority and On_CITES status.

Code Listing 3.4 presents a script we use to create a hybrid model, shown
in Figure 3.6, for the Internet plant sales data. We infer the types of all columns
in the dataset via TypeInferTable, create a separate table Genus_Species explicitly
enforcing two discovered functional dependencies via ExactInfer (described below),
add a standard NaiveBayes on the remainder of tmain, and complete the model by
modeling the determined columns in Genus_Species. Ongoing research efforts build
on this model to investigate how machine learning may aid CITES treaty enforcement
via plant sales inspections.

3.3.1 exactInfer and Exact: Functional Dependencies

ExactInfer implements an algorithm to discover the best functional dependency
given a set of domain columns. “Best” in this case refers to the functional dependence
with largest range. We could for example, only find in the Internet plant sales data
do! TypeInferTable "tmain"
let! efd_rngcols = ExactInfer "tmain" ["Genus";"Species"]
do! NaiveBayes "tmain" "Wild_Propagate"
for col in efd_rngcols do
do! Model "T_Genus_Species" col

Code Listing 3.4: ModelWizard script to construct plant sales model

that Genus and Species functionally determine On_CITES status, but it would lead
to a missed opportunity to find that Genus and Species functionally determine both
On_CITES and conserve_priority.

We implement the derived operation ExactInfer in three phases.

1. Find all columns functionally determined by the given domain columns. Do not
   consider columns that have dependencies.

2. If there is more than one range column, create a new table with domain columns
   as primary keys by calling CreateTableUniques.

3. For each range column, perform an Exact.

   Exact is a primitive operation that performs the steps below to take advantage
   of a functional dependency. Translations of each step to the Internet plant sales Exact
tmain Genus_Species On_CITES are given in brackets.

   Given a main table, a range column in that main table, and a link-type domain
   column linking to a domain table [main table tmain, range column On_CITES, and
domain column Genus_Species in tmain linking to the domain table T_Genus_Species
(created by ExactInfer)],

1. Create a new column in the domain table with the same name, type and model as
   the range column in the main table. [Create On_CITES column in T_Genus_Species.]
2. Set the data of the new column to the values functionally determined by the primary key values in the same row. We implement this by building a map from domain column values to the unique range column value determined by the domain. [Set the data of On_CITES in T.Genus_Species to values determined by the FD in tmain from Genus_Species to On_CITES.]

3. Delete the data of the range column in the main table wherever the domain table link is not missing. There is no actual loss of data here because one may recover the data by joining the main table to the domain table. Instead, think of the data deletion as a form of data compression. [Delete the data of On_CITES in tmain in rows where Genus_Species is not missing.]

4. Modify the model of the range column in the main table to a reference to the range column in the domain table through the domain table link. [Change the model of On_CITES in tmain to Genus_Species.On_CITES.]

Successively applying ExactInfer on a table’s smallest possible domain set forms a basis for table normalization to Boyce-Codd Normal Form (BCNF). Table normalization is the process of decomposing a table into smaller tables to eliminate redundancies. Normalization to BCNF requires that the only FDs present in a table are either trivial FDs where the range is a subset of the domain, or FDs where the domain is a superkey (a superset of a candidate key: a set of columns that uniquely determine the FD’s range). We meet these requirements.

One could imagine extending the ExactInfer infrastructure to discover all the FDs within a table and not just the ones with a particular given domain, similar to automated table normalization work in [BNB08]. However, fully automated table normalization tends to discover spurious FDs, that is, FDs present in a dataset but not true in general. Nevertheless, it is possible to improve ExactInfer’s FD-discovery
algorithms by following recent work in [HQRA+13] and older work in its references.

3.3.2 “Pre-processing” during Modeling

FD-handling is typically a pre-processing step, part of table normalization. In fact, a user that knows about the FDs in a dataset will almost surely account for them before beginning the modeling process at the point where he architects dataset table layout. What if the user does not know about a dataset FD, perhaps when there are hundreds of columns? This is the ideal scenario for ModelWizard to help an analyst discover and take advantage of a dataset fact during the modeling process. We leave it to future studies to determine whether the additional flexibility from conducting pre-processing at the same time as modeling will help in practice.

It is worth considering how the model would work in the case that we do not use a separate table T.Genus.Species to capture functional dependencies. In this case, we would have a single table, tmain, with On.CITES and conserve.priority indexed by Genus and Species. Indexing the range columns by Genus and Species in the main table instead of a separate table models a FD in a looser sense, because we no longer restrict the range columns to a unique value given domain column values.

In the limit of an infinite dataset, the single-table model is equivalent to multi-table one because the CDiscrete distributions on On.CITES and conserve.priority collapse to point mass distributions for each unique (Genus, Species) pair. Fixing a (Genus, Species) pair, the collapse occurs after running Bayesian updating on infinite datapoints that are all the same. In the case of finite data, the single-table model incurs some predictive performance penalty. This penalty grows small quickly if prior distributions are not too strong and dataset size is at least moderately large.

Both the single-table and multi-table model perform better than not capturing a FD at all, i.e., indexing On.CITES and conserve.priority by Wild.Propagate.
This is because using tightly dependent columns—the range and domain columns—too grossly violates the Naive Bayes assumption that features are independent given Wild_Propagate.

A prime future improvement to Figure 3.6’s model is capturing the ordinal nature of column conserve_priority. A common way to do this is to create a table of real-valued thresholds for each value of conserve_priority (H, H-M, M, ...) and model the chosen conserve_priority as a real-valued variable discretized by those thresholds. An “ordinal column template” may make a nice addition to ModelWizard’s primitive operations, and it serves as another activity typically performed during preprocessing that aids users during modeling.

We imagine many other kinds of pre-processing activities from related work may enhance interactive model construction. The Bellman system presents algorithms to discover possible foreign key dependencies, columns formed from a concatenation or format change from other columns, different ways two tables may be joined through intermediate tables, and more, by comparing summary structures computed for database tables [DJMS02]. BayesDB offers capabilities to do similar preprocessing steps in the presence of more general data error through concepts like “stochastic primary key and foreign key,” which can be taken as primary keys containing duplicates due to noise and foreign keys containing changed or non-matching values due to noise [Bax14]. Integrating probabilistic models of internal database structure in the style of BayesDB with models of column value distributions in the style of Tabular is an open avenue for future work.
3.4 User-Movie-Rating Recommendation

For another real world application, we turn to movie recommendation as popularized by the Netflix challenge [BL07]. We show how to build a general clustering model using a ModelWizard script and evaluate its predictive performance. We specifically compare against Singh and Graepel’s application of InfernoDB to movie recommendations, as detailed in their first example that runs on synthetic user-movie-ratings data [SG12, SG13].

Our data is identical to Singh and Graepel’s synthetic dataset, consisting of a table of users with attributes gender and age, a table of movies with attributes category and year, and a table of ratings with a rating from 0 to 10 and links to a user and movie. The dataset is small, having two movie genres, 20 users, 30 movies and 25 ratings. Figure 3.7 illustrates a few rows.

3.4.1 InfernoDB: Schema-Derived Clustering Models

Singh and Graepel introduce the concept of automatically generating machine learning models based on the schema of a database, including types of columns in tables and foreign key relationships between tables.

A column’s type determines its base distribution: Real-valued columns have a Gaussian distribution and discrete (link) columns have a Discrete distribution. We replace the Bernoulli distribution used by Singh and Graepel with equivalent Discrete\(^2\)

\(^2\)Recall that we use Discrete as a synonym for a Categorical distribution.
distributions of dimension two.

Each table has a number of clusters. Tables with no foreign links ("leaf tables") have a fixed number of clusters, chosen by hand since the number of clusters is a crucial hyperparameter. Tables with foreign links ("body tables") have a number of clusters equal to the product of linked tables’ numbers of clusters. Thus, a table with foreign links has clusters equivalent to the cross product of the clusters of tables it links to.

Each row has a distribution over the clusters in its table. The distribution over clusters determines the parameters of each column’s base distribution. The resulting parameters are a weighted average over each cluster’s parameters, with weights determined by a Discrete distribution over clusters. Values for each column are drawn from their base distribution with these resulting parameters. For example, in a table with an age column that has 4 clusters, the age for a row in that table is drawn from a Gaussian distribution with parameters determined by that row’s distribution over the four clusters by taking a weighted average.

Each cluster’s parameters are drawn from an uninformative prior distribution. These priors are Gaussian ($\mu = 0, \sigma = 10^8$) for the mean of a Gaussian, Gamma ($k = 1, \theta = 10$) for the precision of a Gaussian, and Dirichlet $\alpha = 1$ for the probability vector of a Discrete. We chose these hyperparameters to match those used by Singh and Graepel.

Presented another way, Singh and Graepel generate a clustering model formed inductively on tables:\footnote{We assume table links are acyclic; there must exist some table with no outgoing foreign keys.}

1. Table $T$ base case: no foreign links: create a hidden cluster variable that determines parameters of the distribution behind each column of $T$. The distribution behind a column depends on its type. Fix the number of clusters heuristically.
2. Table $T$ recursive case: $T$ has foreign links: create a hidden cluster variable determined by the cross product of clusters of rows in tables that $T$ links to. A particular row’s distribution over clusters is determined by the distribution over clusters in each linked row in foreign tables.

This model uses soft clustering in that we allow a row to take a non-point-mass distribution over clusters. Calculations involving a row’s cluster take weighted averages over this distribution. This is also true of foreign links in the case of missing values for user and movie; we infer distributions over possible users and movies. This process is called link prediction. Its use case is when we have rows in our ratings table with a rating and movie, for example, and we wish to calculate which users are most likely to have given the movie that rating. A challenge to link prediction is high dimension distributions when there are many users or movies.

3.4.2 Inferno Operation with Cluster Setting

Our Inferno implementation in ModelWizard has one major difference from Singh and Graepel’s specification: it returns a map\(^4\) from “leaf” tables to a function that returns a ValidOp that, when later called, modifies the number of clusters in the corresponding leaf table. The extra returned functions allow the user to change the number of clusters after running the Inferno operation. Leaf tables have four clusters by default.

Code Listing 3.5 lists the Inferno operation. Here are a few notes of explanation, matching Code Listing 3.5’s commented annotations:

(A) GetNontrivialLinkedTableNames $ttgt$ returns a list of table names that $ttgt$ links to. We exclude “trivial” links to tables for nominal variables with no

\(^4\)The map is in the form of an association list, with elements of the form (key, value).
let rec Inferno ttgt:ValidOp<(ColumnName list*(int->ValidOp<unit>))list>= OPM {
    let! links = GetNontrivialLinkedTableNames ttgt  // (A)
    let! linkLists = OPM {
        match links with
        | [] ->  // base case
            let! clusterColName =
                NewColumn ttgt "cluster" (NewColType.UptoColumn 4)
            let modFun k = TypeUpto k ttgt clusterColName  // (B)
            return [[clusterColName], modFun]
        | _ ->  // recursive case
            let linkLists = ref []  // (C)
            for (c,t) in links do
                let! ll = Inferno t
                linkLists := List.map (fun (m,vop) -> c::m,vop) ll
                @ !linkLists  // (D)
            return !linkLists}
    let! rngColList = GetConcreteColumns ttgt  // (E)
    for c in rngColList do
        if c.markup = Input then do! Model ttgt c.name
    for ll in linkLists do
        match ll with
        | llhead::llbody,_ ->
            do! Index ttgt c.name llhead llbody
        | [],_ -> failwith "impossible"
    return linkLists}

Code Listing 3.5: Inferno ModelWizard Operation
non-primary-key columns.

(B) \textbf{modFun} is a function to change the number of clusters set one line above.

(C) We construct \texttt{linkLists} by mutable assignment due to an artifact of OpMonad. This has the same effect as a fold with the additional ability to execute \texttt{ValidOps} in the body of the fold.

(D) prepends the current table’s linked ColumnNames to the list of ColumnNames in linked tables, building a correct list of ColumnNames across links to leaf tables.

(E) \texttt{GetConcreteColumns ttgt} returns the columns that will be clustered by \texttt{ttgt}’s new cluster column. These are all the columns in the table that are not link columns to a “nontrivial” table (see (A)) and are not the ID or cluster column. We \texttt{Model} these columns if they are input.

3.4.3 Hyperparameter Sweeps over Number of Clusters

We use the resulting cluster-number-change functions from \texttt{Inferno} to find the optimal numbers of clusters by hyperparameter sweep using cross-validation. We fashion our algorithm as iterative coordinate descent as follows:

Let \texttt{userk} and \texttt{titlek} be numbers of clusters for the user and title table, respectively.

1. Initialize \texttt{userk, titlek := 4} (from \texttt{Inferno}).

2. Hold \texttt{titlek} fixed and calculate the best scoring \texttt{userk} between 1 and 6 by running cross-validation 6 times and comparing scores.

3. Hold \texttt{userk} fixed and calculate the best scoring \texttt{titlek} between 1 and 6 by running cross-validation 6 times and comparing scores.

4. If \texttt{userk} or \texttt{titlek} changed, goto step 2 else stop.
The algorithm generalizes to any number of leaf tables. We may also imagine a variant that does not fix the minimum or maximum number of clusters but instead searches for local score minima.

We use 5-fold cross-validation on the rating column to determine the best scoring numbers of clusters. To do this, we select 20% of the rows in table tmain to hold out their ratings value. We train our model to score on the remaining data and predict the values for the unknown 20% of rows. We use root mean square error (RMSE) to calculate error on predicted ratings versus their held out truths. Repeat for each randomly allocated partition of the dataset into 5 divisions. The best scoring model is the one with lowest mean cross-validation error.

Figure 3.8 shows results of our sweep on Figure 3.7’s dataset, and Figure 3.9 shows the resulting Tabular model (omitting trivial nominal tables of unique values). We graph cross-validation errors of other numbers of clusters as different from the calculated optimal number of clusters: 5 for users and 4 for movies. The \textit{user} line holds \textit{title} constant at its calculated optimal number of clusters and vice versa.

The numbers of clusters are optimal for predicting ratings. They are not necessarily optimal for predicting age, gender, category or year because we do not include prediction error from these columns in our RMSE plots. To include additional column prediction error in our calculation, we would have to define weights representing how much we care about one column’s error relative to others, similar to a utility function. Defining column weights becomes arbitrary, and so we arbitrarily chose weight one on rating and zero everywhere else.

3.4.4 Performance on Missing Data

To evaluate how well our ModelWizard implementation captures the concept behind InfernoDB, we create graphs of the same form as Figure 3 in [SG13]. The graphs
Figure 3.8: Cross-validation mean scores for locally varying numbers of clusters

Figure 3.9: Tabular model after Inferno and sweeping numbers of clusters
show model performance on predicting different columns with different numbers of randomly selected held out values. Unlike the previous section’s procedure to find the optimal number of clusters, we hold out values from all non-link columns: age and gender of a user, category and year of a movie, and rating. There are 125 data values to hold out.

Figure 3.10 shows the performance of the model derived from Inferno using the calculated optimal number of clusters (that is, optimal for predicting ratings). For each number of held out data points on the x-axis, we plot five independent rounds of predicting that many held out values. Each round may have different held out values, and for each we calculate RMSE. Viewing several independent rounds per x-axis value highlights RMSE variance depending on how entries fall into training and test sets. The original InfernoDB set similarly plots multiple rounds of predicting a given number of held out values, except that the number of rounds is not necessarily five; the classic InfernoDB test did not fix the number of rounds.

The ModelWizard version of InfernoDB has roughly equivalent performance as the original version at medium to high numbers of missing data cells. For low numbers of missing data cells, the ModelWizard version appears to perform worse. We are unsure why this is so. The cause could be structural, indicating that there is a major difference between the two versions of the InfernoDB algorithm such as using different numbers of clusters, or inconsequential, perhaps from miscopied data sources or a similar reason.

### 3.4.5 Alternatives

Matrix factorization is a popular alternative to cluster models for recommendation systems. In matrix factorization, each user and movie has a hidden vector of $d$ dimensions, where each dimension can be thought of as a trait. Compatibility between users
Figure 3.10: Inferno model performance comparison varying missing cell count
and movies is determined by the inner product of their trait vectors, resulting in a real-valued number which is shifted to the average rating. Traits of the same sign (in one dimension of the vector) contribute toward a higher rating and opposite-signed traits contribute toward a lower rating. Other models in the literature worth consideration are in the category of collaborative filtering; see [BHK98] for an overview.

Another alternative is to consider rating as an ordinal variable instead of a real-valued one. As in Section 3.3’s Internet plant sales application, this involves ordering ratings and inferring their latent threshold values that delineate and effectively discretize ratings.

As an alternative to Figure 3.7’s multi-table user-movie-ratings schema, the Inferno model also works for denormalized data for which we discover relationships in the dataset. For example, suppose we receive data in the form of Figure 3.11. We may use \texttt{ExactInfer} operations as in Section 3.3 to deduce a table schema that captures exact functional dependencies and then run \texttt{Inferno} on the resulting schema. The result is identical, and it shows how we may explore the space of dataset schemas while we explore the space of machine learning models in ModelWizard.
Chapter 4
Discussion

4.1 Addressing Big Data’s Challenges

A challenge to model construction is modern big data, often characterized by four components [EL13]:

- Volume: large dataset size
- Velocity: high rate of data acquisition, decreasing data value with time
- Veracity: data uncertainty
- Variety: multiple data sources, types and dimensions

Volume was not a consideration in ModelWizard’s initial design, as hinted from small to moderate dataset sizes in the Applications chapter. Luckily, there are many ways we imagine extending ModelWizard to better handle large datasets. A good starting point is adding additional data representations such as sparse data storage. Operating on data stored in a remote database instead of in-memory data could considerably increase scalability to large data. The Excel workbook data model already has the ability to accept remote database connections, which ModelWizard can tap into as it already does for data stored in spreadsheets as outlined in Section 2.7. We may leverage Excel’s remote database support by rewriting operations to build remote queries and updates, perhaps using SQL language, instead of transforming data in memory. Constraints on data map to database column constraints, and user-defined data transformation operations map to stored procedures executed by a SQL engine at the database. NoSQL and NewSQL databases [GHTC13] are
also in scope, though each additional database supported will require a separate set of drivers that operations interface with to access data—unless recent projects such as SQL++ [OPV14], D4M [KCGJ15], or the larger BigDawg proposal [DEK+15] succeed in providing a common language interface to many types of databases.

The shift in thinking is to construct a function that will check and modify data, throwing an exception for data that does not fit an operation rather than eagerly modify data. Viewing operations as database transactions additionally enables parallel execution of nonconflicting operations—that is, operations that do not modify the same part of Schema or Data as another operation that reads or modifies that part.

Sampling, lazy evaluation and background evaluation are further promising techniques that would help ModelWizard handle larger datasets. Instead of running data-transforming operations on a dataset right away, we could run operations on samples from a dataset to see a preview of how the operation will affect the entire dataset. The same principle holds for inference operations; one can gauge how well a model performs by running on a sample. After obtaining preliminary results, ModelWizard can start a background process to run the operation on larger and larger samples, up to the full dataset, asynchronously returning progressively more accurate estimations of an operation’s effect. This allows us to retain interactivity using quick estimations on samples, without losing correctness and accuracy when the user does not mind waiting.

ModelWizard script reuse will help in the case of many datasets with similar columns. A user may create a ModelWizard script that operates on one dataset and share that script with colleagues that have similar datasets, who can then apply the script with little to no change. It is easy to imagine libraries of ModelWizard scripts developed and downloaded for data scientists within and across organizations.
The first component of velocity, high rate of data acquisition, is outside ModelWizard’s scope. ModelWizard is designed to operate on fixed datasets with unknown structure rather than streaming data. A compromise is using ModelWizard to build a well-performing machine learning model for a fixed segment of streaming data on a development server, and then extract the machine learning model and implement it on a production server for streaming analysis. C# code for Tabular models built from ModelWizard is available through the Tabular GUI. Thus to reemphasize: ModelWizard is a tool for model exploration and construction, not for top-performance model deployment.

The second component of velocity, decreasing data value with time, is directly modelable. We can include the time a data value is recorded as itself another column in the dataset. For example, take the problem of object tracking with dataset columns position and time. If our goal is to infer the object’s position at time \( t \), position observations close to time \( t \) are valuable whereas position observations farther before or after time \( t \) yield decreasingly less information. We may account for time dependence in modeling by including time difference between observations in the variance of position difference between observations.

Veracity, the phenomena of data uncertainty, is also directly modelable. Including data accuracy and precision information as additional columns enables us to use those columns in probabilistic modeling. For example, we could imagine extending Section 1.2’s apple freefall example by including the imperfect mechanism by which we record apple elevations. Such an addition will not change the mean, most likely value of a predicted elevation (assuming the same mechanism records all data points), but it will return higher, more realistic variances. It also allows us to more strongly weigh sample rows that we have more confidence in, such as rows from using a higher precision measuring device.
ModelWizard handles data variety fairly well, especially heterogeneous data types. ModelWizard’s machine learning models operate on nominal, string-valued data, numeric data, and in the future, ordinal data. Multiple data sources are no problem as ModelWizard represents each with a separate table, from which we may create cross-table links.

High dimensional data is not a strong suit for ModelWizard. Imagine importing raw image processing data: a single megapixel image in truecolor (one row) will have a million columns, each with a 24-bit integer. Large numbers of columns are not ideal for manual analysis, though one could write ModelWizard operations to process them systematically. A better use case for interactive modeling with ModelWizard is after feature extraction and dimensionality reduction, when each column has an interpretable meaning to data analysts.

4.2 Extending Model Safety to Model Inferability

ModelWizard’s ValidState, ValidOp and OpMonad constructs guarantee a base level of model safety: every model constructed by ModelWizard has a valid Tabular counterpart and will pass Tabular’s type checking. Is it possible to extend model safety to guarantee that models constructed by ModelWizard are inferable, that is, can be run by the back-end inference engine to produce posterior distributions on parameters and missing values? Such a strong guarantee would enable data scientists to freely conjure models using the suite of operations available (respecting types so as not to throw exceptions), without worrying whether the model they construct will run.

The short answer is with great difficulty. Providing inferability guarantees is inherently specific to choice of inference engine. A formal proof requires modeling the syntax and semantics of a probabilistic program to prove that a certain subset
of programs are inferable by a particular inference engine, and then prove that ModelWizard operations will only generate programs (after Tabular compilation) within that inferable subset. All probabilistic programs are theoretically inferable, but different inference engine implementations will support some probabilistic program families more than others.

As a heuristic example derived from the author’s experience, Infer.NET’s expectation propagation algorithm performs more reliably for models with real-valued columns. Infer.NET’s variational message passing algorithm performs more reliably for models with discrete columns. Some models containing both real-valued and discrete columns are inferable by neither algorithm, a problem that surfaced during model exploration for Section 3.3’s Internet Plant Sales application. A chief cause of non-inferability is unimplemented message passing factors due to open research problems in variational inference.

4.3 Extending to Usable Interactivity

Many researchers believe usability is a key factor in the extent of success for probabilistic programming tools [Gor13]. To truly make incremental model construction accessible to data scientists, we imagine a GUI or IDE wrapping ModelWizard’s state, sketched in Figure 4.1. Regular users will find model exploration easier using a GUI, and “power users” who want to create custom operations may do so via script editing.

The GUI would show the currently constructed State, with the ability to zoom in on Tabular Schema and a preview or sample of Data. At the right, we envision a list of operations performed so far. The GUI may tag operations with a model score based on given scoring criteria, such as cross-validation on a particular column of interest. Model log evidence is a useful default.
The menu at the top of Figure 4.1 contains buttons that trigger operations, grouped by category such as “Typing” and “Base Models.” Right clicking on columns in the Schema or Data preview will list operations relevant to that column’s type. At a more advanced stage, we imagine suggesting operations based on common modeling paradigms learned from users modeling similar datasets.

A particularly powerful meta-feature is undo: the ability to roll back an operation and quickly try another one. One can implement undo by extending the OpMonad computation expression to include State monad functionality by tracking past states (or diffs between states) within the monad. Even in the current ModelWizard implementation, users could save intermediate states via ordinary F# let bindings, as demonstrated by state $s_1$ in Figure 3.1, after which performing undo is simply reusing saved state. Undo enables users can quickly try an operation, see whether it makes sense or is silly, and quickly proceed or rollback.

The idea for a ModelWizard GUI is inspired by Microsoft Power Query’s data transformation script editor [Web14] and Proof General’s Coq theorem proving script editor [Asp00]. Both editors lower the barrier for new users, raise situational awareness, and increase productivity while writing scripts. We wish the same for Model-

| Menu of Operations |
|--------------------|
| Current Tabular Schema | Operation History with Inference Performance Scores |
| Data Preview | |

Figure 4.1: ModelWizard GUI Sketch
Wizard users tackling model exploration.

In addition to visualization and interactive editing, a growing theme in systems design is to integrate the “whole machine learning pipeline” from data mining and enrichment to data cleaning and modeling into a common framework, as outlined in [MBGM14] to support the activities of data enthusiasts that do not have formal training in data science. We view ModelWizard as a forward step in creating such an integrated analytics framework, particularly in the combination of preprocessing with modeling. Much future work (or combination with existing tools) is needed to incorporate data enrichment and cleaning.

4.4 Interactive Theorem Proving Analogy

Model construction bears many similarities to theorem proving. Both benefit from interactivity as a happy medium between two extremes.

Manually proving theorems on pencil and paper requires expert knowledge and training to navigate the space of all possible proofs and formalize one that proves the theorem. The approach works as with manual model construction but at high labor cost, sometimes taking years of study in the proof’s domain.

Automatically proving theorems requires powerful algorithms. For example, the automated SMT solver Z3 [DMB08] succeeds for simple theorems but will fail for complex enough theorems due to the size of the space of all proofs. Automated model construction similarly fails in an unrestricted model space.

We aspire to use the design of interactive theorem provers as inspiration for interactive model construction. Imagine operations as model construction tactics, lower ones like ModelDiscrete akin to Coq’s rewrite tactic [BC04] and higher ones like ExactInfer akin to Isabelle’s sledgehammer tactic [PB10]. Like tactics, operations
may fail by throwing an exception and leaving state unchanged.

4.5 Conclusion

Probabilistic programs offer a universal space to create machine learning models for a dataset. ModelWizard presents a new take on constructing machine learning models, focusing on iterative construction one-to-one with model exploration, rather than traditional specification of a probabilistic program entirely at once.

Our primary contribution is planting the seeds for an interactive framework, applicable to any language and inference engine, to view data transformation and machine learning models in terms of composable building blocks we call operations, glued together by program code (F# in our case). In doing so we simultaneously realize realms of pre-processing, manual analysis, automated analysis and modeling itself. We further realize these realms in naturally familiar program structure such as conditionals, iteration, and procedural abstraction, along with opportunity for classic programming language boons such as static analysis, syntactic safety and compilation optimization.

We proffer ModelWizard as a solution scheme to three scientific goals: prediction, retained from inference on constructed machine learning models; understanding, built from model decomposition into understandable operations; and generalization, found through application of operations to new problems and domains. We postulate future work building on our framework’s principles will naturally integrate with and augment data scientists’ *modus operandi* to discover our world’s true structure.
A OpMonad Translation

As a demonstration for how let!, do! and other monadic syntax desugars into vanilla F# code, we present a simplified version of the derived operation TypeInferTable on the target table tmain, followed by its translation into an F# quotation that evaluates to a ValidOp<unit> value. The quotation includes calls to computation expression functions, defined in Code Listing 2.1 and bolded in the code below.

```fsharp
OPM {let! schema = GetSchema
   let! table = getSchemaTableByName schema "tmain"
   for col in table.columns do
     // infer each column's
     do! TypeInferColumn "tmain" col.name } // type in tmain

Quotations.Expr<ValidOp<unit>> =
Call (Some (Value (FSI_0008+OpMonad))), Delay,
Lambda (unitVar,
Call (Some (Value (FSI_0008+OpMonad))), Bind,
[PropertyGet (None, GetSchema, [])],
Lambda (_arg1,
Let (schema, _arg1,
Let (table,
Call (None, getSchemaTableByName,
  [schema, PropertyGet (None, "tmain", [])]),
Call (Some (Value (FSI_0008+OpMonad))), For,
  [Coerce (PropertyGet (Some (table),
    columns, []), IEnumerable`1),
Lambda (_arg2,
  Let (col, _arg2,
    Call (Some (Value (FSI_0008+OpMonad))),
    Bind,[Call (None,
      TypeInferColumn,
      [PropertyGet (None, "tmain", []),
      PropertyGet (Some (col), name, [])]),
Lambda (_arg3,
    Call(Some (Value (FSI_0008+OpMonad)),
    Return, [Value (<null>)]))]))]]))))))
```
B ModelWizard API of Primitive and Derived Operations

P stands for a Primitive operation; others are derived from primitives using \texttt{OpMonad}.

Excel-interfacing and “helper” operations are omitted.

Core bridge from \texttt{State} to F#:

\begin{verbatim}
///P: Return current state (schema, data); does not modify state
val GetState: ValidOp<State>
\end{verbatim}

Column typing:

\begin{verbatim}
///P: Change col’s type to real, ensuring data values are numeric
val TypeReal: TableName -> col:ColumnName -> ValidOp<unit>
///P: Change col’s type to upto(n), ensuring data are integer mod n
val TypeUpto: n: int -> TableName -> col:ColumnName -> ValidOp<unit>
///P: Create all-missing-value column. Return its name, guaranteed fresh
val NewColumn: TableName -> ColumnName -> NewColType -> ValidOp<ColumnName>
\end{verbatim}

Table management:

\begin{verbatim}
///P: Create a unique value table from clist; return new table name
val CreateTableUniques: TableName -> ColumnName list -> ValidOp<TableName>
///P: Transform fkt’s columns into ID references to pkt
val Link: pkt:TableName -> pktofkMap:(ColumnName*ColumnName) list
          -> fkt:TableName -> fklinkcol:ColumnName -> ValidOp<unit>
\end{verbatim}

Derived typing:

\begin{verbatim}
/// Create a new table of col’s unique values and link col to it
val TypeNominal: TableName -> col:ColumnName -> ValidOp<unit>
/// Examine col’s data to infer its type
val TypeInfer: TableName -> col:ColumnName -> ValidOp<unit>
/// TypeInfer each column in the table
val TypeInferTable: TableName -> ValidOp<unit>
\end{verbatim}

Base machine learning models:

\begin{verbatim}
///P: Place a \texttt{CGaussian} distr. on col, independent of other columns
val ModelGaussian: TableName -> col:ColumnName -> ValidOp<unit>
///P: Place a \texttt{CDiscrete} distr. on col, independent of other columns
val ModelDiscrete: TableName -> col:ColumnName -> ValidOp<unit>
/// Place an appropriate default model on a column based on its type
val Model: TableName -> col:ColumnName -> ValidOp<unit>
\end{verbatim}
Model coupling:

/// P: Use different distr. params on crng for each discrete cdom value
/// The list is for indexing across table links.
val Index: TableName -> crng:ColumnName -> cdom:ColumnName
    -> tableLinkList:ColumnName list -> ValidOp<unit>

/// P: Create linear dependence: crng (modeled Input) on cdom (typed real)
val LinReg: TableName-> crng:ColumnName-> cdom:ColumnName->ValidOp<unit>

/// P: Create quadr. dependence: crng (modeled Input) on cdom (typed real)
val QuadReg: TableName-> crng:ColumnName-> cdom:ColumnName->ValidOp<unit>

Derived machine learning models:

/// Construct Naive Bayes model taking 'free' columns of tn as features.
val NaiveBayes : tn:TableName -> className:ColumnName -> ValidOp<unit>

/// Construct Inferno clustering model, recursing on linked tables.
/// Return a list of column links and functions to modify # of clusters
val Inferno: TableName->ValidOp<(ColumnName list*(int->ValidOp<unit>)) list>

Exact functional dependencies:

/// P: If valid functional dependency, moves crng to cdom’s linked table
val Exact: TableName-> cdom:ColumnName-> crng:ColumnName->ValidOp<unit>

/// Find, capture & return columns exactly determined by the column list
val ExactInfer: TableName->domCols:ColumnName list->ValidOp<ColumnName list>

Inference:

/// Compile current state, run inference and return data log evidence
val ScoreLogEvidence: ValidOp<float>

/// Return average RMSE from k runs of cross-validation on a real column
val CrossValidate: TableName -> ColumnName -> k:int -> ValidOp<float>

/// Find best number of clusters using the modify-#-of-cluster functions
/// & scoring function, e.g. ScoreLogEvidence (higher scores better) or
/// CrossValidate (lower scores better). Returns plottable score data.
val SweepNumberClusters: clusterFun:(int->ValidOp<unit>) -> scoreFun:
    ValidOp<float> ->isHighBest:bool -> ValidOp<int*float* (int*float) list>

/// Run Cross Validation, holding out and scoring data in arbitrary
/// columns. Data held out ranges from 0 to all. Return scores averaged
/// numRepeats times, for each column, for each # of held out points.
val MissingDataAnalysis: colsHoldOut:(TableName*ColumnName) list
    -> colsScore:(TableName*ColumnName) list -> numRepeats:int
    -> ValidOp<Map<TableColumn,(int*float) list>
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