Toward Interactive Statistical Modeling

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Workshop on Automated Program Generation for Computational Science at ICCS 2010
The team

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Yale University
*programming languages, optimization*

Alexander Gray
Georgia Institute of Technology
*machine learning, optimization*

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Georgia Institute of Technology
*high-performance computing, linear algebra*
Statistics is everywhere

finance

astrophysics

EEG analysis

bioinformatics

retail demand prediction

computational chemistry
But the workflow is still mostly manual
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**Vision:** reduce development time while retaining correctness & efficiency.
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- **key ideas:** mechanization, type theory
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- **key contribution**: first rigorous symbolic formalization of statistics
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- **key contribution**: first rigorous symbolic formalization of statistics
Example: Modeling height data

Gaussian model

Height (cm)
Trying alternative statistical models

Formulation:

\[ X_i \sim \text{Normal}(\theta, 1) \]
\[ \hat{\theta} = \arg \max_{\theta} f(x \mid \theta) \]
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Solution: closed form

\[ \hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} x_i \]
Example: Modeling height data

mixture of Gaussians model

![Graph showing mixture of Gaussians model for height data.](image-url)
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Formulation:

\[ Z_i \sim \text{Bernoulli}(0.5) \]
\[ X_i \sim \text{Normal}((1 - Z_i)\theta_0 + Z_i\theta_1, 1) \]
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Solution: \textit{an EM algorithm (type of optimizer)}

\[(\hat{\theta}_0, \hat{\theta}_1) := \text{rand}();\]
while (…)
  for i = 1 to n do
    \[ \gamma_i := \frac{\phi(x_i; \hat{\theta}_1, 1)}{\phi(x_i; \hat{\theta}_0, 1) + \phi(x_i; \hat{\theta}_1, 1)} \]
    \[ \hat{\theta}_0 := \frac{\sum_{i=1}^{n} (1 - \gamma_i) \cdot x_i}{\sum_{i=1}^{n} (1 - \gamma_i)} \]
    \[ \hat{\theta}_1 := \frac{\sum_{i=1}^{n} \gamma_i \cdot x_i}{\sum_{i=1}^{n} \gamma_i} \]
  return \((\hat{\theta}_0, \hat{\theta}_1)\);
Trying alternative statistical models

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- Minor conceptual changes lead to vastly different algorithms.
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• Minor conceptual changes lead to vastly different algorithms.
• AutoBayes (2003) handles varying models for MLE/MAP – but there are many more possible axes of variation.
Idea: Let’s mechanize these derivations

**Goal:** declarative specification $\rightarrow$ executable code
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$\Rightarrow$ need a symbolic representation of statistics
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Goal: declarative specification $\rightarrow$ executable code

$\Rightarrow$ need a symbolic representation of statistics

Our approach

1. Rigorously defined mathematical language
   - enables stating statistical problems

2. Schemas – program transformations
   - embodiments of mathematical reformulations

3. Interactive algorithm assistant
   - enables exploring the space of correct solutions
Challenge 1: Statistics is big

Many types of mathematics

- probability, optimization, calculus, linear algebra, ...
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Computational aspects
- algorithms & datastructures
- numerical stability, robustness
- programming expertise and code tuning
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Myriad solution strategies
  - e.g., SVMs, EM, L2E, NMF, various optimizers, \ldots
  - domain-driven customizations
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⇒ Need an *expressive* symbolic representation of mathematics.
Challenge 2: Ensuring correctness

Expressive representation $\rightarrow$ easier to create nonsensical expressions

- especially true for mechanically generated expressions
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Many schemas $\rightarrow$ more chances for errors to sneak in
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Expressive representation → easier to create nonsensical expressions
  especially true for mechanically generated expressions

Many schemas → more chances for errors to sneak in

⇒ We use type theory to promote correctness.
The usual story: Types are a way to rule out ill-formed expressions.
Type Theory 101

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The bigger story: Type theory connects mathematics and computation.
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The bigger story: Type theory connects mathematics and computation.

1. Advanced type theories can be used to formalize mathematics.
   - an alternative to set theory
   - forms the basis of several modern theorem provers

2. These type theories have a computational interpretation.
   - Curry-Howard: type systems are logics
   - increased mathematical precision about programs
Language

\[ \text{language} = \text{syntax} + \text{type system} + \text{semantics} \]
language = syntax + type system + semantics

Core language

Optimization  Probability
Language: Core

\[ T ::= \text{Bool} \mid \text{Int} \mid \text{Real} \mid T_1 \times \ldots \times T_n \mid T_1 \rightarrow T_2 \]

\[ E ::= \text{true} \mid \text{false} \mid \neg E \mid E_1 \lor E_2 \mid E_1 \land E_2 \]
\[ \mid r \mid E_1 + E_2 \mid E_1 \ast E_2 \mid E_1^{E_2} \mid \log E \]
\[ \mid (E_1, \ldots, E_n) \mid E.k \]
\[ \mid \text{if } E_1 \text{ then } E_2 \text{ else } E_3 \mid E_1 = E_2 \mid E_1 \leq E_2 \]
\[ \mid x \mid \lambda x : T \cdot E \mid E_1 E_2 \mid \text{fix } E \]

- A typed lambda calculus + recursion.
\[
E \models \arg \max_{x_1: T_1, \ldots, x_n: T_n} \left\{ E_1 \mid E_2 \right\} \quad \text{optimization}
\]

- Full account: “Automating Mathematical Program Transformations” (Agarwal et al., PADL 2010).
Challenges in modeling continuous probability distributions

Continuous random variables arise naturally in numerous applications.
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- Computation and semantics are not as straightforward anymore.
  - weighted lists & summation vs. integration
  - We use symbolic reasoning.
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- Probability density functions now require more attention.
  - Mixed discrete-continuous densities require extra bookkeeping.
  - Not all distributions have a density.
  - We implement the necessary bookkeeping and restrictions.
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- Functions must be measurable.
  - Non-measurable functions are not constructible in our language.
$T \leftarrow \text{Prob } T$

$E \leftarrow \text{bernoulli } E \mid \text{normal } E_1 E_2 \mid \cdots$
\hspace{2cm} distributions
\hspace{2cm} singleton distribution
\hspace{2cm} random variables
\hspace{2cm} conditional distributions
\hspace{2cm} expectation
\hspace{2cm} density functions
\hspace{2cm} \\
\hspace{2cm} \text{return } E
\hspace{2cm} \text{var } x \sim E_1 \text{ in } E_2
\hspace{2cm} \text{condition } E_1 \text{ in } E_2
\hspace{2cm} \mathbb{E}_{x \sim E_1}(E_2)
\hspace{2cm} \text{pdf } E

- **Continuous random variables!** (e.g., Prob Real)
- Semantics in terms of measure theory.
Modeling example revisited

Recall the example from before:

\[ X_i \sim \text{Normal}(\theta, 1) \]
\[
\arg \max_{\theta} f(x \mid \theta)
\]
Modeling example revisited

Recall the example from before:

$$X_i \sim \text{Normal}(\theta, 1)$$

$$\arg \max_\theta f(x \mid \theta)$$

In our language:

```plaintext
let F \theta =
    var X_1 \sim \text{normal} \theta 1 \text{ in}
    var X_2 \sim \text{normal} \theta 1 \text{ in}
    var X_3 \sim \text{normal} \theta 1 \text{ in}
    return (X_1, X_2, X_3)

in

\arg \max_\theta \{ \text{pdf} (F \theta) (x_1, x_2, x_3) \mid \text{true} \}

\theta : \text{Real}
```
Modeling example revisited

Recall the example from before:

\[ X_i \sim \text{Normal}(\theta, 1) \]

\[ \arg \max_{\theta} f(x | \theta) \]

In our language:

\[
\text{let } F \theta = \begin{align*}
\var X_1 & \sim \text{normal } \theta 1 \text{ in} \\
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\var X_3 & \sim \text{normal } \theta 1 \text{ in} \\
\text{return } (X_1, X_2, X_3) \\
\end{align*}
\]

\[
\text{in} \begin{align*}
\arg \max_{\theta: \text{Real}} \{ \text{pdf} (F \theta) (x_1, x_2, x_3) | \text{true} \} \\
\end{align*}
\]

Mechanization requires a higher level of formalism.
Schemas

Logically: expression reformulation theorems

- example: $\forall a, b \in \mathbb{R}, \ a \ast b = 0 \iff a = 0 \lor b = 0$
Schemas

Logically: expression reformulation theorems

- example: $\forall a, b \in \mathbb{R}, \ a \ast b = 0 \iff a = 0 \lor b = 0$

Operationally: rewrite rules (implemented as OCaml functions)
Schemas

Logically: expression reformulation theorems
- example: $\forall a, b \in \mathbb{R}, a \cdot b = 0 \iff a = 0 \lor b = 0$

Operationally: rewrite rules (implemented as OCaml functions)

Current schema library contains 100+ schemas
- computer algebra
- propositional logic
- equation manipulation
- calculus
- optimization
- probability & statistics
The *Expectation-Maximization (EM)* schema

EM is widely used for maximum likelihood estimation (MLE).

- will require everything introduced so far
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\[
\arg \max_{\theta: \text{Real}} \text{pdf} \left( \begin{array}{c} \vdots \\
\end{array} \right) \times \rightarrow
\]
The *Expectation-Maximization (EM)* schema

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\[
\arg \max_{\theta: \text{Real}} \text{pdf} \left( \begin{array}{l}
\text{var } Z \sim F_Z \text{ in } \\
\text{var } X \sim F_X \text{ in } \\
\text{return } X
\end{array} \right) \times \rightarrow
\]
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\text{return } X
\end{array} \right) x \quad \rightarrow
\]

let rec loop \( \hat{\theta} = \\
\text{if } (...) \text{ then } \hat{\theta} \\
\text{else loop } \arg\max_{\theta: \text{Real}} \mathbb{E}_{z \sim C} (\log(\text{pdf } J (x, z)))
\in
\text{loop } \theta_0
\]
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if (...) then \(\boldsymbol{\hat{\theta}}\)

else loop \(\arg\max_{\theta: \text{Real}} \mathbb{E}_{Z \sim C}(\log(\text{pdf } J(x, z)))\)

in

loop \(\theta_0\)

\[
J = \left( \begin{array}{l}
\text{var } Z \sim F_Z \text{ in } \\
\text{var } X \sim F_X \text{ in } \\
\text{return } (X, Z)
\end{array} \right) \quad C' = \left( \begin{array}{l}
\text{var } Z \sim F_Z \text{ in } \\
\text{var } X \sim F_X \text{ in } \\
\text{condition } X = x \text{ in }
\text{return } Z
\end{array} \right) \quad C = C'[\theta := \boldsymbol{\hat{\theta}}]
\]
The *Expectation-Maximization (EM)* schema

EM is widely used for maximum likelihood estimation (MLE).

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\[
\text{arg max } \theta \left( \begin{array}{l}
v \text{ar } Z \sim F_Z \text{ in} \\
v \text{ar } X \sim F_X \text{ in} \\
r \text{eturn } X
\end{array} \right) \xrightarrow{\Rightarrow} \text{let rec loop } \hat{\theta} = \\
\quad \text{if } (...) \text{ then } \hat{\theta} \\
\quad \text{else loop } \text{arg max } \theta : \text{Real } E_{Z \sim C} \text{log(pdf } J(x, z))) \\
\quad \text{in} \\
\quad \text{loop } \theta_0
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Relies crucially on symbolic operations.
Interactive algorithm assistant

Features

- enter problems
- apply schemas
- undo/redo
- combinator

Status

- can solve several textbook examples of MLE, incl. via EM
- autotuning + more sophisticated code generation is planned

Come see me for a demo!
Conclusions

- The first symbolic formalization of statistics for freely expressing statistical problems and reformulations
  - type-theoretic formalization of probability & optimization
  - continuous probability distributions

- An implementation of the language & schemas
  - the Expectation-Maximization (EM) schema
  - interactive algorithm assistant

- Future plans include incorporating feedback
  - autotuning, high-performance code generation
  - model selection, causal inference
Thank you

Fin.