Application of Mathematical Components to probabilities and program formalization

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December 7, 2022

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This Talk

- We have been interested in applying formal verification to information security
- We have been led to look at topics such as information theory, error-correcting codes, probabilistic programs, etc.
- We would like to report on a few formal theories that might be of general interest
- The common topic is probability, the work spans several years
- Our message is that MATHCOMP has been providing us with a reliable environment for our experiments

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Information Theory using $\operatorname{MATHCOMP}$

Monadic Equational Reasoning for Probabilistic Programs

Formal Semantics for Statistical Modeling

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SSREFLECT Early Adopters?

- Starting in 2004, we were working on formal proof of imperative programs in CoQ using separation logic
- We were facing productivity issues that we failed to analyze correctly
- By chance, we ran into



and realized that many of our concerns were addressed by $\ensuremath{\mathrm{SSReFLeCT}}$

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SSReflect/MathComp in Japan

- 1. We have been trying to promote $\operatorname{MATHCOMP}$ in Japan with lectures
- 2. These lectures turned into a book in 2018



- 3. In this book, tactics are given mascots, e.g.:
 - 3.2 タクティク move=>, move:, move: =>, move/ タクティク move=>, move:はサブゴールとコンテキスト

■の型・変数・関数などを移動します(→表 3.2).



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The SSREFLECT Zoo According to

move



rewrite

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case



apply







Outline

Information Theory using $\operatorname{MATHCOMP}$

Monadic Equational Reasoning for Probabilistic Programs

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Formal Semantics for Statistical Modeling

Fundamental Questions Answered Information Theory

- 1. What is the ultimate data compression rate¹?
- 2. What is the ultimate encoding $rate^2$ for communication?

Setting:

- a source is a probability distribution
- a channel is a stochastic matrix
 (e.g., the binary symmetric channel ^{1-p}
 ^p
 ^{1-p}
 ¹⁻

Shannon answered the fundamental questions in 1948:

- 1. Source coding theorem: One cannot minimize the compression rate below the *entropy*
- 2. Channel coding theorem: One cannot maximize the encoding rate beyond the *capacity* of a channel

¹compressed bitstring size / original message size

²original message size / encoded message size

Information Theory: Basic Definitions [CT01]

- The entropy of a random variable taking *n* values with probabilities p_i is $H = -\sum_{i=0}^{n-1} p_i \log p_i$
- Given two probability mass functions p and q, the divergence is $D(p||q) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}$
- The mutual information between two random variables X, Y with joint probability mass function p(x, y) and marginals p(x) and p(y) is I(X; Y) = D(p(x, y)||p(x)p(y))
- Consider an input X and an output Y. A channel is a conditional probability distribution p_{Y|X}(y|x). The capacity is C = max_{p(x)} I(X; Y), p(x) ranging over all the input distributions

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 \Rightarrow It looks like a good fit for $\mathrm{SSReFLECT}$'s iterated operators [BGBP08]

Finite Probabilities with SSREFLECT and COQ (We are in 2009)

Finite probability theory with the iterated operators and the finite sets of MATHCOMP and the real numbers of COQ:

Distributions over a finite type:

Record fdist (A : finType) := mk {
 f :> A ->R+ ;
 _ : \sum_(a in A) f a == 1 :> R }.

- Probability of an event E given a distribution P: Definition Pr P (E : {set A}) := \sum_(a in E) P a.
- Random variables:

Definition RV U T (P : fdist U) := U -> T.

Distribution of a random variable X: `Pr[X = a], shortcut for Pr P (X @^-1: [set a]) or for fdistmap X P a

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Information Theory with MATHCOMP

Starting from:

- H = -∑_{i=0}ⁿ⁻¹ p_i log p_i
 Definition entropy := \sum_(a in A) P a * log (P a).

 ∑_{x∈X} p(x) log $\frac{p(x)}{q(x)}$ Definition div := \sum_(a in A) P a * log (P a / Q a).

 D(p(x, y) || p(x) p(y))
 - Definition mutual_info := D(PQ || PQ¹ x PQ²).

We completely formalized an introductory textbook to information theory:

- Šhannon's theorems [AH12, AHS14]
- Error-correcting codes (Hamming, BCH, Reed-Solomon, LDPC) [AG15, AGS20b]
- Presentations to information theorists [OHA14, AGS16, AGS18]

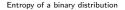


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Convexity of Information-theoretic Definitions Statements from [CT01]

Theorem H(p) is a concave function of p.





Theorem

D(p||q) is convex in the pair (p,q), i.e., if (p_1,q_1) and (p_2,q_2) are pairs of probability mass functions, then

$$D(\lambda p_1 + (1-\lambda)p_2 \|\lambda q_1 + (1-\lambda)q_2) \leq \lambda D(p_1\|q_1) + (1-\lambda)D(p_2\|q_2)$$

for all $0 \le \lambda \le 1$.

Theorem

Let $(X, Y) \sim p(x, y) = p(x)p(y|x)$. The mutual information I(X; Y) is a concave function of p(x) for fixed p(y|x) and a convex function of p(y|x) for fixed p(x).

Convex Space

A convex space is a carrier together with a family of binary operators $a \triangleleft p \triangleright b$ with $0 \le p \le 1$ such that [Sto49, Fri09]:

• $a \triangleleft p \triangleright a = a$ (idempotence)

•
$$a \triangleleft p \triangleright b = b \triangleleft 1 - p \triangleright a$$
 (skewed commutativity)

▶ $a \triangleleft p \triangleright (b \triangleleft q \triangleright b) = (a \triangleleft r \triangleright b) \triangleleft s \triangleright c$ (quasi-associativity) with $s = \overline{p}\overline{q}$ and $r = \frac{p}{s}$ (where $\overline{x} = 1 - x$)

Examples: real numbers (pa + (1 - p)b), functions to a convex space, finite distributions, etc.

Allows for generic definitions (U convex space, V ordered convex space):

- $f: U \to U'$ is affine $\stackrel{def}{=} \forall a, b, 0 \le p \le 1, f(a \lhd p \triangleright b) = f(a) \lhd p \triangleright f(b)$
- $f: U \to V$ is convex $\stackrel{def}{=} \forall a, b, 0 \le p \le 1, f(a \lhd p \rhd b) \le f(a) \lhd p \rhd f(b)$
- also convex sets and hulls

Convex Space in MATHCOMP

Conveniently defined using HIERARCHY-BUILDER [CST20]:

1. Declare an interface:

HB.mixin Record isConvexSpace (T : Type) := {
 _ <| _ |> _ : forall p, T -> T -> T ;
 conv1 : forall a b, a <| 1%:pr |> b = a ;
 convm : forall p a, a <| p |> a = a ;
 convC : forall p a b, a <| p |> b = b <| p.~%:pr |> a;
 convA : forall (p q : prob) (a b c : T),
 a <| p |> (b <| q |> c) =
 (a <| [r_of p, q] |> b) <| [s_of p, q] |> c }.

2. Declare a structure:

```
#[short(type=convType)]
HB.structure Definition ConvexSpace := {T of isConvexSpace T }.
```

 Build instances: any lmodType (and thus real numbers), the type "fdist A", the type "A -> fdist B", etc. Application of Convex Spaces to Information Theory

- Short statements for convexity properties of information theoretic definitions:
 - Lemma entropy_concave : concave_function (fun P : fdist A => `H P).

Lemma mutual_information_concave W :
 concave_function (fun P => mutual_info (P `X W)).

where P X W is the product distribution $\lambda(x, y) \cdot P x \cdot W \times y$

Lemma mutual_information_convex P : convex_function (fun W : A -> fdist B => mutual info (P `X W)).

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Real Cones

A practical tool to reason about convexity

- In a convex space, quasi-associativity and skewed commutativity make for cumbersome symbolic computations
- It is actually possible to transpose such computations into real cones where addition is commutative and associative [VW06]:

```
HB.mixin Record isQuasiRealCone A := {
   addpt : A -> A -> A ;
   zero : A ;
   addptC : commutative addpt ;
   addptA : associative addpt ;
   addpt0 : right_id zero addpt ;
   scalept : R -> A -> A ;
   scaleopt : forall x, scalept 0 x = zero ;
   scaleopt : forall x, scalept 1 x = x ;
   scaleoptDr : forall r, {morph scalept r : x y / addpt x y >-> addpt x y}
   scaleptA : forall p q x, 0 <= p -> 0 <= q ->
      scaleopt p (scalept q x) = scaleopt (p * q) x }.
```

From Convex Spaces to Real Cones

Consider the following inductive type:

Inductive scaled (A : Type) := Scaled of Rpos & A | Zero.

When A is a convex space:

- ▶ scaled A can be equipped with a real cone structure (take addpt (Scaled r x) (Scaled q y) to be (r + q)(x ⊲ r/(r+q) ⊳ y))
- > scaled A can be equipped with a convex space structure (take x ⊲ p ▷ y to be addpt (scalept p x) (scalept (1 - p) y) [VW06])

We can transpose symbolic computations using the fact that Scaled 1 is injective and affine:

- ▶ a <|p|> b
 - \rightarrow Scaled 1 a <|p|> Scaled 1 b
 - \rightarrow addpt (scalept p (Scaled 1 a)) (scalept (1 p) (Scaled 1 b)) where addition is associative and commutative

See $\operatorname{INFOTHEO}$ online or [AGS20a] for details



Information Theory using MATHCOMP

Monadic Equational Reasoning for Probabilistic Programs

Formal Semantics for Statistical Modeling

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Monadic Equational Reasoning

This is an approach to verify programs with effects using equational reasoning [GH11]

- effects are represented by monad interfaces with typically:
 - ▶ an operator (failure, arbitrary choice, probabilistic choice, etc.)
 - rewriting laws in the form of equations
- monad interfaces can inherit from other interfaces and can be combined

Our starting idea:

build a hierarchy of interfaces using packed classes [GGMR09]

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use SSREFLECT's rewrite [GT12] to perform equational reasoning

Example of Monadic Laws

Monad laws (two operators: $ret(\cdot)$ and $\cdot \gg \cdot$):

1. $ret(a) \gg f = f a$ (left neutral)2. $m \gg (\lambda x. ret(x)) = m$ (right neutral)3. $(m \gg f) \gg g = m \gg (\lambda x. f x \gg g)$ (associativity)Arbitrary choice (one operator: $\cdot \Box \cdot$):(associativity)1. $(m_1 \Box m_2) \Box m_3 = m_1 \Box (m_2 \Box m_3)$ (associativity)2. $(m_1 \Box m_2) \gg k = (m_1 \gg k) \Box (m_2 \gg k)$

(left-distributivity of bind w.r.t. arbitrary choice)

etc.

Functors and Monads with HIERARCHY-BUILDER

- We consider COQ's Type to be the category Set of sets and functions [TJ16]
- Let us start with functors:
 - action on objects: F : Type -> Type (carrier)
 - action on morphisms: actm below

```
HB.mixin Record isFunctor (F : Type -> Type) := {
    actm : forall A B, (A -> B) -> F A -> F B;
    functor_id : FunctorLaws.id actm ;
    functor_o : FunctorLaws.comp actm }.
```

Next, monads (ret/bind interface):

```
HB.factory Record isMonad_ret_bind (F : Type -> Type) := {
  ret' : forall A, A -> F A ;
  bind : forall A B, F A -> (A -> F B) -> F B ;
  bindretf : BindLaws.left_neutral bind ret' ;
  bindmret : BindLaws.right_neutral bind ret' ;
  bindA : BindLaws.associative bind }.
```

The Interface of the Probability Monad

Probability monad:

- extends the type of Monad
- similar interface to convex spaces
- with left-distributivity of bind w.r.t. probabilistic choice

```
HB.mixin Record isMonadProb (M : Type -> Type) of Monad M := {
    _ <| _ |> _ : forall p T, M T -> M T -> M T;
    choice0 : forall T a b, a <| 0 |> b = b;
    choiceC : forall T p a b, a <| p |> b = b <| 1 - p |> a;
    choiceA : forall T p q r s a b c,
        p = r * s -> 1 - s = (1 - p) * (1 - q) ->
        a <| p |> (b <| q |> c) = (a <| r |> b) <| s |> c;
    choice_bindDl : forall p a b,
        (a <| p |> b) >>= f = (a >>= f) <| p |> (b >>= f) }.
```

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Model of the Probability Monad

The interface do have an implementation

- Finite distributions do not form a monad because fdist : finType -> Type is not an endofunction
- Hence finitely-supported distributions with finmap [CS15]: Record fsdist (A : choiceType) := mk { f :> {fsfun A -> R with 0} ; _ : all (fun x => 0 <b f x) (finsupp f) && \sum_(a <- finsupp f) f a == 1}.</pre>
- The required operators $(ret(\cdot), \cdot \gg \cdot, \cdot \triangleleft \cdot \triangleright \cdot)$:
 - fsdist1 : forall A : choiceType, A -> {dist A}
 def
 [fsfun b in [fset a] => 1 | 0]
 - fsdistbind : forall A B : choiceType,
 {dist A} -> (A -> {dist B}) -> {dist B}

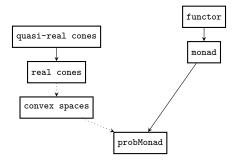
$$\stackrel{\text{def}}{=} \lambda b. \sum_{a \in \text{supp}(d)} d(a) \times (f(a))(b) \text{ over } \bigcup_{x \in f(\text{supp}(d))} \text{supp}(x)$$

$$\bullet \text{ fsdist_conv : forall } A : \text{ choiceType},$$

prob -> {dist A} -> {dist A} -> {dist A}

 $\stackrel{def}{=} \lambda a.p d_1(a) + (1-p) d_2(a) \text{ over } \operatorname{supp}(d_1) \cup \operatorname{supp}(d_2)$

The Start of a Hierarchy of Effects



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Solid arrow: inherits Dotted arrow: uses

Probabilistic Program Verification using Rewriting

```
A biased coin with probability p:
Definition bcoin {M : probMonad} p : M bool := Ret T < | p |> Ret F.
Simple statement:
Definition two_coins p q : M (bool * bool) :=
  do a <- bcoin p; do b <- bcoin q; Ret (a, b).
Lemma two_coinsE p q : two_coins p q = two_coins q p.
Proof:
rewrite /two coins /bcoin.
  (\text{Ret } T < |p| > \text{Ret } F) >>=
  (fun a \Rightarrow (Ret T < |q| > Ret F) >>= (fun b \Rightarrow Ret (a, b)))
rewrite ![in LHS](choice bindDl,bindretf).
  (* choice_bindDl -> probability monad law *)
  (* bindret f = ret x \ge f = f x \longrightarrow monad law *)
  (\text{Ret } (T, T) < |q| > \text{Ret } (T, F)) < |p| > (\text{Ret } (F, T) < |q| > \text{Ret } (F, F))
rewrite -choiceACA.
  (* interchange > </g> -> real cones *)
  (\text{Ret} (T, T) < |p| > \text{Ret} (T, F)) < |q| > (\text{Ret} (F, T) < |p| > \text{Ret} (F, F))
```

Examples Formalized with The MONAE Library



- tree relabeling [GH11], Spark aggregation [Mu19b], Monty-Hall problem [GH11, Gib12]
- n-queens [GH11], completed by [Mu19a] (we fixed an earlier version of the latter)
- quicksort [MC20] (we completed a pre-existing formalization in Agda)
- Jaskelioff's theory of modular monad transformers [Jas09] (we actually proposed a fix for this theory)

Experiments documented in the following papers [ANS19, AN21, AGNS21, SA22]

Combination of Monad Interfaces Can be Difficult

It was observed in [ASCG16] that [GH11] contains a mistake³:

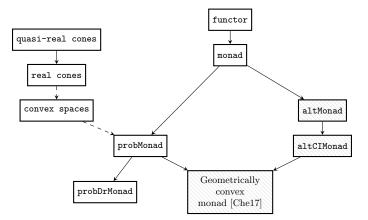
- right-distributivity of bind over probabilistic choice
 m ≫ λx.(kx ⊲ p ▷ k'x) = (m ≫ k) ⊲ p ▷ (m ≫ k')
 combined with
- distributivity of probabilistic choice over arbitrary choice
 m ⊲ p ▷ (a □ b) = (m ⊲ p ▷ a) □ (m ⊲ p ▷ b)

result in a degenerated theory:

- distributivity of arbitrary choice over probabilistic choice
 m□ (a ⊲ p ▷ b) = (m□ a) ⊲ p ▷ (m□ b)
- which implies a ⊲ p ▷ b = a ⊲ q ▷ b for all p, q ∈]0;1[
 [KP17, Thm A.3]
- \Rightarrow It is important to provide implementations for interfaces

³We checked with MONAE that [GH11] was not relying on this mistake. 📱 🥠

Hierarchy of Effects (cont'd)



The probDrMonad adds:

•
$$m \gg \lambda x.(k x \triangleleft p \triangleright k' x) = (m \gg k) \triangleleft p \triangleright (m \gg k')$$

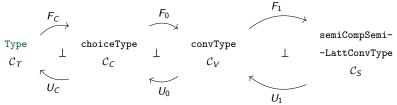
The geometrically convex monad adds:

Model of the Geometrically Convex Monad

What is a computation in this monad?

- Gibbons observes that it should be a convex-closed sets of probability distributions [Gib12]
- Cheung provides a construction using adjunctions between categories [Che17]

We formalized Cheung's construction [AGNS21]:



This relies on an extension of MONAE with *concrete categories* (to go beyond **Set**)

Ask Takafumi here in this room! \rightarrow

Outline

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Formal Semantics for Statistical Modeling

Statistical Model as Probabilistic Programs

 Example: guessing whether or not today's a weekday by looking at the number of buses passing by [Sta20]

```
normalize (
   let x = sample (bernoulli (2 / 7)) in
   let r = if x then 3 else 10 in
   let _ = score (r ^ 4 / 4! * e ^ (- r)) in
   return x)
```

- Intuitive explanation:
 - sample takes a probability measure
 - normalize returns a probability measure
 - score (f x) means that we observe x from the distribution corresponding to the density f

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- here, observe 4 from the Poisson distribution (of density $\frac{r^k}{k!}e^{-r}$)
- Problem: existing formalizations in COQ use axioms [HcS19, ZA22]

Formalization of Kernels using $\operatorname{MathCOMP-Analysis}$

Staton proposed a semantics for programs with sampling, scoring, and normalization using *s*-finite kernels [Sta17] Definition:

- A kernel $X \rightsquigarrow Y$ is a function $k : X \to \Sigma_Y \to [0, \infty]$ such that
 - 1. for all x, kx is a measure
 - 2. for all measurable set $U, x \mapsto k \times U$ is measurable

Reminder: measure theory	in	MATHCOMP-ANALYSIS	[AC22]
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measurable spaces	type measurableType
measure	type {measure set T -> $\ R$ }
measurable functions	predicate measurable_fun

Formal definition of kernel (notation R.-ker X ~> Y):

HB.mixin Record isKernel

```
X Y R (k : X -> {measure set Y -> bar R} :=
```

{ measurable_kernel :

forall U, measurable U -> measurable_fun setT (fun x => k x U) }.

S-Finite and Finite Kernels

A circular-looking definition

Definition:

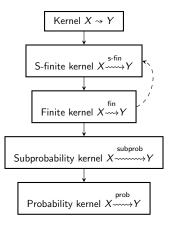
- A kernel k : X → Y is finite when ∃r s.t. ∀x, kxY < r (uniformly upper bounded)
- A kernel k is s-finite when there exists a sequence of finite kernels s such that k = ∑_{i=0}[∞] s_i

Circularity?

- s-finite kernels are more general than finite kernels (so they should be defined first)
- finite kernels are needed to define s-finite kernels...

Wanted: Hierarchy of Kernels

To implement Staton's semantics of probabilistic programs



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S-Finite and Finite Kernels

A recipe using HIERARCHY-BUILDER

1. Interface for s-finite kernels using a predicate for finite kernels:

```
HB.mixin Record Kernel_isSFinite_subdef
X Y R (k : X -> {measure set Y -> \bar R}) := {
    sfinite_subdef : exists2 s : (R.-ker X ~> Y)^nat,
    forall n, measure_fam_uub (s n) &
    forall x U, measurable U -> k x U = kseries s x U }.
```

```
Notation: R.-sfker X ~> Y, inherits from R.-ker X ~> Y
```

2. Interface for finite kernels:

```
HB.mixin Record SFiniteKernel_isFinite
X Y R (k : X -> {measure set Y -> \bar R}) :=
{ measure_uub : measure_fam_uub k }.
```

Notation: R.-fker X ~> Y, inherits from R.-sfker X ~> X

3. Definitive interface for s-finite kernels:

```
HB.factory Record Kernel_isSFinite
X Y R (k : X -> {measure set Y -> \bar R})
of isKernel _ _ _ _ k := {
sfinite : exists s : (R.-fker X ~> Y)^nat,
forall x U, measurable U -> k x U = kseries s x U }.
```

Composition of S-finite Kernels

The main property of s-finite kernels is that they are stable by composition (this provides a semantics for let x := e in e')

Given *l* : X → Y and *k* : X × Y → Z, the composition *l*; *k* is defined by

$$\lambda x U. \int_{y} k(x, y) U(\mathbf{d} / x)$$

- Reminder: integral theory in MATHCOMP-ANALYSIS [AC22] $\int_{x \in A} f(x)(\mathbf{d}\,\mu) \quad [\operatorname{mu}]_{(x \text{ in } A) \ f \ x}$
- Formal definition of composition:

Definition kcomp l k x U := $int[l x]_y k (x, y) U.$

Staton proved that the composition of s-finite kernels is a s-finite kernel [Sta17]. He skipped the proof that it is a kernel. It is not trivial but it can be achieved it by adapting existing lemmas from Fubini's theorem available in MATHCOMP-ANALYSIS.

Semantics of Sampling using S-finite Kernels

For illustration

What is the semantics of sample (bernoulli (2 / 7))?

- 1. Build the measurable space of probability measures pprobability Y R $\,$
 - generated from the set of probability measures μ such that $\mu(U) < r$ for all measurable sets U and $0 \le r \le 1$
 - The type X -> pprobability Y R is essentially X -> {measure set Y -> \bar R}
- 2. P : X -> pprobability Y R is a kernel
 - for any measurable set U, fun x => P x U is measurable
- 3. P : X \rightarrow pprobability Y R is a probability kernel
 - because for all x, P x setT = 1
 - it is therefore automatically a s-finite kernel
- 4. For our example, take for P the (constant) Bernoulli probability measure (built out of Dirac measures)

Staton's Buses in Coq

```
normalize (
   let x = sample (bernoulli (2 / 7)) in
   let r = if x then 3 else 10 in
   let _ = score (r ^ 4 / 4! * e ^ (- r)) in
   return x)
```

₽

```
Definition kstaton_bus : R.-sfker T ~> mbool :=
  letin (sample (bernoulli p27))
  (letin
      (letin (ite var2of2 (ret k3) (ret k10))
      (score (measurable_fun_comp mh var3of3)))
      (ret var2of3)).
  (* NB: density function parameterized,
            "De Bruijn indices" for variables *)
Definition staton_bus := normalize kstaton_bus.
```

Symbolic Evaluation of Statistical Models

We can evaluate a model to a distribution:

Lemma staton_busE P (t : R) U :
 let N := ((2 / 7) * poisson4 3 + (5 / 7) * poisson4 10)%R in
 staton_bus mpoisson4 P t U =
 ((2 / 7)%:E * (poisson4 3)%:E * \d_true U +
 (5 / 7)%:E * (poisson4 10)%:E * \d_false U) * N^-1%:E.

(Proof by rewriting) In mathematical notation:

$$\frac{\frac{2}{7}\frac{3^4}{4!}e^{-3}}{N}\delta_1 + \frac{\frac{5}{7}\frac{10^4}{4!}e^{-10}}{N}\delta_0 = 0.780369\delta_1 + 0.219631\delta_0$$

So it is more likely that we are in the weekend

Commutativity Property of Probabilistic Programs

The main motivation for Staton's work

Is the following program transformation correct?

let x :=	t in	\leftrightarrow	let y	:= u in	L
<pre>let y :=</pre>	u in		let x	:= t in	L
ret (x, y	y)		ret (x, y)	

This is a consequence of Tonelli-Fubini's theorem for *s*-*finite measures*:

```
(* f measurable non-negative, m1, m2 s-finite *)
Lemma sfinite_fubini :
    \int[m1]_x \int[m2]_y f (x, y) =
    \int[m2]_y \int[m1]_x f (x, y).
```

(This is a consequence of Tonelli-Fubini's theorem for σ -finite measures—the one you find in a standard undergraduate textbook on integration).

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Conclusion

The $\operatorname{MathCOMP}$ project has been providing us with

- good tactic support (e.g., rewrite in monadic equational reasoning)
- a rich, stable, flexible framework (we could combine MATHCOMP and the COQ standard library)

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- libraries (finmap, MATHCOMP-ANALYSIS)
- methodologies (packed classes, naming conventions)
- tools (HIERARCHY-BUILDER)

which let us

- develop original formalizations (INFOTHEO, MONAE)
- develop libraries for (probabilistic) program verification
- fix existing pencil-and-paper proofs
- retrofit results to MATHCOMP (in particular MATHCOMP-ANALYSIS)

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