#### Probabilistic Programming from the Ground Up

Lecture 2: Conditioning, sampling

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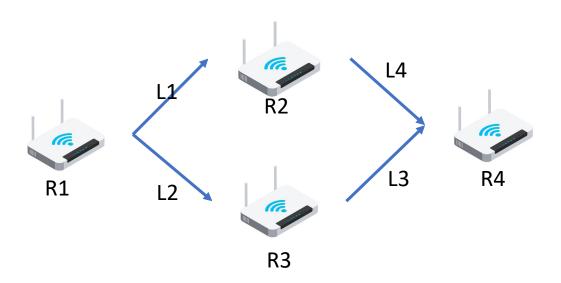
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https://www.khoury.northeastern.edu/home/sholtzen/oplss24-ppl/





#### TinyPPL Exercise: Network Reliability



#### Suppose:

- each link fails independently with probably 1/50
- each router chooses which router to forward an incoming packet to with uniform probability.

#### Network reliability

# TinyCond

Bayesian conditioning and observation

## What is conditioning

- Conditioning updates your beliefs about the world given observations
- Classic example: medical diagnosis
- Your COVID-19 test comes back positive. Does that mean you have COVID?
  - Not necessarily!
  - The probability that you have COVID should go up, but by how much? This depends on the test, prevalence of COVID, etc.

# COVID Test Motivating Example

- Query: What is the probability that I have COVID given the test came back positive?
- Required data:
  - True positive probability: the probability that the test will be positive if you do have COVID

$$Pr(Test = T \mid Covid = T) = 0.99$$

 False positive probability: the probability that the test will be positive if you do not have COVID

$$Pr(Test = T \mid Covid = F) = 0.05$$

Latent rate: the probability that an average person has COVID

$$Pr(Covid = T) = 0.01$$

Possible worlds

Check that probability of all worlds sums to 1

COVID	Test	Pr(COVID, Test)
Т	Т	0.01*0.99=0.0099
Т	F	0.01*0.01=0.0001
F	Т	0.99*0.05=0.0495
F	F	0.99*0.95=0.9405

# Possible worlds after conditioning on Test = T

COVID	Test	
Т	Т	0.0099
Т	F	0
F	Т	0.0495
F	F	0

Called *unnormalized probability distribution*, since it does not sum to 1.

# Possible worlds after renormalizing (Bayes's Rule)

COVID	Test	Pr(Test   Covid = True)
Т	T	0.0099/(0.0099+0.0495)=0.1666666
Т	F	0.0001
F	Т	0.0495/(0.0099+0.0495)=0.8333333
F	F	0.9405

Note: Even though the test came back positive, it is still more likely that we do not have COVID!

Probability can be surprisingly unintuitive.

# Modeling the COVID Diagnosis Scenario in a PPL

#### TinyCond Grammar

#### Pure computations

```
::=
    | <ident>
    | true
    | false
    | if  then  else 
    |  && 
    |  || 
    | !
```

#### **Probabilistic computations**

```
<e> ::=
    | flip <float>
    | <id> <- <e>; <e>
    | observe <e>; <e>
    | return
```

# Semantics of TinyCond

• Unnormalized semantics: denoted  $\|\mathbf{e}\|_U$  essentially the same as TinyPPL, but with added rule for observe:

$$[\![\text{observe }e_1;e_2]\!]_U(\rho)(v) = \begin{cases} [\![e_2]\!](\rho)(v) & \text{ if } [\![e_1]\!](\rho) = \text{true} \\ 0 & \text{otherwise}. \end{cases}$$

 Simply assigns probability 0 to all executions that do not satisfy the observation.

#### Normalized semantics

• Then, we can compute the normalized semantics from the unnormalized semantics:

$$\llbracket \mathbf{e} \rrbracket(\rho)(v) = \frac{\llbracket \mathbf{e} \rrbracket(\rho)(v)}{\llbracket \mathbf{e} \rrbracket(\rho)(\mathtt{tt}) + \llbracket \mathbf{e} \rrbracket(\rho)(\mathtt{ff})}$$

# Example Semantics of TinyCond

$$\begin{bmatrix} x & <- & \text{flip } 1/2; \\ y & <- & \text{flip } 1/2; \\ \text{observe } x & || & y; \\ \text{return } x \end{bmatrix} (ff) = \frac{1}{4}$$

To keep the code concise, we added in an effectful if

#### Bayesian Learning

- Suppose I want to learn whether a coin is biased
  - If it's biased, then it lands heads with probability 0.9
- Initially you think there is a 50% chance the coin is biased; this is called your prior
- You observe three coin outcomes, True, True, False. Now you want to know the **posterior** probability of whether the coin is biased.

```
biased <- flip 0.5;
flip1 <- if biased then flip 0.9 else flip 0.5;
observe flip1;
flip2 <- if biased then flip 0.9 else flip 0.5;
observe flip2;
flip3 <- if biased then flip 0.9 else flip 0.5;
observe flip3;
return biased</pre>
```

# Non-locality of Conditioning

```
x <- flip 0.5;
y <- flip 0.5;
observe x || y;
return x</pre>
x <- flip 0.6666;
y <- flip 0.6666;
return x</pre>
```

Semantically, observation "reaches back in time" to affect previous probabilistic operations in the program!

# Sampling semantics

#### Context

 Last time we discussed semantics and modeling in TinyPPL and TinySamp

We gave small implementations of both these languages

 Problem: These implementations were inefficient and inexpressive

# Challenge 1: Scalability

 What is the probability that this program returns true?

```
let big program = tinyppl e of string
  "(bind x (flip 0.5)
   (bind x (flip 0.5)
  (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
  (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (bind x (flip 0.5)
   (return x))))))))))))))))))"
```

Takes a long time to compute for TinyCond and TinyPPL, even though we can easily see it's 0.5

## Challenge 2: Expressivity

• TinyPPL and TinyCond are quite restrictive languages: very few language features.

Limits ability to model realistic scenarios

#### Direct Sampling Semantics

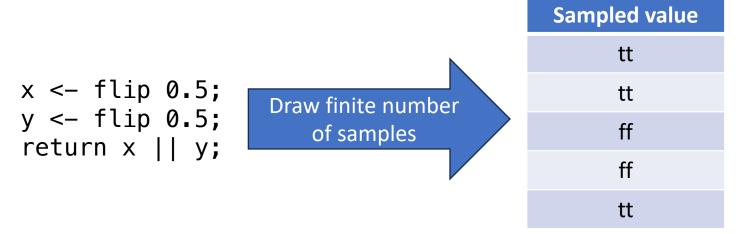
- Simple intuition: sample all probabilistic quantities as they are encountered
  - Then you're left with a pure program you can run with standard semantics

```
x \leftarrow flip 0.5; x \leftarrow return true; x \leftarrow return true; y \leftarrow flip 0.5; \rightarrow y \leftarrow return false; return x \mid \mid y; return x \mid \mid y; return true \mid \mid false;
```

**↓** 

#### Approximation Semantics Intuition

 We can approximate the semantics of a program by drawing many samples



 Suppose we draw the above 5 samples; then we would conclude that program outputs T with probability approximately 3/5

#### Expectations

- Let  $Pr: \Omega \to [0,1]$  be a **probability distribution** on a set  $\Omega$  (we will assume countable sets)
  - Required that  $\sum_{\omega \in \Omega} \Pr(\omega) = 1$ .
- A **random variable** is a map out of the sample space; we will assume it is real-valued  $f: \Omega \to real$
- Then, the expectation of f with respect to Pr is defined as:

$$\mathbf{E}_{\Pr}[f] = \sum_{\omega \in \Omega} \Pr(\omega) f(\omega).$$

## Law of large numbers

A few different theorems of the general shape:

$$\mathbf{E}_{\Pr}[f] = \lim_{N o \infty} rac{1}{N} \sum_{\omega_i \sim \Pr}^{N} f(\omega_i).$$

This notation means "draw N independent samples from Pr"

#### **Expectation Estimator**

For a fixed finite N:

$$\mathbf{E}_{\Pr}[f] \approx \frac{1}{N} \sum_{\omega_i \sim \Pr}^{N} f(\omega_i).$$

 Lots of interesting theorems on bounding how quickly this estimator approaches the true expectation; see "concentration inequalities"

## Direct Sampling Semantics

 Let's give a sampling semantics for TinyPPL with only fair coin flips

#### Pure computations

#### Probabilistic computations

```
::=
    | <ident>
    | true
    | false
    | if  then  else 
    |  && 
    |  |  |  | !
```

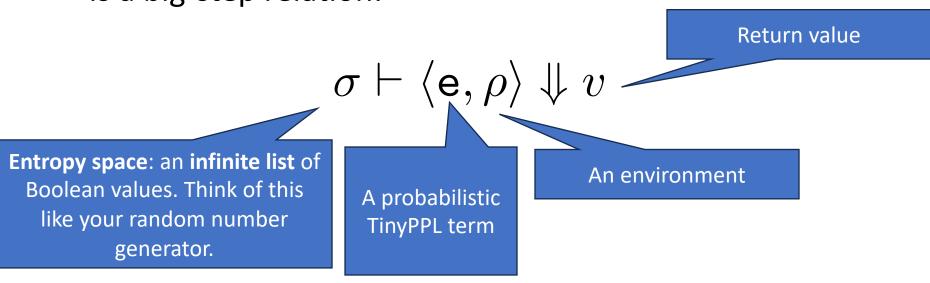
```
<e> ::=
    | flip 1/2
    | <id> <- <e>; <e>
    | return
```

## High level goal

- 1. Give a semantics to TinyPPL that formalizes "drawing a sample". Call this the (direct) sampling semantics.
- 2. Relate the expectation of direct sampling semantics to the denotation of TinyPPL programs
- 3. Use this relationship to establish (asymptotic) correctness of sampling using expectation estimator

#### Direct Sampling Semantics

• Is a big-step relation:



- "In the context of the entropy space, the term e with environment  $\rho$  steps to value v"
- Will be defined inductively on terms

$$f:: \sigma \vdash \langle \mathtt{flip}\ 1/2, \rho \rangle \Downarrow f$$

To handle coin flips, step to the first element of the entropy space.

$$\frac{\langle \mathbf{p}, \rho \rangle \Downarrow v}{\sigma \vdash \langle \mathbf{return} \ \mathbf{p}, \rho \rangle \Downarrow v}$$

To handle returning pure values, run the pure term and return the value it runs to.

 To handle bind, we need to split up the entropy space into two independent streams of random values

- We do this with two auxiliary functions:  $\pi_L$  and  $\pi_R$ .
  - Define  $\pi_L$  to take all even-indexed elements of the entropy space, and  $\pi_R$  to take all odd-indexed elements.

$$\frac{\pi_L(\sigma) \vdash \langle \mathbf{e}_1, \rho \rangle \Downarrow v \qquad \pi_R(\sigma) \vdash \langle \mathbf{e}_2, \rho[x \mapsto v] \rangle \Downarrow v'}{\sigma \vdash \langle x \leftarrow \mathbf{e}_1; \mathbf{e}_2, \rho \rangle \Downarrow v'}$$

#### Evaluation function

 Auxiliary function called eval that runs a program to its returned value:

$$\operatorname{eval}(\sigma, \rho, \mathbf{e}) = v \quad \text{if } \sigma \vdash \langle \mathbf{e}, \rho \rangle \Downarrow v$$

- This is a well-defined function because sampling semantics is deterministic (check!)
- It's a partial function: if the available entropy is too small, it will get stuck.

#### Theorem: Adequacy of sampling semantics

- Let e be a probabilistic TinyPPL program
- Let  $\rho$  be an environment that is well-typed for e (i.e., contains all free variables in e)
- Let  $\sigma$  be an entropy space that is "big enough" (i.e., eval cannot get stuck)
- Let  $\Pr(\sigma)$  be a uniform probability distribution on entropy spaces (i.e., assigns probability  $\frac{1}{|\sigma|}$  to every entropy space  $\sigma$ , where  $|\sigma|$  is the length of the list
- Then,

$$\mathbf{E}_{\sigma}([\mathtt{eval}(\mathtt{e}, \rho, \sigma) = \mathtt{tt}]) = \llbracket \mathtt{e} \rrbracket(\rho)(\mathtt{tt})$$

#### Lemmas

Left as exercises for the curious

1. (Constant) For k constant:  $\mathbf{E}_{\sigma}(k) = k$ 

2. (Splitting) 
$$\mathbf{E}_{\sigma}(f(\sigma)) = \mathbf{E}_{\sigma}\left(\frac{1}{2}f(\mathtt{tt}::\sigma) + \frac{1}{2}f(\mathtt{ff}::\sigma)\right)$$

3. (Independent) For f and g independent:

$$\mathbf{E}_{\sigma}(f(\sigma) \times g(\sigma)) = \mathbf{E}_{\sigma}(f(\sigma)) \times \mathbf{E}_{\sigma}(g(\sigma))$$

#### Proof for flip

```
\begin{split} \mathbf{E}_{\sigma} & ([\texttt{eval}(\texttt{flip}, \sigma, \rho) = \texttt{tt}]) \\ &= \mathbf{E}_{\sigma} \left( 1/2 [\texttt{eval}(\texttt{flip}, \texttt{tt} :: \sigma, \rho) = \texttt{tt}] + 1/2 [\texttt{eval}(\texttt{flip}, \texttt{ff} :: \sigma, \rho) = \texttt{tt}] \right) \\ &= \mathbf{E}_{\sigma} \left( 1/2 \right) \\ &= \mathbf{E}_{\sigma} \left( 1/2 \right) \end{split} \qquad \qquad \text{Def. of eval} \\ &= [\![\texttt{flip} \ 1/2]\!] (\rho) (\texttt{tt}). \end{split}
```

#### Proof for bind

$$\begin{split} &\mathbf{E}_{\sigma}\left([\operatorname{eval}(x\leftarrow \mathtt{e}_1;\mathtt{e}_2,\sigma,\rho)=\mathtt{tt}]\right) \\ &= \mathbf{E}_{\sigma}\left(\sum_{v'}[\operatorname{eval}(\mathtt{e}_1,\pi_L(\sigma),\rho)=v'] \times [\operatorname{eval}(\mathtt{e}_2,\pi_R(\sigma),\rho[x\mapsto v'])=\mathtt{tt}]\right) \\ &= \sum_{v'}\mathbf{E}_{\sigma}\left([\operatorname{eval}(\mathtt{e}_1,\pi_L(\sigma),\rho)=v'] \times [\operatorname{eval}(\mathtt{e}_2,\pi_R(\sigma),\rho[x\mapsto v'])=\mathtt{tt}]\right) \\ &= \sum_{v'}\mathbf{E}_{\sigma}\left([\operatorname{eval}(\mathtt{e}_1,\pi_L(\sigma),\rho)=v']\right) \times \mathbf{E}_{\sigma}\left([\operatorname{eval}(\mathtt{e}_2,\pi_R(\sigma),\rho[x\mapsto v'])=\mathtt{tt}]\right) \\ &= \sum_{v'}[\![\mathtt{e}_1]\!](\rho)(v') \times [\![\mathtt{e}_2]\!](\rho[x\mapsto v'](\mathtt{tt}) \\ &= [\![x\leftarrow \mathtt{e}_1;\mathtt{e}_2]\!](\rho)(\mathtt{tt}). \end{split}$$
 I.H.

#### TinySamp

# Rejection sampling

#### Adding observe

#### Pure computations

# ::= | <ident> | true | false | if then else | && | | | !

#### Probabilistic computations

```
<e> ::=
    | flip 1/2
    | <id> <- <e>; <e>
    | observe e; e
    | return
```

#### Direct Sampling Semantics

- Simple intuition: just like sampling semantics, we sample all probabilistic quantities as they are encountered
  - If an observation is violated, **reject** the sample: do not count it towards the estimate

```
x \leftarrow flip 0.5; \quad x \leftarrow return false; \quad x \leftarrow return false; \\ y \leftarrow flip 0.5; \quad y \leftarrow flip 0.5; \quad y \leftarrow return false; \\ observe x \mid\mid y; \quad observe x \mid\mid y; \quad observe x \mid\mid y; \\ return x; \quad return true; \quad \downarrow
```

# Rejection sampling

```
x <- flip 0.5;
y <- flip 0.5;
observe x || y;
return x;</pre>
Draw finite number
of samples

I

ff
```

 Suppose we draw the above 5 samples; then we would conclude that program outputs T with probability approximately 1/3

# Rejection Sampling Semantics

$$v :: \sigma \vdash \langle \mathtt{flip} \ \theta, \rho \rangle \Downarrow v \qquad \qquad \frac{\langle p, \rho \rangle \Downarrow v}{\sigma \vdash \langle \mathtt{return} \ p, \rho \rangle \Downarrow v}$$
 
$$\frac{\langle p, \rho \rangle \Downarrow \mathtt{tt} \qquad \sigma \vdash \langle \mathtt{e}, \rho \rangle \Downarrow v}{\sigma \vdash \langle \mathtt{observe} \ p; \mathtt{e}, \rho \rangle \Downarrow v} \qquad \qquad \frac{\langle p, \rho \rangle \Downarrow \mathtt{ff}}{\sigma \vdash \langle \mathtt{observe} \ p; \mathtt{e}, \rho \rangle \Downarrow \bot}$$
 
$$\frac{\pi_L(\sigma) \vdash \langle \mathtt{e}_1, \rho \rangle \Downarrow \bot}{\sigma \vdash \langle x \leftarrow \mathtt{e}_1; \mathtt{e}_2, \rho \rangle \Downarrow \bot} \qquad \frac{\pi_L(\sigma) \vdash \langle \mathtt{e}_1, \rho \rangle \Downarrow v}{\sigma \vdash \langle x \leftarrow \mathtt{e}_1; \mathtt{e}_2, \rho \rangle \Downarrow v}$$