Paradoxes of Probabilistic Programming

and how to condition on events of measure zero with infinitesimal probabilities (to appear at POPL'21)

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November 25, 2020

- ▶ Domain specific language for statistical and machine learning models
- Normal programming language extended with rand, observe, and run

Example:

- \blacktriangleright Men's height is distributed according to Normal(1.8, 0.5) meters
- \blacktriangleright Women's height is distributed according to *Normal*(1.7, 0.5) meters
- A scientist randomly samples a man and a woman and compares their height
- ► The scientist tells us that the heights are equal

Question: What's the expected value of the height in this situation?

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Question: What's the expected value of the height in this situation?

```
function meters(){
  h = rand(Normal(1.7, 0.5))
  observe(Normal(1.8, 0.5), h)
  return h
}
samples = run(meters, 1000)
estimate = average(samples)
```

Example:

- ▶ Men's height is distributed according to *Normal*(1.8, 0.5) meters
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}
samples = run(meters, 1000)
estimate = average(samples)
```

```
Answer: \approx 1.75
```

```
function centimeters(){
  h = rand(Normal(170, 50))
  observe(Normal(180, 50), h)
  return h
}
samples = run(meters, 1000)
estimate = average(samples)
```

Answer: ≈ 175

Suppose the scientist is lazy, and only does the measurement half of the time...

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Meters:

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h = rand(Normal(1.7, 0.5))
if(flip(0.5)){
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Meters:

```
h = rand(Normal(1.7, 0.5))
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}
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```

Answer: ≈ 1.721

Centimeters:

```
h = rand(Normal(170, 50))
if(flip(0.5)){
  observe(Normal(180, 50), h)
}
return h
```

Answer: ≈ 170.2

▶ The answer depends on whether the scientist uses meters or centimeters!

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- ► Happens if we run this with importance sampling in Anglican
- ► The issue is fundamental and not limited to Anglican
- ▶ Even happens in formal operational semantics (e.g. Commutative or Quasi-Borel)
- ▶ Unclear what the answer *should* be, or whether this program should be disallowed

Objection: you shouldn't do observe a variable number of times based on coin flip

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```
h = rand(Normal(1.7, 0.5))
w = rand(Normal(60, 10))
if(flip(0.5)){
  observe(Normal(1.8, 0.5), h)
}else{
  observe(Normal(70, 10), w)
}
return h
Answer: ≈ 1.75
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                                    Answer: \approx 170
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- ▶ The same number of observes regardless of the outcome of the coin flip
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Original program:

h = rand(Normal(1.7,0.5)) observe(Normal(1.8,0.5),h) return h

Answer: 1.75

Logarithmic ruler program:

```
H = rand(LogNormal(1.7,0.5))
observe(LogNormal(1.8,0.5),H)
return log(H)
```

Answer: 1.62

▶ Whether we use linear scale or log scale shouldn't matter, just like meters or centimeters shouldn't matter

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- What does probililistic conditioning really mean?

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- No conditionals at all, but the output still depends on the scale we use
- What do probabilistic programs really mean?
- ▶ What does probililistic conditioning really mean?
- Related to the Borel-Komolgorov paradox

Overview

Problem:

- ▶ Probabilistic programs are not invariant under parameter transformations
- ▶ It's not clear what observe really means

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Key ideas:

- 1. Figure out what observe should do, by analogy with the discrete case
- 2. Change the language: observe conditions on intervals instead of points
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Overview

Problem:

- Probabilistic programs are not invariant under parameter transformations
- ▶ It's not clear what observe really means

Key ideas:

- 1. Figure out what observe should do, by analogy with the discrete case
- 2. Change the language: observe conditions on intervals instead of points
- 3. Take interval width to be infinitesimally small to condition on measure zero events

Result:

- ▶ New language is invariant under arbitrary parameter transformations
- ▶ Programs have clear probabilistic meaning via rejection sampling
- Implemented as a DSL in Julia

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

What's the probability distribution of x now?

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```
samples = []
for(i in 1..1000){
    x = rand(DiscreteUniform(1,6))
    y = rand(DiscreteUniform(1,6))
    z = rand(DiscreteUniform(1,6))
    if(z == x + y){
        samples.append(x)
    }
}
```

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

```
samples = []
                            0.4
for(i in 1..1000){
  x = rand(DiscreteUnif
   = rand(DiscreteUnif
  z = rand(DiscreteUnife
  if(z == x + y){
    samples.append(x)
                            0.1
                            0.0
                                            samples (1000)
```

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

```
samples = []
for(i in 1..1000){
  x = rand(DiscreteUnif
  v = rand(DiscreteUnif)
  z = rand(DiscreteUnife
  if(z == x + y){
    samples.append(x)
                            0.1
                            0.0
                                            samples (2000)
```

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

```
samples = []
                            0.4
for(i in 1..1000){
  x = rand(DiscreteUnif
  v = rand(DiscreteUnif)
  z = rand(DiscreteUnife
  if(z == x + y){
    samples.append(x)
                            0.1
                            0.0
                                            samples (3000)
```

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

```
samples = []
                            0.4
for(i in 1..1000){
  x = rand(DiscreteUnif
  v = rand(DiscreteUnif
  z = rand(DiscreteUnife
  if(z == x + y){
    samples.append(x)
                            0.1
                            0.0
                                            samples (10000)
```

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

```
samples = []
for(i in 1..1000){
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  v = rand(DiscreteUnif
  z = rand(DiscreteUnif()
  if(z == x + y){
    samples.append(x)
                            0.0
                                           samples (10000)
```

Key idea of PP: answer probabilistic inference questions by repeated simulation + filtering

Someone: "I rolled three dice $x, y, z \in \{1, 2, 3, 4, 5, 6\}$ and observed that x + y = z."

What's the probability distribution of x now? Use **rejection sampling**:

```
samples = []
for(i in 1..1000){
  x = rand(DiscreteUnif
  v = rand(DiscreteUnif
  z = rand(DiscreteUnife
  if(z == x + v){
    samples.append(x)
                           0.0
                                           samples (10000)
```

Key idea of PP: answer probabilistic inference questions by repeated simulation + filtering ⇒ **Probabilistic Programming Language** = **DSL for probabilistic simulations**

Probabilistic programming 101: DSL for rejection sampling

Probabilistic programming language:

- ► Normal programming language + rand(D)
- observe(b) filtering/conditioning
- run(func, k) run simulation func() k times, return array of samples

Probabilistic programming 101: DSL for rejection sampling

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- ► Normal programming language + rand(D)
- observe(b) filtering/conditioning
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```
function threeDice(){
   x = rand(DiscreteUniform(1,6))
   y = rand(DiscreteUniform(1,6))
   z = rand(DiscreteUniform(1,6))
   observe(z == x + y)
   return x
}
samples = run(threeDice, 1000)
```

Probabilistic programming 101: DSL for rejection sampling

Probabilistic programming language:

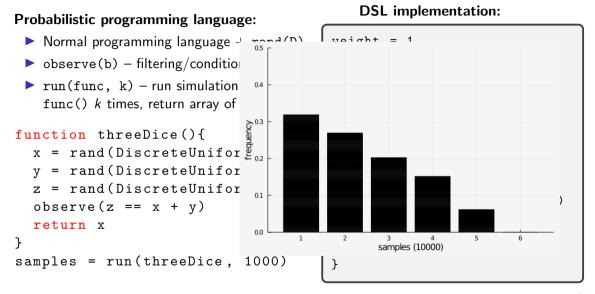
- ► Normal programming language + rand(D)
- observe(b) filtering/conditioning
- run(func, k) run simulation func() k times, return array of samples

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function threeDice(){
   x = rand(DiscreteUniform(1,6))
   y = rand(DiscreteUniform(1,6))
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   observe(z == x + y)
   return x
}
samples = run(threeDice, 1000)
```

DSL implementation:

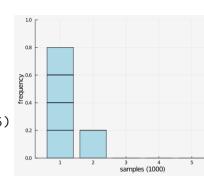
```
weight = 1
function observe(b){
  if(!b) weight = 0
function run(func, k){
  samples = []
  for(i in 1..k){
    weight = 1
    result = func()
    if(weight == 1){
      samples.append(result)
  return samples
```

Probabilistic programming 101: DSL for rejection sampling

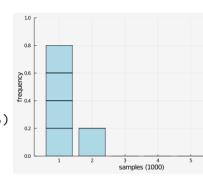


```
function multiDice(){
x = rand(DiscreteUniform(1.6))
 for (i in 1:x){
 v = rand(DiscreteUniform(1,6))
  observe(rand(DiscreteUniform(1,y)) == 3)
 observe(rand(DiscreteUniform(1,6))+x == 5)
 return x
samples = run(multiDice, 1000)
```

```
function multiDice(){
x = rand(DiscreteUniform(1.6))
 for(i in 1:x){
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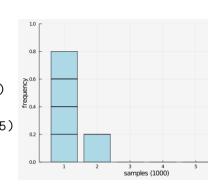


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Problem: most samples get rejected ⇒ convergence is slow

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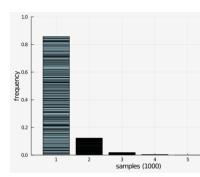


Problem: most samples get rejected ⇒ convergence is slow **Standard solution:** importance sampling

- ▶ change observe(rand(D) == x) \mapsto observe(D,x)
- function observe(D,x){ weight *= probability(D,x) }
- weights are now numbers between 0..1 instead of only 0,1
- run returns an array of weighted samples

Probabilistic programming 101: importance sampling

```
function multiDice(){
 x = rand(DiscreteUniform(1.6))
 for (i in 1:x){
 v = rand(DiscreteUniform(1,6))
  observe(DiscreteUniform(1,y), 3)
 }
 observe(DiscreteUniform(1,6), 5-x)
 return x
samples = run(multiDice, 1000)
```



Problem: most samples get rejected ⇒ convergence is slow **Solution:**

- ▶ change observe(rand(D) == x) \mapsto observe(D,x)
- function observe(D,x){ weight *= probability(D,x) }
- ▶ weights are now numbers between 0..1 instead of only 0,1
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Continuous distributions are problematic because probability(D,x) = 0.

When doing observe(D, x) for continuous distributions D,

- ► Rejection sampling rejects 100% of the trials
- ▶ Importance sampling only produces trials with weight = 0

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Intuition: $pdf(D,x) \propto the probability that <math>rand(D)$ is close to x. **Formally:**

$$cdf(D, x) = \mathbb{P}[rand(D) < x]$$
 $pdf(D, x) = \frac{d}{dx}cdf(D, x)$

End of probabilistic programming 101.

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 $\operatorname{pdf}(D,x) = \frac{d}{dx}\operatorname{cdf}(D,x)$

End of probabilistic programming 101.

Using the pdf instead of the probability is the source of the strange behaviour!

What went wrong: conditionals

Recall the drunk scientist:

```
if(flip(0.5)){
  observe(Normal(1.8, 0.5), h)
}else{
  observe(Normal(70, 10), w)
}
```

```
function observe(D,x){
  weight *= pdf(D,x)
}
```

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Recall the drunk scientist:

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  weight *= pdf(D,x)
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```

- An observe(D,x) call multiplies the weight by pdf(D,x)
- ► The pdf is not unitless! pdf(Normal(μ, σ), x) = $\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$
- ▶ The weight has units m^{-1} in some trials and kg^{-1} in other trials
- ▶ Results in unit errors when computing the weighted average:

$$\mathbb{E}[bmi] \approx \frac{\sum_{k=1}^{N} (weight_k) \cdot (bmi_k)}{\sum_{k=1}^{N} (weight_k)}$$

▶ The sum adds $m^{-1} + kg^{-1}$!

What went wrong: nonlinear parameter transformations

Recall the log scale scientist:

```
observe(Normal(1.8, 0.5), h) vs observe(LogNormal(1.8, 0.5), H)
```

Conditioning on events of measure zero is ambiguous!

What went wrong: nonlinear parameter transformations

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observe(Normal(1.8, 0.5), h) vs observe(LogNormal(1.8, 0.5), H)

Conditioning on events of measure zero is ambiguous!

$$A_{\epsilon} = \{(x, y) \in \mathbb{R}^2 : |x - y| \le \epsilon\}$$

$$B_{\epsilon} = \{(x, y) \in \mathbb{R}^2 : |\exp(x) - \exp(y)| \le \epsilon\}$$

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"Although the sequences A_{ϵ} and B_{ϵ} tend to the same limit "x=y", the conditional densities $\mathbb{P}(x|A_{\epsilon})$ and $\mathbb{P}(x|B_{\epsilon})$ tend to different limits. As we see from this, merely to specify "x=y" without any qualifications is ambiguous. Whenever we have a probability density on one space and we wish to generate from it one on a subspace of measure zero, the only safe procedure is to pass to an explicitly defined limit by a process like A_{ϵ} and B_{ϵ} . In general, the final result will and must depend on which limiting operation was specified. This is extremely counter-intuitive at first hearing; yet it becomes obvious when the reason for it is understood."

– E.T. Jaynes (paraphrased)

Solution: don't condition on measure zero events

Problem: conditioning on events of measure zero is ambiguous.

Solution: condition on intervals.

observe(D, Interval(x,w))

Meaning: rand(D) is in an interval of width w around x.

Solution: don't condition on measure zero events

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Rejection sampling:

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function observe(D,I){
  if(abs(rand(D) - I.midpoint) > I.width/2){ weight = 0 }
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Rejection sampling:

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function observe(D,I){
  if(abs(rand(D) - I.midpoint) > I.width/2){ weight = 0 }
}
```

Importance sampling:

```
function observe(D,I){ weight *= probability(D,I) }
```

For intervals, probability(D,I) is nonzero.

Example of conditioning on intervals

Example:

```
function centimeters(){
 h = rand(Normal(170, 50))
  if(flip(0.5)){
    observe(Normal(180, 10), Interval(h, 10))
function meters(){
 h = rand(Normal(1.7, 0.5))
  if(flip(0.5)){
    observe(Normal(1.8, 0.1), Interval(h, 0.1))
```

Example of conditioning on intervals

Example:

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function meters(){
 h = rand(Normal(1.7, 0.5))
  if(flip(0.5)){
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```

Same output & no unit errors, even though observe is conditionally executed!

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    observe(Normal(180, 10), Interval(h, 10))
function meters(){
 h = rand(Normal(1.7, 0.5))
  if(flip(0.5)){
    observe(Normal(1.8, 0.1), Interval(h, 0.1))
```

Same output & no unit errors, even though observe is conditionally executed! Rejection sampling and importance sampling converge to the same answer!

We still want to condition on measure zero events

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Idea: parameterize the program by the width of the interval, and take the limit width o 0

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Idea: parameterize the program by the width of the interval, and take the limit $width \rightarrow 0$

```
function drunk(width){
  h = rand(Normal(1.7, 0.5))
  w = rand(Normal(60, 10))
  if(flip(0.5)){
    observe(Normal(1.8, 0.1), Interval(h, A*width))
  }else{
    observe(Normal(70, 10), Interval(w, B*width))
  }
}
```

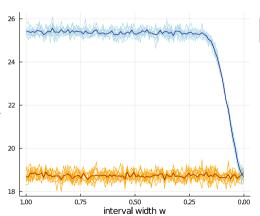
Since *width* is unitless, we must introduce constants A and B with units m and kg. The relative size matters even as $width \rightarrow 0$!

We still want to condition on measure zero events

Idea: parameterize the program by the width of the interval, and take the limit $width \rightarrow 0$

```
function drunk(width){
  h = rand(Normal(1.7, 0.5))
  w = rand(Normal(60, 10))
  if(flip(0.5)){
    observe(Normal(1.8, 0.1), Int
  }else{
    observe(Normal(70, 10), Inter-
  }
}
```

Since *width* is unitless, we must introduce constants A and B with units m and kg. The relative size matters even as $width \rightarrow 0$!

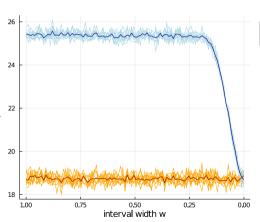


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  }else{
    observe(Normal(70, 10), Inter
  }
}
```

Since width is unitless, we must introduce constants A and B with units m and kg. The relative size matters even as width $\rightarrow 0!$



Can we compute the limit $w \to 0$ directly?

Definition

An infinitesimal number is a pair $(r, n) \in \mathbb{R} \times \mathbb{Z}$, which we write as $r\epsilon^n$.

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Arithmetic with infinitesimals:

$$r\epsilon^n \pm s\epsilon^k = egin{cases} (r\pm s)\epsilon^n & ext{if } n=k \ r\epsilon^n & ext{if } n < k \ \pm s\epsilon^k & ext{if } n > k \end{cases}$$
 $(r\epsilon^n)\cdot(s\epsilon^k) = (r\cdot s)\epsilon^{n+k}$ $(r\epsilon^n)/(s\epsilon^k) = egin{cases} (r/s)\epsilon^{n-k} & ext{if } s
eq 0 \ ext{undefined} & ext{if } s = 0 \end{cases}$

The probability that rand(D) lies in the interval $[x - r\epsilon^n, x + r\epsilon^n]$:

probability(
$$D$$
, Interval(x , re^n)) =
$$\begin{cases} \operatorname{cdf}(D, x + \frac{1}{2}r) - \operatorname{cdf}(D, x - \frac{1}{2}r) & \text{if } n = 0 \\ \operatorname{pdf}(D, x) \cdot re^n & \text{if } n > 0 \end{cases}$$

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Infinitesimals unify cdf and pdf!

Correctness properties

Consistency with existing probabilistic programming languages:

 ${\tt observe(D,Interval(x,eps))} \ \ {\tt gives} \ \ {\tt the} \ \ {\tt same} \ \ {\tt result} \ \ {\tt as} \ \ {\tt observe(D,x)} \ \ {\tt outside} \ \ {\tt conditionals}$

Correctness properties

Consistency with existing probabilistic programming languages:

observe(D,Interval(x,eps)) gives the same result as observe(D,x) outside conditionals

Consistency with non-zero width intervals:

observe(D,Interval(x,eps)) gives the same result as observe(D,Interval(x,width)) and then taking the limit width $\to 0$

Theorem

If f(x) is given by a "probability expression" and $f(\epsilon) = r\epsilon^n$, then $\lim_{x\to 0} \frac{f(x)}{x^n} = r$.

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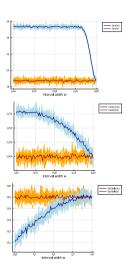
Definition

We say that f(x) is a "probability expression" in the variable x if f(x) is defined using the operations $+, -, \cdot, /$, constants, and probability $(D, \operatorname{Interval}(s, rx))$ where $r, s \in \mathbb{R}$ are constants, and D is a probability distribution with differentiable cdf.

Importance sampling computes a probability expression.

Example programs:

```
function bmi(width){
 h = rand(Normal(1.70, 0.2))
 w = rand(Normal(70.30))
  if (flip (0.5)) {
      observe(Normal(2.0,0.1), Interval(h,10*width))
  }else{
      observe(Normal(90.5), Interval(w.width))
  return w / h^2
function meters(width){
 h = rand(Normal(1.7, 0.5))
  if (flip (0.5)) {
      observe(Normal(2.0.0.1), Interval(h, width))
  return h
function decibels (width) {
 x = rand(Normal(10.5))
  observe(Normal(15.5).Interval(x.width))
  return v
```



Theorem works: we can condition on events of measure zero without paradoxes

The factor in front of ϵ allows us to do parameter transformations correctly:

A function f maps $Interval(x, \epsilon)$ to $Interval(f(x), f'(x)\epsilon)$.

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Original program:

Answer: 1.75

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A function f maps $Interval(x, \epsilon)$ to $Interval(f(x), f'(x)\epsilon)$.

Original program:

return h

Answer: 1.75

Logarithmic ruler program:

Answer: 1.75

Same output ⇒ parameter transformation correctly applied

Language support for parameter transformations $f : \mathbb{R} \to \mathbb{R}$.

- ▶ Define f(D) for distributions by defining rand, pdf, cdf of f(D)
- ightharpoonup Define f(I) for finite width intervals and infinitesimal width intervals

Requires that f is monotone and differentiable.

Original program:

```
observe(Normal(1.8,0.5),
Interval(h,eps))
```

Answer: 1.75

Language support for parameter transformations $f : \mathbb{R} \to \mathbb{R}$.

- ▶ Define f(D) for distributions by defining rand, pdf, cdf of f(D)
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Requires that f is monotone and differentiable.

Original program:	Logarithmic ruler program:		
observe(Normal(1.8,0.5),	observe(exp(Normal(1.8,0.5)),		
<pre>Interval(h,eps))</pre>	<pre>exp(Interval(h,eps)))</pre>		
Answer: 1.75	Answer: 1.75		

Language support for parameter transformations $f : \mathbb{R} \to \mathbb{R}$.

- ▶ Define f(D) for distributions by defining rand, pdf, cdf of f(D)
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Requires that f is monotone and differentiable.

\sim					
U	rıgı	inal	pro	ogra	ım:

Logarithmic ruler program:

```
observe(Normal(1.8,0.5),
Interval(h,eps))
```

Answer: 1.75 **Answer:** 1.75

In general: observe(f(D), f(I)) \equiv observe(D, I)

 \implies programs are invariant under parameter transformations

Recap

- Paradoxical behaviour: seemingly equivalent probabilistic programs give different outputs
- ▶ Root of the problem: conditioning on measure-zero events is ambiguous
- Solution: condition on intervals
- Restores rejection sampling as ground truth semantics
- Model measure-zero events as a limit, computed using infinitesimal arithmetic
- ► Semantics of observe(D, Interval(x, eps)) agrees with the old observe(D, x) in most cases
- Programs are now invariant under parameter transformations
- ► Implementation in Julia

Comments or questions?

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Acknowledgements I thank Sriram Sankaranarayanan and the anonymous POPL reviewers for their outstanding feedback. I'm grateful to Ike Mulder, Arjen Rouvoet, Paolo Giarrusso, Dongho Lee, Ahmad Salim Al-Sibahi, Sam Staton, Christian Weilbach, and Robbert Krebbers for help, inspiration, and discussions.