Semantic Foundations for Probabilistic Programming

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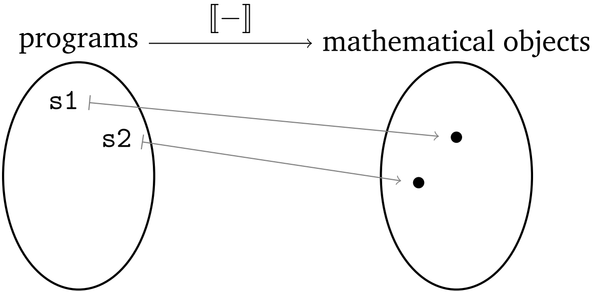
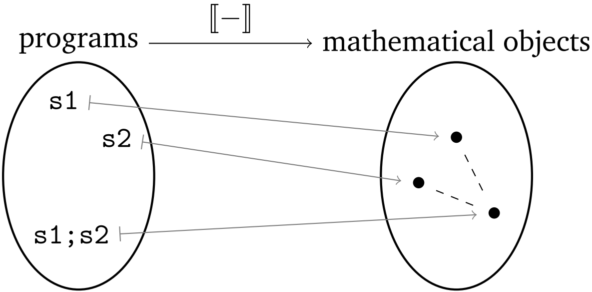
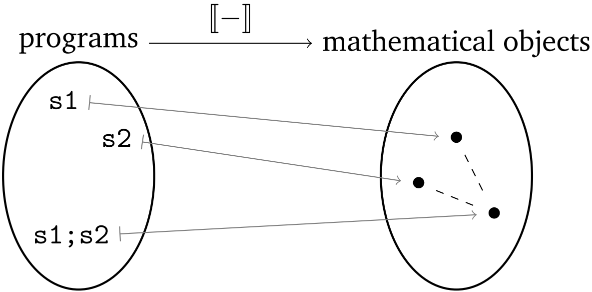
Semantic foundations



Semantic foundations

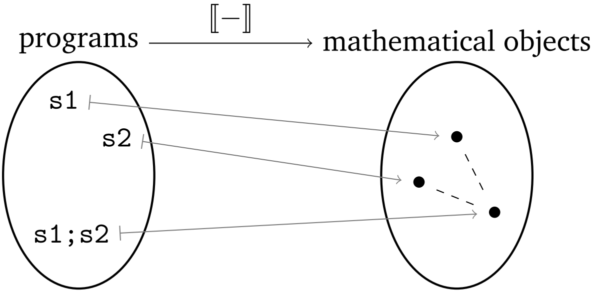


Semantic foundations



- *Operational*: remember implementation details (efficiency)
- *Denotational*: see what program does conceptually (correctness)

Semantic foundations

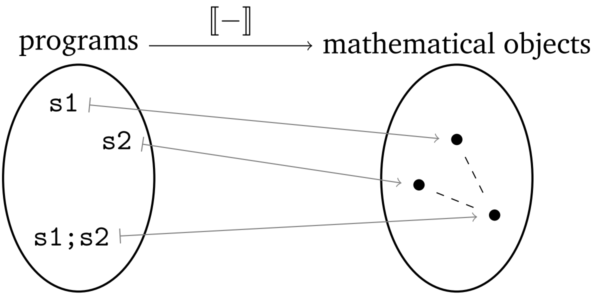


- *Operational*: remember implementation details (efficiency)
- *Denotational*: see what program does conceptually (correctness)

Motivation:

- Ground programmer's unspoken intuitions
- Justify/refute/suggest program transformations
- Understand programming through mathematics

Semantic foundations



- *Operational*: remember implementation details (efficiency)
- *Denotational*: see what program does conceptually (correctness)

Motivation:

- Ground programmer's unspoken intuitions
- Justify/refute/suggest program transformations
- Understand *probability* through *program equations*

Probabilistic programming

$$\mathrm{P}(A \mid B) \;=\; \frac{\mathrm{P}(B \mid A) \times \mathrm{P}(A)}{\mathrm{P}(B)}$$

Probabilistic programming

$$P(A \mid B) \propto P(B \mid A) \times P(A)$$

Probabilistic programming

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$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

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idealized Anglican = functional programming +

normalize **observe** **sample**

http://www.robots.ox.ac.uk/~fwood/anglican

Overview

- Interpret types as measurable spaces e.g. $[\![\texttt{real}]\!] = \mathbb{R}$
- Interpret (open) terms as kernels
- Interpret closed terms as measures
- Inference normalizes measures posterior $\propto$ likelihood $\times$ prior

[Kozen, "Semantics of probabilistic programs", J Comp Syst Sci, 1981]

Overview

- Interpret types as measurable spaces — e.g. $[\![\texttt{real}]\!] = \mathbb{R}$
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- Inference normalizes measures — posterior $\propto$ likelihood $\times$ prior

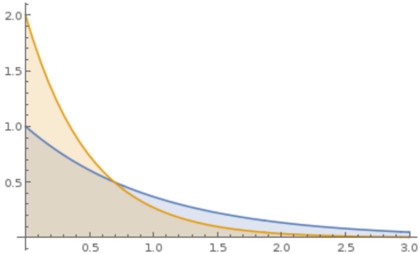
But:

- Commutativity? — Fubini not true for all kernels
- Higher order functions? — $\mathbb{R} \to \mathbb{R}$ not a measurable space
- Extensionality?
- Recursion?

[Kozen, "Semantics of probabilistic programs", J Comp Syst Sci, 1981]
[Aumann, "Borel structures for function spaces", Ill J Math, 1961]

Example

1. Toss a fair coin to get outcome x
2. Set up exponential decay with rate r depending on x
3. Observe immediate decay
4. What is the outcome x?



Example

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```
let x = sample(bern(0.5)) in
let r = if x then 2.0 else 1.0
observe(0.0 from exp(r));
return x
```

Example

1. Toss a fair coin to get outcome x
2. Set up exponential decay with rate r depending on x
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4. What is the outcome x?

two traces:

	0.5	0.5
`let x = sample(bern(0.5)) in`	`x=true`	`x=false`

```
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Code	0.5	0.5
`let x = sample(bern(0.5)) in`	`x=true`	`x=false`
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`observe(0.0 from exp(r));`	`score 2`	
`return x`	`return true`	

Example

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two traces:

```
                                           0.5            0.5
let x = sample(bern(0.5)) in               x=true         x=false
let r = if x then 2.0 else 1.0             r=2.0          r=1.0
observe(0.0 from exp(r));                  score 2        score 1
return x                                   return true    return false
```

Example

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two traces:

0.5	0.5
x=true	x=false
r=2.0	r=1.0
score 2	score 1
return true	return false

posterior $\propto$ likelihood $\times$ prior

2×0.5: true
1×0.5: false

Example

1. Toss a fair coin to get outcome x
2. Set up exponential decay with rate r depending on x
3. Observe immediate decay
4. What is the outcome x?

$\mathrm{P}(\texttt{true}) = 1, \mathrm{P}(\texttt{false}) = 0.5$

```
let x = sample(bern(0.5)) in
let r = if x then 2.0 else 1.0
observe(0.0 from exp(r));
return x
```

two traces:

0.5	0.5
`x=true`	`x=false`
`r=2.0`	`r=1.0`
`score 2`	`score 1`
`return true`	`return false`

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Example

1. Toss a fair coin to get outcome x
2. Set up exponential decay with rate r depending on x
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4. What is the outcome x?

model evidence (score): 1.5

$P(\texttt{true}) = 66\%$, $P(\texttt{false}) = 33\%$

```
let x = sample(bern(0.5)) in
let r = if x then 2.0 else 1.0
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return x
```

two traces:

0.5	0.5
`x=true`	`x=false`
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`return true`	`return false`

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Example

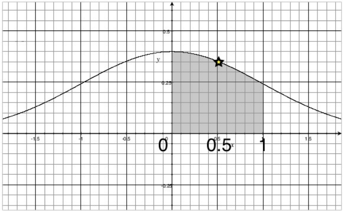
1. Toss a fair coin to get outcome x
2. Set up exponential decay with rate r depending on x
3. Observe immediate decay model evidence (score): 1.5
4. What is the outcome x? $\mathrm{P}(\texttt{true}) = 66\%$, $\mathrm{P}(\texttt{false}) = 33\%$

Programs may also sample continuous distributions so have to deal with uncountable number of traces:

```
let y = sample(gauss(7,2))
```

Measure theory

Impossible to sample 0.5 from standard normal distribution
But sample in interval $(0, 1)$ with probability around 0.34



Measure theory

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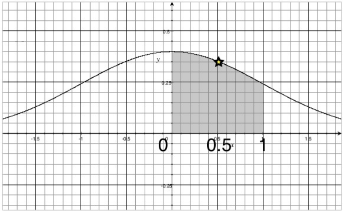

A measurable space is a set X with a family Σ_X of subsets
that is closed under countable unions and complements

A (probability) measure on X is a function $p \colon \Sigma_X \to [0, \infty]$
that satisfies $p(\sum U_n) = \sum p(U_n)$ (and has $p(X) = 1$)

First order language

- Types: $\mathbb{A}, \mathbb{B} ::= \mathbb{R} \mid P(\mathbb{A}) \mid 1 \mid \mathbb{A} \times \mathbb{B} \mid \sum_{i \in I} \mathbb{A}_i$

  real numbers ($\mathbb{R}$); distributions over $\mathbb{A}$ ($P(\mathbb{A})$); finite products ($\mathbb{A} \times \mathbb{B}$); countable sums ($\sum_{i \in I} \mathbb{A}_i$)

  $\texttt{bool} := 1 + 1$

  $\texttt{nat} := \sum_{i \in \mathbb{N}} 1$

First order language

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- Deterministic terms may not sample:
  - variables — $\mathtt{x}, \mathtt{y}, \mathtt{z}$
  - constructors for sums and products — $\mathtt{case}, \mathtt{in}_i, \mathtt{if}, \mathtt{false}, \mathtt{true}$
  - measurable functions — $\mathtt{bern}, \mathtt{exp}, \mathtt{gauss}, \mathtt{dirac}$

$$\vdash_{\mathrm{d}} \mathtt{42.0} : \mathbb{R}$$
$$\vdash_{\mathrm{d}} \mathtt{gauss}(\mathtt{2.0}, \mathtt{7.0}) : \mathrm{P}(\mathbb{R})$$
$$\mathtt{x} : \mathbb{R}, \mathtt{y} : \mathbb{R} \vdash_{\mathrm{d}} \mathtt{x} + \mathtt{y} : \mathbb{R}$$
$$\mathtt{x} : \mathbb{R}, \mathtt{y} : \mathbb{R} \vdash_{\mathrm{d}} x < y : \mathtt{bool}$$

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  - variables — `x, y, z`
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  - measurable functions — `bern`, `exp`, `gauss`, `dirac`
- Probabilistic terms may sample:
  - sequencing — `return`, `let`
  - constraints — `score`
  - priors — `sample`

$$\frac{\Gamma \vdash_{\mathrm{d}} t \colon \mathbb{A}}{\Gamma \vdash_{\mathrm{p}} \texttt{return}(t) \colon \mathbb{A}} \qquad \frac{\Gamma \vdash_{\mathrm{p}} t \colon \mathbb{A} \quad x \colon \mathbb{A} \vdash_{\mathrm{p}} u \colon \mathbb{B}}{\Gamma \vdash_{\mathrm{p}} \texttt{let } x = t \texttt{ in } u \colon \mathbb{B}}$$

$$\frac{\Gamma \vdash_{\mathrm{d}} t \colon \mathbb{R}}{\Gamma \vdash_{\mathrm{p}} \texttt{score}(t) \colon 1} \qquad \frac{\Gamma \vdash_{\mathrm{d}} t \colon P(\mathbb{A})}{\Gamma \vdash_{\mathrm{p}} \texttt{sample}(t) \colon \mathbb{A}}$$

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- Deterministic terms may not sample:
  - variables — `x, y, z`
  - constructors for sums and products — `case`, $\mathtt{in}_i$, `if`, `false`, `true`
  - measurable functions — `bern`, `exp`, `gauss`, `dirac`
  - inference — `norm`
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$$\frac{\Gamma \vdash_{\mathrm{d}} t : \mathbb{A}}{\Gamma \vdash_{\mathrm{p}} \mathtt{return}(t) : \mathbb{A}} \qquad \frac{\Gamma \vdash_{\mathrm{p}} t : \mathbb{A} \quad x : \mathbb{A} \vdash_{\mathrm{p}} u : \mathbb{B}}{\Gamma \vdash_{\mathrm{p}} \mathtt{let}\ x = t\ \mathtt{in}\ u : \mathbb{B}}$$

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First order semantics

Interpret

- type $\mathbb{A}$ as measurable space $[\![\mathbb{A}]\!]$
- deterministic term $\Gamma \vdash_{\mathrm{d}} t \colon \mathbb{A}$ as measurable function $[\![\Gamma]\!] \to [\![\mathbb{A}]\!]$
- probabilistic term $\Gamma \vdash_{\mathrm{p}} t \colon \mathbb{A}$ as kernel $[\![t]\!] \colon [\![\Gamma]\!] \times \Sigma_{[\![\mathbb{A}]\!]} \to [0, \infty]$
  fixing first argument: measure, fixing second argument: measurable

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Example

$$\left[\!\!\left[\begin{array}{l}\texttt{let x = sample(bern(0.5)) in}\\ \texttt{let r = if x then 2.0 else 1.0}\\ \texttt{observe(0.0 from exp(r));}\\ \texttt{return x}\end{array}\right]\!\!\right]$$

The meaning of a program returning values in X is a measure on X

$$\begin{array}{rll} \emptyset & \text{has measure} & 0.0 \\ \{\texttt{true}\} & \text{has measure} & 1.0 = 0.5 \times 2.0 \\ \{\texttt{false}\} & \text{has measure} & 0.5 = 0.5 \times 1.0 \\ \{\texttt{true}, \texttt{false}\} & \text{has measure} & 1.5 \end{array}$$

Normalization: **posterior** $\propto$ **likelihood** $\times$ **prior**

$$\frac{\Gamma \vdash_{\mathrm{p}} t : \mathbb{A}}{\Gamma \vdash_{\mathrm{d}} \texttt{norm}(t) : \mathbb{R} \times \mathrm{P}(\mathbb{A}) \; + \underbrace{1 + 1}}$$

model evidence

errors

normalized posterior

Normalization: **posterior** $\propto$ **likelihood** $\times$ **prior**

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Interpretation of probabilistic term is kernel $[\![\Gamma]\!] \times \Sigma_{[\![\mathbb{A}]\!]} \to [0, \infty]$ so

fixing first argument gives measure

$$\frac{[\![t]\!](\gamma, -)}{[\![t]\!](\gamma, [\![\mathbb{A}]\!])}$$

is normalized probability measure

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model evidence

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(constant is 0 or ∞)

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normalizing constant is model evidence

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$$\left[\!\!\left[\begin{array}{l} \texttt{let x = sample(bern(0.5)) in} \\ \texttt{let r = if x then 2.0 else 1.0} \\ \texttt{observe(0.0 from exp(r));} \\ \texttt{return x} \end{array} \right]\!\!\right] = \begin{pmatrix} \texttt{true}: & 2.0 \times 0.5 \\ \texttt{false}: & 1.0 \times 0.5 \end{pmatrix}$$

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model evidence

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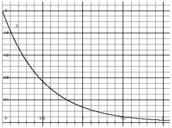
$$\left[\!\left[\begin{array}{l} \texttt{norm(} \\ \quad \texttt{let x = sample(bern(0.5)) in} \\ \quad \texttt{let r = if x then 2.0 else 1.0} \\ \quad \texttt{observe(0.0 from exp(r));} \\ \quad \texttt{return x)} \end{array} \right]\!\right] = \mathrm{in}_1\big(1.5,\ \texttt{bern}(0.66)\big)$$

Example: sequential Monte Carlo

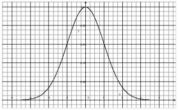
$$\left[\!\!\left[\begin{array}{l}\texttt{norm(let x=t}\\ \texttt{\ \ \ \ \ \ in u)}\end{array}\right]\!\!\right] = \left[\!\!\left[\begin{array}{l}\texttt{norm(let (e,d) = norm(t) in}\\ \texttt{\ \ \ \ \ \ score(e); let x=sample(d)}\\ \texttt{\ \ \ \ \ \ in u)}\end{array}\right]\!\!\right]$$

Example: importance sampling

$$[\![\quad \texttt{sample(exp(2))} \quad]\!]$$

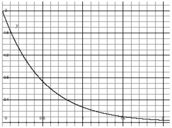


$$= \left[\!\!\left[\begin{array}{l} \texttt{let x = sample(gauss(0,1)))} \\ \texttt{score(exp-pdf(2,x) / gauss-pdf(0,1,x));} \\ \texttt{return x} \end{array} \right]\!\!\right]$$

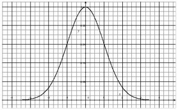


Example: importance sampling

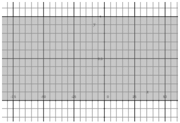
```
⟦ sample(exp(2)) ⟧
```



```
= ⟦ let x = sample(gauss(0,1))
    score(exp-pdf(2,x) / gauss-pdf(0,1,x));
    return x ⟧
```

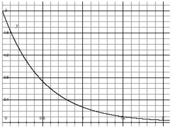


```
= ⟦ let x = sample(gauss(0,1))
    score(1 / gauss-pdf(0,1,x));
    score(exp-pdf(2,x));
    return x ⟧
```

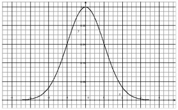


Example: importance sampling

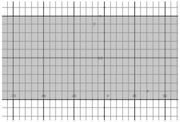
```
⟦norm( sample(exp(2)) )⟧
```



```
= ⟦norm(
    let x = sample(gauss(0,1)))
    score(exp-pdf(2,x) / gauss-pdf(0,1,x));
    return x  )⟧
```



```
≠ ⟦norm( norm(
    let x = sample(gauss(0,1)))
    score(1 / gauss-pdf(0,1,x));  );
    score(exp-pdf(2,x));
    return x )⟧
```



Don't normalize as you go

Commutativity

Reordering lines is very useful program transformation

$$\left[\!\left[\begin{array}{l}\texttt{let x=t in}\\ \texttt{let y=u in}\\ \texttt{v}\end{array}\right]\!\right] = \left[\!\left[\begin{array}{l}\texttt{let y=u in}\\ \texttt{let x=t in}\\ \texttt{v}\end{array}\right]\!\right]$$

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Not true for arbitrary kernels, only for s-finite kernels

kernel is s-finite when countable sum of bounded ones

$k \colon [\![\Gamma]\!] \times \Sigma_{[\![\mathbb{A}]\!]} \to [0, \infty]$ bounded if $\exists n \forall \gamma \forall U \colon k(\gamma, U) < n$

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- kernel k is s-finite iff it can be built from sub-probability distributions, `score`, and *binding*
  $k \gg= l$ is $(\gamma, V) \mapsto \int_{[\![\mathbb{A}]\!]} l(\gamma, x, V) k(\gamma, \mathrm{d}x)$
- measurable spaces and s-finite kernels form distributive symmetric monoidal category

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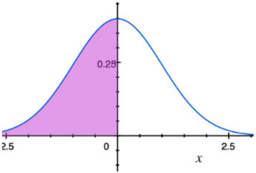
Interpret terms as s-finite kernels

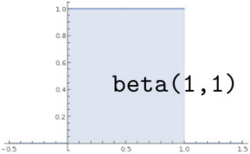
Example: facts about distributions

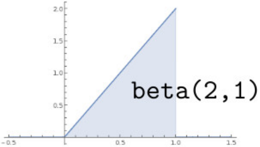
$$\left[\!\!\left[\begin{array}{l}\texttt{let x = sample(gauss(0.0,1.0))}\\ \texttt{in return (x<0)}\end{array}\right]\!\!\right] = [\![\,\texttt{sample(bern(0.5))}\,]\!]$$



Example: conjugate priors

$$\left[\!\!\left[\begin{array}{l}\texttt{let x = sample(beta(1,1))}\\ \texttt{in observe(bern(x), true);}\\ \texttt{return x}\end{array}\right]\!\!\right] = \left[\!\!\left[\begin{array}{l}\texttt{observe(bern(0.5), true);}\\ \texttt{let x = sample(beta(2,1))}\\ \texttt{in return x}\end{array}\right]\!\!\right]$$





Higher order functions

Allow probabilistic terms as input/output for other terms

```
(define (ibp-stick-breaking-process concentration base-measure)
  (let ((sticks (mem (lambda j (random-beta 1.0 concentration))))
        (atoms  (mem (lambda j (base-measure)))))
    (lambda ()
      (let loop ((j 1) (dualstick (sticks 1))}
        (append (if (flip dualstick)              ;; with prob. dualstick
                    (atoms j)                     ;;   add feature j
                    '())                          ;; otherwise, next stick
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[Roy et al, “A stochastic programming perspective on nonparametric Bayes”, ICML 2008]

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$\mathbb{R} \to \mathbb{R}$ is not a measurable space
Easy to handle operationally.
What to do denotationally?

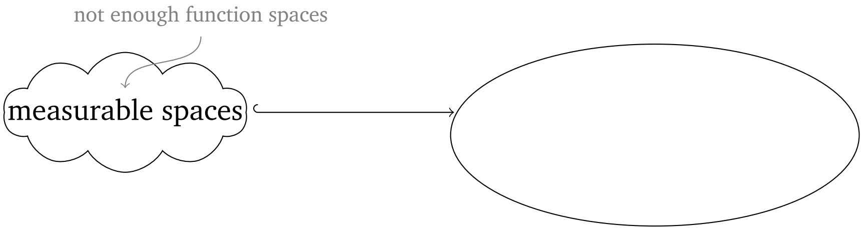
[Roy et al, "A stochastic programming perspective on nonparametric Bayes", ICML 2008]

[Aumann, "Borel structures for function spaces", Ill J Math, 1961]

[Borgström et al, "Measure transformer semantics for Bayesian machine learning", ESOP2011]

Higher order semantics

Use category theory to extend measure theory



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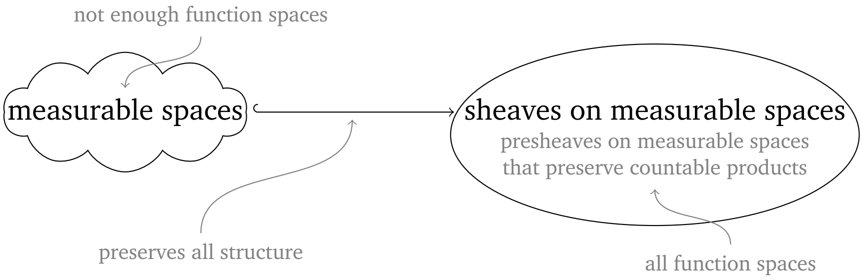

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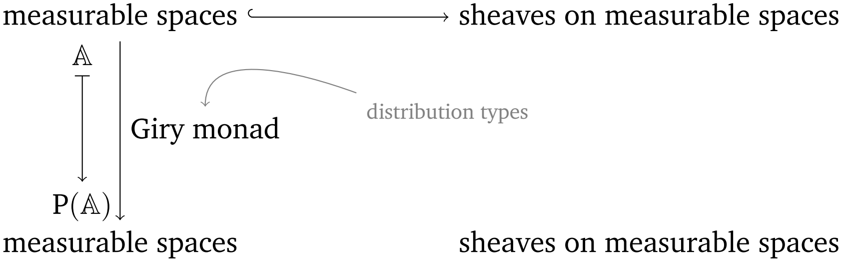

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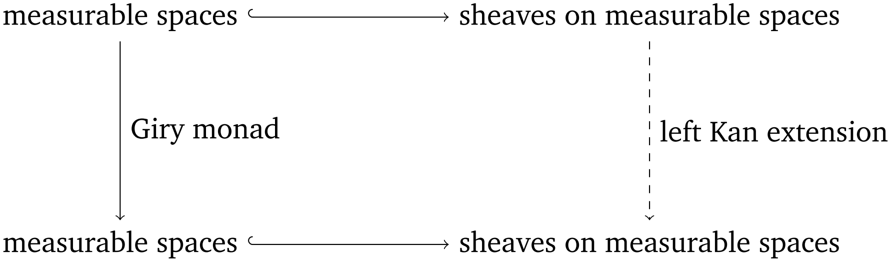

[Power, “Generic models for computational effects”, Th Comp Sci 2006]

Higher order semantics

Use category theory to extend measure theory

$$\text{measurable spaces} \hookrightarrow \text{sheaves on measurable spaces}$$

- $[\![1 \to (\mathbb{R} \to \mathbb{R})]\!]$ consists of random functions   measurable $\Omega \times \mathbb{R} \to \mathbb{R}$
- All definable functions $\mathbb{R} \to \mathbb{R}$ are measurable   “Church-Turing”
- Denotational and operational semantics match   soundness & adequacy

Extensionality

Not extensional: $1 \xrightarrow{p} \mathbb{A} \underset{g}{\overset{f}{\rightrightarrows}} \mathbb{B}$ for all $p \;\not\Rightarrow\; f = g$

Solution: restrict to subcategory that *is* extensional

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Solution: restrict to subcategory that *is* extensional

A quasi-measurable space is a set X with $M_X \subseteq [\mathbb{R} \to X]$ satisfying

- if $f \colon \mathbb{R} \to \mathbb{R}$ is measurable and $g \in M$, then $gf \in M$
- if $f \colon \mathbb{R} \to X$ is constant, then $f \in M$
- if $f \colon \mathbb{R} \to \mathbb{N}$ is measurable and $g_n \in M$, then $[g_n]f \in M$ $\quad t \mapsto g_{f(t)}(t)$

morphisms are functions $f \colon X \to Y$ with $g \in M_X \Rightarrow fg \in M_Y$

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Example: X measurable space, M_X measurable functions $\mathbb{R} \to X$
morphism $X \to Y$ is measurable function

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Theorem: this gives cartesian closed category with countable sums

Corollary: if term t has first order type, then $[\![t]\!]$ is measurable

even if t involves higher order functions

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A measure on (X, M_X) is a measure μ on $\mathbb{R}$ with a function $f \in M$

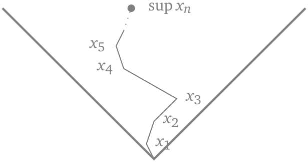
Proposition: measures on $[X \to Y]$ are random functions

measurable map $\mathbb{R} \times X \to Y$ modulo measure on $\mathbb{R}$

Recursion

No recursion / least fixed points
Idea: restrict to presheaves over domains

An ω-complete partial order has suprema of increasing sequences
morphisms preserve suprema of increasing sequences and infima



A quasi-measurable space is ordered when X is an ωcpo and M is closed under pointwise increasing suprema

Example: Any ωcpo, e.g. [0,1]   take M all measurable functions $\mathbb{R} \to X$
where X has the Borel σ-algebra on the Lawson topology

Theorem: this gives a cartesian closed category with countable sums

Example: von Neumann's trick

$$\left[\!\!\left[\begin{array}{l}\texttt{let g = bern(0.66) in}\\ \texttt{letrec f() = (let x = sample(g)}\\ \qquad\qquad\quad\texttt{let y = sample(g)}\\ \qquad\qquad\quad\texttt{if x=y then f()}\\ \qquad\qquad\qquad\quad\texttt{else return x)}\\ \texttt{in f()}\end{array}\right]\!\!\right] \stackrel{?}{=} [\![\texttt{sample(bern(0.5))}]\!]$$

Conclusion

Foundational semantics for probabilistic programming:

- continuous distributions
- soft constraints
- commutativity
- higher order functions
- recursion

can verify/suggest program transformations. Approximations?