Quasi-Borel spaces and the validation of Bayesian inference algorithms

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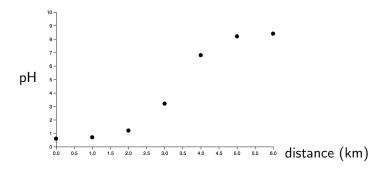


Bayesian data modelling

- 1. Develop a probabilistic (generative) model.
- 2. Design an inference algorithm for the model.
- 3. Using the algorithm, fit the model to the data.

Example

Acidity in soil



Generative model

$$\begin{array}{ll} s & \sim \mathsf{normal}(0,2) \\ b & \sim \mathsf{normal}(0,6) \\ f(x) = s \cdot x + b \\ y_i & = \mathsf{normal}(f(i), 0.5) \\ & \qquad \qquad \mathsf{for} \ i = 0 \dots 6 \end{array}$$

Generative model

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Conditioning

$$y_0 = 0.6, y_1 = 0.7, y_2 = 1.2, y_3 = 3.2, y_4 = 6.8, y_5 = 8.2, y_6 = 8.4$$

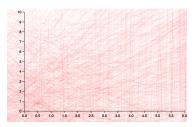
Predict f?

Bayesian inference

$$P(s, b|y_0, \dots, y_6) = \frac{P(y_0, \dots, y_6|s, b) \cdot P(s, b)}{P(y_0, \dots, y_6)}$$

Bayesian inference

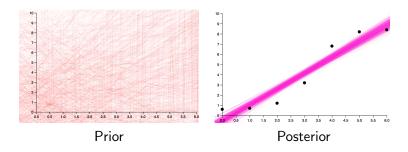
$$P(s, b|y_0, \dots, y_6) = \frac{P(y_0, \dots, y_6|s, b) \cdot P(s, b)}{P(y_0, \dots, y_6)}$$



Prior

Bayesian inference

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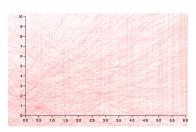
Probabilistic programming models

- Develop a probabilistic (generative) model.
 Write a program.
- 2. Design an inference algorithm for the model.
- 3. Using the built-in algorithm, fit the model to the data.

In Anglican [Wood et al.'14]

```
(let [s (sample (normal 0.0 2.0))
    b (sample (normal 0.0 6.0))
    f (fn [x] (+ (* s x) b)))]
```

(predict :f f))



```
(let [s (sample (normal 0.0 2.0))
      b (sample (normal 0.0 6.0))
      f (fn [x] (+ (* s x) b)))]
 (observe (normal (f 1.0) 0.5) 2.5)
 (observe (normal (f 2.0) 0.5) 3.8)
 (observe (normal (f 3.0) 0.5) 4.5)
 (observe (normal (f 4.0) 0.5) 6.2)
 (observe (normal (f 5.0) 0.5) 8.0)
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```
(let [F (fn [] (let [s (sample (normal 0.0 2.0))
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      f (F)]
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 (observe (normal (f 1.0) 0.5) 2.5)
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(let [F (fn [] (let [
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Components

- ▶ Control flow, e.g.: simply typed λ -calculus
- data types, e.g.: lists, functions, thunks
- ► Continuous probabilistic choice: (sample (normal 0.0 2.0))
- ► Conditioning: (observe (normal (f 2.0) 0.5) 3.8)
- ▶ Inference

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posterior \propto liklihood \times prior

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- Inference

posterior \propto liklihood \times prior

Which we refine to:

 $posterior = weight \odot prior$

Some measure theory

Rescaling

$$\nu = w \odot \mu$$

when for all $\chi: X \to [0, \infty]$:

$$\int_X \chi(x)\nu(\mathrm{d} x) = \int_X \chi(x) \cdot w(x)\mu(\mathrm{d} x)$$

(where X measurable space, $\mu \in MX$ measures on X , $w: X \to [0, \infty]$ measurable function)

A probabilistic program is a measure

For t:X

$$[\![t]\!]=w\odot\operatorname{prior}[\![t]\!]$$

where prior $[\![t]\!]$ is the **prior** (ignore conditioning), and $w=\frac{\mathrm{d}[\![t]\!]}{\mathrm{d}(\mathrm{prior}[\![t]\!])}$

Conditioning

$$\frac{t:x \qquad \varphi:X \rightarrow [0,+\infty]}{\operatorname{observe}(t,\varphi):1}$$

and

$$[\![\texttt{observe}]\!](x, \varphi) = \varphi(x) \odot \delta_{()}$$

A probabilistic program is a measure

For t:X

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Conditioning

Replace observe by score:

$$\frac{r:[0,\infty]}{\mathrm{score}\, r:1}$$

and

$$\llbracket \mathsf{score} \, \rrbracket \, (r) = r \odot \delta_{()}$$

A probabilistic program is a measure

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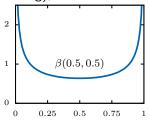
where prior [t] is the **prior** (ignore conditioning),

and
$$w = \frac{\mathrm{d} \llbracket t \rrbracket}{\mathrm{d} (\mathsf{prior} \llbracket t \rrbracket)}$$

Note

For probability measures prior [t]:

▶ It's possible that $\max w > 1$, e.g.:



or even $\max w = \infty$

▶ If we insist that all measures are sub-probability measures, then w and $[\![t]\!]$ are **not** compositional (i.e., global)

A probabilistic program is an s-finite measure [Staton'17]

For t:X

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where prior $[\![t]\!]$ is the **prior** (ignore conditioning), and $w = \frac{\mathrm{d}[\![t]\!]}{\mathrm{d}(\mathrm{prior}[\![t]\!])}$ Sampling manipulates prior.

Conditioning affects w, sequenced multiplicatively.

S-finite measures

$$\sum_{i\in\mathbb{N}}\mu_i$$

$$\mu_i$$
 finite: $\mu_i(X) < \infty$

What is inference?

Computing distributions

For t:X

$$[\![t]\!]=w\odot\operatorname{prior}[\![t]\!]$$

we want to:

- ▶ Plot [[t]].
- ▶ Sample [t] (e.g., to make prediction)

Challenge

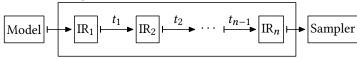
Given a fair coin $(\frac{1}{2}\delta_1 + \frac{1}{2}\delta_0)$, how do we sample from a biased coin $(p\delta_1 + (1-p)\delta_0)$?

Generalise:

Given a prior distribution prior [t], how do we sample from [t]?

What is inference?

Inference engine



Programming-language experts needed

In the traditional areas:

Verification

Semantics

Correctness

Optimisation

Static analysis

- Programming abstractions
- Type systems

This talk

Correctness of inference

Inference algorithm: distribution/meaning preserving transformation from one inference representation to another

Requirements

- Represented data is continuous
- Compositional inference representations (IRs)
- ► IRs are higher-order

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Traditional measure theory is unsuitable:

Theorem (Aumann'61)

The set $\mathbf{Meas}(\mathbb{R},\mathbb{R})$ cannot be made into a measurable space with

$$eval: \mathbf{Meas}(\mathbb{R}, \mathbb{R}) \times \mathbb{R} \to \mathbb{R}$$

measurable.

Contribution

Correctness of inference

- Modular validation of inference algorithms: Sequential Monte Carlo, Trace Markov Chain Monte Carlo By combining:
- Synthetic measure theory [Kock'12]: measure theory without measurable spaces
- Quasi-Borel spaces: a convenient category for higher-order measure theory [LICS'17]

Talk structure

- Probabilistic programming and Bayesian inference
- Synthetic measure theory
- Quasi-Borel spaces
- ► Inference representations
- Ongoing work
- Conclusion

Measure category [Kock'12]

A pair $(\mathcal{C}, \underline{M})$

lacktrian Cartesian-closed category ${\cal C}$

Measure category [Kock'12]

A pair (C, \underline{M})

- ightharpoonup Cartesian-closed category ${\cal C}$
- Countable coproducts and countable limits

Measure category [Kock'12]

A pair (C, \underline{M})

- ightharpoonup Cartesian-closed category ${\cal C}$
- Countable coproducts and countable limits
- ▶ $\underline{\mathbf{M}} = (\mathbf{M}, \mathbf{return}, \gg =)$ a strong commutative monad, i.e.:

$$\mathbf{M}: |\mathcal{C}| \to |\mathcal{C}|$$
 $\operatorname{return}_X: X \to \mathbf{M} X$ $\gg_{X,Y}: \mathbf{M} X \times (\mathbf{M} Y)^X \to \mathbf{M} Y$

satisfying the monad laws and

$$\underline{T}.\mathbf{do} \left\{ x \leftarrow a; y \leftarrow b; \mathbf{return}(x, y) \right\} \\ = \\ \underline{T}.\mathbf{do} \left\{ y \leftarrow b; x \leftarrow a; \mathbf{return}(x, y) \right\}$$

Measure category [Kock'12]

A pair $(\mathcal{C}, \underline{M})$

- ightharpoonup Cartesian-closed category ${\cal C}$
- Countable coproducts and countable limits
- ▶ $\underline{\mathbf{M}} = (\mathbf{M}, \text{return}, \gg =)$ a strong commutative monad, i.e.:
- Canonical morphisms are invertible:

$$M \mathbb{O} \cong \mathbb{1}$$
 $M(\coprod_{n \in \mathbb{N}} X) \cong \prod_{n \in \mathbb{N}} M X$

Synthetic measure theory: consequences

Surprisingly rich structure

- \triangleright 0:1 \rightarrow M0
- $R := M \mathbb{1}$ a σ -semiring:

$$(\cdot): R \times R \xrightarrow{\text{double strength}} R \qquad 1 := \operatorname{return}() \in R$$

▶ Every algebra is an *R*-module:

$$\odot: R \times MX \xrightarrow{\mathsf{strength}} MX$$

Associated affine monad:

$$P X \xrightarrow{\sup_{--} X} M X \xrightarrow{M!} R$$

Synthetic measure theory: notation

Kock integration

$$\iint\limits_X f(x)\underline{\mu}(\mathrm{d}x) \coloneqq \underline{\mu} \gg = f$$

Measure-valued, hence analogous to

$$\int_X \chi(x) \cdot f(x) \underline{\mu}(\mathrm{d}x)$$

for generic $\chi: X \to [0, \infty)$

η-expanded integrand

Synthetic measure theory: notation

Notation	Meaning	Terminology
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$\stackrel{\circ}{w}\odot\mu$	$:= \overline{\oint}_X (w(x) \odot \underline{\delta}_x) \underline{\mu}(\mathrm{d}x)$	Rescaling
$\oint_Y f(x,y)k(x,\mathrm{d}y)$	$= \oint_Y f(x,y)k(x)(\mathrm{d}y)$	Kernel integration
$\iint_{X\times Y} f(x,y)\underline{\mu}(\mathrm{d}x,\mathrm{d}y)$	$y) \coloneqq \oint_{X \times Y} f(z)\underline{\mu}(\mathrm{d}z)$	Iterated integrals

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$\mu \otimes \underline{ u}$	$:= \oint_X \left(\oint_Y \underline{\delta}_{(x,y)} \underline{\nu}(\mathrm{d}y) \right) \mu(\mathrm{d}x)$	Product measure

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$\mathbb{E}^{A}_{x \sim \underline{\mu}}[f(x)]$	$=\underline{\mu} \gg f$	Expectation

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$\mathbb{E}_{x \sim \mu}^{A}[f(x)]$	$=\mu\gg f$	Expectation
$\int_X \overline{f}(x)\underline{\mu}(\mathrm{d}x)$	$:= \overline{\mathbb{E}}_{x \sim \underline{\mu}}^{R}[f(x)]$	Lebesgue integral

Synthetic measure theory: Radon-Nikodym

Radon-Nikodym derivatives

- ▶ $\underline{\nu} \ll \mu$ when $\underline{\nu} = w \odot \mu$;
- w and v are **equal** $\underline{\mu}$ -almost everywhere when $w\odot \mu = v\odot \mu.$
- ▶ Measurable property: $P: X \to \mathsf{bool}$, induces $[P]: X \to [0, \infty]$
- ▶ P over X holds $\underline{\mu}$ -a.e. when [P] = 1 $\underline{\mu}$ -a.e..

Theorem (Radon-Nikodym)

Let $(\mathcal{C}, \mathrm{M})$ be a well-pointed measure category. For every $\underline{\nu} \lessdot \underline{\mu}$ in $\mathrm{M}\, X$, there exists a $\underline{\mu}$ -a.e. unique morphism $\frac{\mathrm{d}\underline{\nu}}{\mathrm{d}\underline{\mu}}: X \to R$ satisfying $\frac{\mathrm{d}\underline{\nu}}{\mathrm{d}\underline{\mu}} \odot \underline{\mu} = \underline{\nu}$.

Talk structure

- Probabilistic programming and Bayesian inference
- Synthetic measure theory
- Quasi-Borel spaces
- Inference representations
- Ongoing work
- ► Conclusion

Brief measure theory

Measures subsets of \mathbb{R}

Borel subsets $\mathcal{B}(\mathbb{R})$ as closure under:

- ▶ Intervals [a, b].
- Countable unions.
- Complements.

 $\varphi: \mathbb{R} \to \mathbb{R}$ is **measurable** when:

$$B \in \mathcal{B}(\mathbb{R}) \Longrightarrow \varphi^{-1}[B] \in \mathcal{B}(\mathbb{R})$$

Source of randomness

Key idea

Propagating randomness from discrete and continuous sampling:

$$\alpha: \mathbb{I} \to X$$

along "random elements":

- for measurable spaces: derived through measurable functions;
- ► for quasi-Borel spaces: axiomised through structure.

Objects

A quasi-Borel space $X = (|X|, M_X)$ consists of:

- ▶ a carrier set X;
- ightharpoonup a set of **random elements** $M_X\subseteq |X|^{\mathbb{I}}$

such that the random elements are closed under:

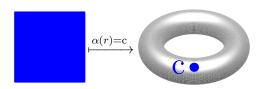
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▶ constant functions <u>c</u>;



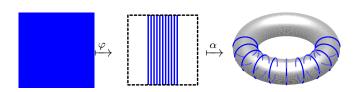
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such that the random elements are closed under:

- constant functions c;
- lacktriangledown precomposition with a measurable $arphi:\mathbb{I} o\mathbb{I}$



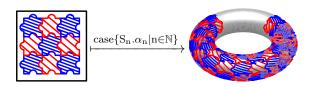
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- ▶ constant functions <u>c</u>;
- lacktriangledown precomposition with a measurable $arphi:\mathbb{I} o\mathbb{I}$
- countable measurable case split.



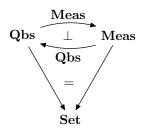
Morphisms
$$f:X\to Y$$
 Functions $f:|X|\to |Y|$ such that:
$$\alpha\in M_X \qquad \Longrightarrow \qquad f\circ\alpha\in M_Y$$

Measurable spaces

Adjunction with measurable spaces $(M \in \mathcal{C}Meas, X \in \mathbf{Qbs})$:

$$M_{\mathbf{Qbs}M} := \mathcal{C}Meas(\mathbb{R}, M)$$

 $\Sigma_{(\mathcal{C}MeasX)} := \{ B \subseteq X | \forall \alpha \in M_X, \alpha^{-1}[X] \in \mathcal{B}(\mathbb{R}) \}$



NB: $CMeas \circ \mathbf{Qbs}X = X$ for standard Borel spaces X.

Free and cofree spaces

Equip a set $A \in \mathbf{Set}$ with:

$$\begin{array}{ll} M_{\mathrm{Free}A} \ := \big\{ \mathrm{case} \, \{S_n.\underline{a}_n | n \in \mathbb{N} \} \big| (S_n) \ \text{a measurable partition} \big\} \\ M_{\mathrm{Cofree}A} := A^{\mathbb{R}} \end{array}$$



Products

Correlated random elements:

$$M_{X\times Y}:=\left\{r\mapsto \left(\alpha(r),\beta(r)\right)\middle|\alpha\in M_X,\beta\in M_Y\right\}$$

Function spaces

$$\begin{split} \left| Y^X \right| &:= \mathbf{Qbs}(X,Y) \\ M_{Y^X} &:= \left\{ f: \mathbb{R} \to \left| Y^X \right| \middle| \mathsf{uncurry} \ f \in \mathbf{Qbs}(\mathbb{R} \times X,Y) \right\} \end{split}$$

$$\mathsf{NB} \colon X^\mathbb{R} = M_X$$

Subspaces

Every subset $S \subseteq |X|$ inherits the subspace structure:

$$M_S := \{ \alpha : \mathbb{R} \to S | \alpha \in M_X \}$$

equiv. a strong sub-object.

Subspaces

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More structure

Coproducts, limits, colimits, Grothendieck quasi-topos, locally presentable, . . .

The commutative monad

Measures

 (Ω, α, μ) :

- $ightharpoonup \Omega$ is a standard Borel space
- $\alpha \in X^{\Omega}$
- and μ is a σ -finite measure on Ω

Induced integration operator

For $f: X \to [0, \infty]$:

$$\int f d(\Omega, \alpha, \mu) := \int_{\Omega} f(\alpha(x)) \mu(dx)$$

Monad of measures

 $(\Omega,\alpha,\mu)\approx (\Omega',\alpha',\mu')$ when they determine the same integration operator.

MX consists of equivalence classes of \approx .

A synthetic model

The measure category $(\mathbf{Qbs}, \underline{\mathbf{M}})$

- $\mathbf{Qbs}(\mathbb{1}, R) \cong_{\sigma} [0, \infty];$
- ▶ $\mathbf{Qbs}(R, \mathbb{1} + \mathbb{1}) \cong \mathcal{B}([0, \infty])$ as characteristic functions
- ▶ $\mathbf{Qbs}(R,R) \cong \mathbf{Meas}([0,\infty],[0,\infty])$
- ▶ Giry $[0,\infty] \rightarrowtail \mathbf{Qbs}(\mathbb{1},\mathrm{M}(R)) \rightarrowtail \mathsf{Measures}\ [0,\infty]$
- ▶ $R^R \times M(R) \to R$, $(f,\underline{\mu}) \mapsto \int f(x)\,\underline{\mu}(\mathrm{d}x)$ is the Lebesgue integral

Talk structure

- Probabilistic programming and Bayesian inference
- Synthetic measure theory
- Quasi-Borel spaces
- ► Inference representations
- Ongoing work
- ► Conclusion

$$\boxed{\text{Model}} \vdash \boxed{\text{IR}_1} \vdash \stackrel{t_1}{\longleftarrow} \boxed{\text{IR}_2} \vdash \stackrel{t_2}{\longleftarrow} \cdots \vdash \stackrel{t_{n-1}}{\longleftarrow} \boxed{\text{IR}_n} \vdash \boxed{\text{Sampler}}$$

Program representation

A representation \underline{T} $(T, \text{return}^{\underline{T}}, \gg \underline{T}, m^{\underline{T}})$ consists of:

- ▶ $(T, \text{return}^{\underline{T}}, \gg = \underline{T})$: monadic interface;
- ▶ $m_X^T: TX \to MX$: meaning morphism for every space X and m^T preserves return^T and $\gg = T$:

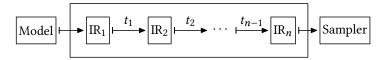
$$\operatorname{return}^{\underline{\mathbf{M}}} x = m(\operatorname{return}^{\underline{T}} x)$$

$$m(a \gg T f) = (m a) \gg M \lambda x. m(f x)$$

$$\boxed{\text{Model}} \longmapsto \boxed{\text{IR}_1} \longmapsto \boxed{\text{IR}_2} \longmapsto \cdots \longmapsto \boxed{\text{R}_n} \longmapsto \boxed{\text{Sampler}}$$

Example representation: lists

$$\begin{array}{ll} \textbf{instance} \ Rep \ (\textbf{List}) \ \textbf{where} \\ \textbf{return} \ x &= [x] \\ x_s \gg = f &= \mathsf{foldr} [\] \\ &\qquad \qquad (\lambda(x,y_s). \\ &\qquad \qquad f(x) + y_s) \ x_s \\ m_{\mathsf{List}} [x_1, \dots, x_n] = \sum_{i=1}^n \underline{\delta}_{x_i} \end{array}$$

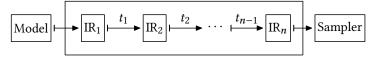


Sampling representation

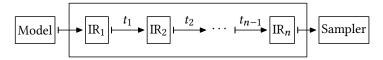
$$(T, \text{return}^{\underline{T}}, \gg = \underline{T}, m^{\underline{T}}, \mathbf{sample}^{\underline{T}})$$

- ► $(T, \text{return}^{\underline{T}}, \gg = \underline{T}, m^{\underline{T}})$: program representation
- $ightharpoonup \mathbf{sample}^{\underline{T}}: \mathbb{1} \to T\mathbb{I}$

and
$$m^{\underline{T}} \circ \mathbf{sample}^{\underline{T}} = \mathbf{U}_{\mathbb{I}}$$



Example: free sampler

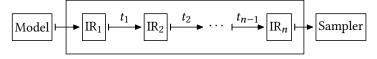


Conditioning representation

$$(T, \text{return}_{\underline{T}}, \gg \underline{T}, m_{\underline{T}}, \text{score}_{\underline{T}})$$

- $ightharpoonup (T, \text{return} \underline{T}, \gg \underline{T}, m\underline{T})$: program representation
- $\operatorname{score}^{\underline{T}}:[0,\infty)\to T\,\mathbb{1}$

and
$$m^{\underline{T}} \circ \operatorname{score}^{\underline{T}} r = r \odot \underline{\delta}_{()}$$



Weighted values

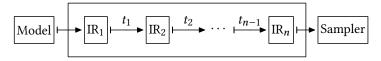
For every representation \underline{T} , $W \underline{T} X := T(\mathbb{R}_+ * X)$

instance Conditioning Rep (W
$$\underline{T}$$
) where

return_{W \underline{T}} $x = \text{return}^{\underline{T}}(1, x)$
 $a \gg_{\underline{W}\underline{T}} f = \underline{T}.\mathbf{do} \{(r, x) \leftarrow a;$
 $(s, y) \leftarrow f(x);$

return $(r \cdot s, y)$ }
 $m_{\underline{W}\underline{T}} a = \lambda x. \oint_{\mathbb{R}_{+} \times X} r \odot \underline{\delta}_{x} m^{\underline{T}}(a) (dr, dx)$

score_{W \underline{T}} $r = \text{return}^{\underline{T}}(r, ())$



Inference representation

 $(T, \text{return}^{\underline{T}}, \gg =^{\underline{T}}, \mathbf{sample}^{\underline{T}} \text{score}^{\underline{T}}, m^{\underline{T}})$: sampling and conditioning

Example: weighted sampler

$$\operatorname{WSam} X := \operatorname{W} \operatorname{Sam} X = \operatorname{Sam}([0,\infty) \times X)$$

Inference transformations

$$\underline{t}: \underline{T} \to \underline{S}$$

 $\underline{t}:T\:X\to S\:X$ for every space X such that:

$$m_{\underline{S}} \circ \underline{t} = m_{\underline{T}}$$

A single compositional step in an inference algorithm

Inference transformations

$$\underline{t}: \underline{T} \to \underline{S}$$

 $\underline{t}:TX\to SX$ for every space X such that:

$$m_{\underline{S}} \circ \underline{t} = m_{\underline{T}}$$

A single compositional step in an inference algorithm

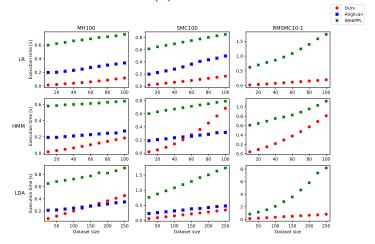
Unnaturality

$$\operatorname{aggr}_X : \operatorname{List}(\mathbb{R}_+ * X) \to \operatorname{List}(\mathbb{R}_+ * X)$$
 aggregating (r,x) , (s,x) to $(r+s,x)$ Then $\operatorname{aggr} : \operatorname{List} \to \operatorname{List}$ but not natural:

$$\begin{split} \operatorname{aggr} \circ \mathsf{List!} \ & [(\tfrac{1}{2},\mathsf{False}),(\tfrac{1}{2},\mathsf{True})][(1,())] \\ & \neq [(\tfrac{1}{2},()),(\tfrac{1}{2},())] \ \mathsf{Enum!} \circ \operatorname{aggr} \ [(\tfrac{1}{2},\mathsf{False}),(\tfrac{1}{2},\mathsf{True})] \end{split}$$

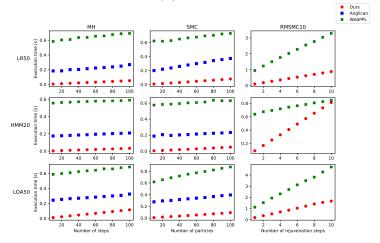
MonadBayes: Modular implementation

Performance evaluation (1)



MonadBayes: Modular implementation

Performance evaluation (2)



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Ongoing work: term and type recursion

ω -quasi-Borel spaces

$$P = (|P|, \leq_P, M_P)$$
:

- ▶ (P, \leq_P) is an ω -cpo;
- $ightharpoonup (P, M_P)$ is a qbs; and
- $Qbs \xrightarrow{\simeq} Mod(qbs, Set) \xrightarrow{\simeq} Qbs$ $Set \xrightarrow{Set} Set$

→ Mod(ωabs, Set) -

• M_P is pointwise ω -chain closed.

and Scott-continuous qbs-morphisms

Axiomatic domain theory [Fiore'94]

Model of Fiore's axiomatic domain theory, with admissible maps $f:P\rightarrowtail Q$ are Scott-open and **Borel open**:

$$f[P] \in \Sigma_Q = \left\{ S \subseteq |Q| \middle| \forall \alpha \in M_Q.\alpha^{-1}[S] \in \mathcal{B} \right\}$$

Contribution

Correctness of inference

- Modular validation of inference algorithms: Sequential Monte Carlo, Trace Markov Chain Monte Carlo By combining:
- Synthetic measure theory [Kock'12]: measure theory without measurable spaces
- Quasi-Borel spaces: a convenient category for higher-order measure theory [LICS'17]

Conclusion

Summary

- Bayesian inference: (continuous) sampling and conditioning
- Inference representation: monadic interface, sampling, conditioning, and meaning
- Plenty of opportunities for traditional programming language expertise

Further topics

- Sequential Monte Carlo (SMC)
- Markov Chain Monte Carlo (MCMC) and Metropolis-Hastings-Green Theorem for Qbs
- Combining SMC and MCMC into Move-Resample SMC