## Quantitative Equational Reasoning

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# Outline

## Introduction

- 2 Equational reasoning
- 3 Categorical algebra

## 4 Metrics

Quantitative equations

## 6 Examples

- Equations are at the heart of mathematical reasoning.
- Reasoning about programs is also based on program equivalences.
- A trinity of ideas: Equationally given algebras, Lawvere theories, Monads on Set
- The dawning of the age of quantitative reasoning.
- We want quantitative analogues of algebraic reasoning.
- (Pseudo)metrics instead of equivalence relations.
- Equality indexed by a real number  $=_{\epsilon}$ .
- Monads on Met.
- Enriched Lawvere theories?

- Signature  $\Omega = \{(Op_i, n_i) | i = 1 \dots k\}$
- Terms  $t ::= x | Op(t_1, \ldots, t_n)$
- Equations s = t
- Axioms, sets of equations Ax
- Deduction  $Ax \vdash s = t$
- Usual rules for deduction: equivalence relation, congruence,...
- Theories: set of equations closed under deduction.

## Equational deduction rules

• Axiom  $Ax \vdash s = t$  if  $s = t \in Ax$ 

Equivalence

$$\overline{Ax \vdash t = t}$$

$$\underline{Ax \vdash s = t, Ax \vdash t = u}$$

$$\overline{Ax \vdash s = u}$$

$$\underline{Ax \vdash s = t}$$

$$\overline{Ax \vdash t = s}$$

#### Congruence

$$\frac{Ax \vdash t_1 = s_1, \dots, Ax \vdash t_n = s_n}{Ax \vdash Op(t_1, \dots, t_n) = Op(s_1, \dots, s_n)}$$

Substitution

$$\frac{Ax \vdash t = s}{Ax \vdash t[u/x] = s[u/x]}$$

- We assume that that there is one set of "basic things" one-sorted algebras.
- Fix a set  $\Omega$  of *operations*, each with a fixed arity  $n \in \mathbb{N}$ . These include *constants* as arity zero "operations." Such an  $\Omega$  is called a signature.
- Everything has finite arity.
- As Ω-algebra A is a set A to interpret the basic sort and, for each operation f of arity n a function f<sub>A</sub> : A<sup>n</sup> → A.

- Can define homomorphisms and subalgebras easily.
- What about equations that are required to hold?
- Given a set X we define the term algebra generated by X, TX
- The elements of *X* are in *TX*.
- If  $t_1, \ldots, t_n$  are in *TX* and *f* has arity *n* then  $f(t_1, \ldots, t_n)$  is in *TX*.

- Want to write things like  $\forall x, y, z; f(x, f(y, z)) = f(f(x, y), z)$ .
- X, set of variables.
- Let *s*, *t* be terms in *TX*, we say the equation s = t holds in an  $\Omega$ -algebra  $\mathcal{A}$  if for every homomorphism  $h : TX \to \mathcal{A}$  we have h(s) = h(t) where, in the latter, = means identity.
- Let S be a set of equations between pairs of terms in TX. We define a *congruence relation* ∼<sub>S</sub> on TX in the evident way.

- Easy to check that if  $t_1 \sim_S s_1, \ldots, t_n \sim_S s_n$  then  $f(t_1, \ldots, t_n) \sim_S f(s_1, \ldots, s_n)$  we can define  $f_{\sim_S}$  on  $TX / \sim_S$ .
- Let [t] be an equivalence class of ∼<sub>S</sub>; f<sub>∼S</sub>([t<sub>1</sub>],..., [t<sub>n</sub>]) is well defined by [f(t<sub>1</sub>,..., t<sub>n</sub>)].
- A class of Ω-algebras satisfying a set of equations is called a variety of algebras (not the same as an algebraic variety!).
- When are a set of equations bad? If we can derive *x* = *y* from *S* then the only algebras have one element.

- Monoids, groups, rings, lattices, boolean algebras are all examples.
- Vector spaces have two sorts.
- Fields are annoying because we have to say *x* ≠ 0 implies *x*<sup>-1</sup> exists. Fields do not form an equational variety.
- Sometimes we need to state conditional equations; these are called *Horn clauses*. Example: cancellative monoids, x ⋅ y = x ⋅ z ⊢ y = z.
- Stacks are equationally definable but queues are not.

• Signature:

$$\{+_{\varepsilon}|\varepsilon\in[0,1]\}$$

Axioms:

$$(B_1) \vdash t + t t' = t$$
  

$$(B_2) \vdash t + \epsilon t = t$$
  

$$(SC) \vdash t + \epsilon t' = t' + 1 - \epsilon t$$
  

$$(SA) \vdash (t + \epsilon t') + \epsilon' t'' = t + \epsilon \epsilon' (t' + \frac{\epsilon' - \epsilon \epsilon'}{1 - \epsilon \epsilon'} t'')$$

# Universal properties

- Let K(Ω, S) be the collection of algebras satisfying the equations in S. K(Ω, S) becomes a category if we take the morphisms to be Ω-homomorphisms.
- Let X be a set of generators. We write T[X] for TX/ ∼<sub>S</sub>. There is a map η<sub>X</sub> : X → T[X] given by η<sub>X</sub>(x) = [x].
- Universal property.

Set 
$$\mathbb{K}(\Omega, S)$$

### Birkhoff

A collection of algebras is a variety of algebras if and only if it is closed under homomorphic images, subalgebras and products.

There are analogoues results for algebras defined by Horn clauses: quasivariety theorems.

#### Example

Consider  $\mathbb{Z}_2 \times \mathbb{Z}_2$ . It's not a field because, *e.g.*  $(1,0) \times (0,1) = (0,0)$ . Hence fields cannot be described by equations!

- Capturing universal algebra categorically.
- Data: (i) Endofunctor  $T : \mathbb{C} \to \mathbb{C}$ , (ii)  $\eta : I \to T$  natural, and (iii)  $\mu : T^2 \to T$  also natural.
- Some diagrams are required to commute.



• Examples: powerset, "free" constructions *e.g.* monoid, group, the Giry monad.

- From a monad *T* : C → C make a new category: the Kleisli category C<sub>T</sub>.
- Objects, the same as those of C.
- Morphisms  $f : A \to B$  in  $\mathcal{C}_T$  are  $f : A \to TB$  in  $\mathcal{C}$ .
- Composition?  $f : A \rightarrow TB$  and  $g : B \rightarrow TC$  don't match.
- $f: A \rightarrow TB$  and  $Tg: TB \rightarrow T^2C$  to match but we are in  $T^2C$ .
- Compose with  $\mu_C: T^2C \to TC$  to get  $A \to TC$ .
- The Kleisli category of the powerset monad is the category of sets and relations.

- Mes: objects are sets equipped with a  $\sigma$ -algebra  $(X, \Sigma)$ , morphisms  $f : (X, \Sigma) \to (Y, \Lambda)$  are functions  $f : X \to Y$  such that  $\forall B \in \Lambda, f^{-1}(B) \in \Sigma$ .
- $\mathcal{G}$  : Mes  $\rightarrow$  Mes,  $\mathcal{G}(X, \Sigma) = \{p | p \text{ is a probability measure on } \Sigma\}.$
- For each  $A \in \Sigma$ , define  $e_A : \mathcal{G}(X) \to [0, 1]$  by  $e_A(p) = p(A)$ . Equip  $\mathcal{G}(X)$  with the smallest  $\sigma$ -algebra making all the  $e_A$  measurable.
- $f: X \to Y, \ \mathfrak{G}(f): \mathfrak{G}(X) \to \mathfrak{G}(Y)$  given by  $\mathfrak{G}(f)(p)(B \in \Lambda) = p(f^{-1}(B)).$

- $\eta_X : X \to \mathcal{G}(X)$  given by  $\eta_X(x) = \delta_x$ , where  $\delta_x(A) = 1$  if  $x \in A$  and 0 if  $x \notin A$ .
- $\mu_X(Q \in \mathcal{G}^2(X))(A) = \int e_A dQ$ . Averaging over  $\mathcal{G}$  using Q.
- Probabilistic analogue of the powerset.

- Objects: Same as **Mes**, morphisms from *X* to *Y* are measurable functions from *X* to  $\mathcal{G}(Y)$ .
- Compose: h: X → G(Y), k: Y → G(Z) by the formula: (kõh) = (µZ) ∘ (G(k)) ∘ h where õ is the Kleisli composition and ∘ is composition in Mes.
- Curry the definition of morphism:  $h: X \times \Sigma_Y \rightarrow [0, 1]$ . Markov kernels. We call this category **Ker**. Probabilistic relations.
- Composition in terms of kernels: (kõh)(x, C ⊂ Z) = ∫k(y, C)h(x, ·). Relational composition, matrix multiplication.

# The Eilenberg-Moore category

- From *T* we can construct a category of algebras: objects  $a : TA \rightarrow A$
- and morphisms  $f : A \rightarrow B$  such that

$$TA \xrightarrow{a} A$$

$$Tf \downarrow \qquad \qquad \downarrow f$$

$$TB \xrightarrow{b} B$$

commute.

- Many categories of algebras (monoids, groups, rings, lattices) can be reconstructed this way.
- The Kleisli category = the category of "free" algebras.
- We get a monad on Set from X → T[X]. The Eilenberg-Moore category for this monad is isomorphic to K(Ω, S).
- Algebras for a monad 
   Algebras given by equations and operations.

- Quantitative analogue of an equivalence relation.
- Space *M*, (pseudo)metric  $d: M \times M \to \mathbb{R}^{\geq 0}$
- d(x, x) = 0, d(x, y) = d(y, x) and  $d(x, z) \le d(x, y) + d(y, z)$ .
- If d(x, y) = 0 implies x = y we say d is a **metric**.
- We can define usual notions of convergence, completeness, topology, continuity etc.
- Maps:  $f(X, d) \rightarrow (Y, d')$  are *nonexpansive*  $d'(f(x), f(y)) \leq d(x, y)$ ; automtically continuous
- We define  $\mathcal{M}$ : objects metric spaces, morphisms are nonexpansive functions.
- Quantitative equations give monads on  $\mathcal{M}$ .

## Metrics between probability distributions

Let p, q be probability distributions on  $(X, d, \Sigma)$ .

• Total variation  $tv(p,q) = \sup_{E \in \Sigma} |p(E) - q(E)|$ .

• Kantorovich:  $\kappa(p,q) = \sup_{f} |\int f dp - \int f dq|$  where f is nonexpansive.

- A *coupling* π between *p*, *q* is a distribution on *X* × *X* such that the marginals of π are *p*, *q*. Write C(*p*, *q*) for the space of couplings.
- Kantorovich:  $\kappa(p,q) = \inf_{\mathfrak{C}(p,q)} \int_{X \times X} d(x,y) d\pi(x,y).$ Kantorovich-Rubinshtein duality.
- Wasserstein:  $W^{(l)}(p,q) = \inf_{\mathcal{C}(p,q)} \left[ \int_{X \times X} d(x,y)^l d\pi(x,y) \right]^{1/l}$ . l = 1 gives Kantorovich.
- $W^{(l)}(\delta_x, \delta_y) = d(x, y).$

- Signature  $\Omega$ , variables *X* we get terms  $\mathbb{T}X$ .
- Quantitative equations:  $\mathcal{V}(\mathbb{T}X)$ :

$$s =_{\varepsilon} t$$
,  $s, t \in \mathbb{T}X$ ,  $\varepsilon \in \mathbb{Q} \cap [0, 1]$ 

- A substitution σ is a map X → TX; we write Σ(X) for the set of substitutions.
- Any  $\sigma$  extends to a map  $\mathbb{T}X \to \mathbb{T}X$ .
- Quantitative inferences:  $\mathcal{E}(\mathbb{T}X) = \mathcal{P}_{fin}(\mathcal{V}(\mathbb{T}X)) \times \mathcal{V}(\mathbb{T}X)$

$$\{s_1 =_{\varepsilon_1} t_1, \ldots, s_n =_{\varepsilon_n} t_n\} \vdash s =_{\varepsilon} t$$

# **Deducibility relations**

(Refl) 
$$\emptyset \vdash t =_0 t$$
  
(Symm)  $\{t =_{\varepsilon} s\} \vdash s =_{\varepsilon} t$ .  
(Triang)  $\{t =_{\varepsilon} s, s =_{\varepsilon'} u\} \vdash t =_{\varepsilon + \varepsilon'} u$ .  
(Max) For  $e' > 0$ ,  $\{t =_{\varepsilon} s\} \vdash t =_{\varepsilon + \varepsilon'} s$ .  
(Arch) For all  $\varepsilon \ge 0$ ,  $\{t =_{\varepsilon'} s \mid \varepsilon' > \varepsilon\} \vdash t =_{\varepsilon} s$ . Infinitary!  
(NExp) For  $f : n \in \Omega$ ,  
 $\{t_1 =_{\varepsilon} s_1, \dots, t_n =_{\varepsilon} s_n\} \vdash f(t_1, \dots t_n) =_{\varepsilon} f(s_1, \dots s_i, \dots s_n)$   
(Subst) If  $\sigma \in \Sigma(X)$ ,  $\Gamma \vdash t =_{\varepsilon} s$  implies  $\sigma(\Gamma) \vdash \sigma(t) =_{\varepsilon} \sigma(s)$ .  
(Cut) If  $\Gamma \vdash \phi$  for all  $\phi \in \Gamma'$  and  $\Gamma' \vdash \psi$ , then  $\Gamma \vdash \psi$ .  
(Assumpt) If  $\phi \in \Gamma$ , then  $\Gamma \vdash \phi$ .

- Given S ⊂ E(TX), ⊢<sub>S</sub>: smallest deducibility relation containing S.
- Equational theory:  $\mathcal{U} = \vdash_{S} \bigcap \mathcal{E}(\mathbb{T}X)$ .

•  $\Omega$ : signature;  $\mathcal{A} = (A, d)$ ,

A an  $\Omega$ -algebra and (A, d) a metric space.

- All functions in  $\Omega$  are nonexpansive.
- Morphisms are Ω-algebra homomorphisms that are nonexpansive.
- $\mathbb{T}X$  is an  $\Omega$ -algebra.  $\sigma : \mathbb{T}X \to A$ ,  $\Omega$ -homomorphism.

• (A, d) satisfies 
$$\{s_i = \varepsilon_i t_i / i = 1, ..., n\} \vdash s = \varepsilon t$$
 if

$$\forall \sigma, \ d(\sigma(s_i), \sigma(t_i)) \leq \varepsilon_i, \ i = 1, \dots, n$$
  
implies  
$$d(\sigma(s), \sigma(t)) \leq \varepsilon.$$

- We write  $\{s_i =_{\varepsilon_i} t_i / i = 1, ..., n\} \models_{\mathcal{A}} s =_{\varepsilon} t$ .
- We write  $\mathbb{K}(\mathcal{U}, \Omega)$  for the algebras satisfying  $\mathcal{U}$ .

$$d^{\mathcal{U}}(s,t) = \inf\{\varepsilon \mid \emptyset \vdash s =_{\varepsilon} t \in \mathcal{U}\}$$

Why not use the following?

 $d^{\mathcal{U}}(s,t) = \inf\{\varepsilon \mid \forall V \in \mathcal{P}_f(\mathcal{V}(X)), V \vdash s =_{\varepsilon} t \in \mathcal{U}\}$ 

- They are the same!
- The (pseudo)metric can take on infinite values.
- The kernel is a congruence for  $\Omega$ .
- If we take the quotient we get an (extended) metric space.
- The resulting algebra is in  $\mathbb{K}(\Omega, \mathcal{U})$ .
- We can do this for any set M of generators and produce a "free" quantitative algebra.

#### $\forall \mathcal{A} \in \mathbb{K}(\mathcal{U}, \Omega), \Gamma \models_{\mathcal{A}} \varphi \text{ if and only if } [\Gamma \vdash \varphi] \in \mathcal{U}.$

- Analogue of the usual completeness theorem for equational logic.
- Right to left is by definition.
- Left to right is by a model construction.
- The proof needs to deal with quantitative aspects and uses the archimedean property.

- Starting from a metric space (M, d) we can define TM by adding constants for each m ∈ M
- and axioms  $\emptyset \vdash m =_e n$  for every rational e such that  $d(m, n) \leq e$ .
- Call this extended signature  $\Omega_M$  and the extended theory  $\mathcal{U}_M$ .
- Any algebra in K(U<sub>M</sub>, U<sub>M</sub>) can be viewed as an algebra in K(Ω, U) by forgetting about the interpretation of the constants from M.
- Given any α : M → A non-expansive we can turn A = (A, d) into an algebra in K(Ω<sub>M</sub>, U<sub>M</sub>) by interpreting each m ∈ M as α(m) ∈ A.



 $\mathcal{U}_M$  is consistent if and only if the map  $\eta_M$  is an isometry.

We have a monad on  $\mathcal{M}$ .

- $\Omega = \{+_e : 2 | e \in [0, 1]\};$  uncountably many operations!
- **(B1)**  $\emptyset \vdash x +_1 y =_0 x$
- (B2)  $\emptyset \vdash x +_e x =_0 x$
- (SC)  $\emptyset \vdash x +_e y =_0 y +_{1-e} x$
- $(SA)(x + e_1 y) + e_2 z =_0 x + e_1 e_2 (y + \frac{e_2 e_1 e_2}{1 e_1 e_2} z)$  where  $e_1, e_2 \in (0, 1)$
- (LI)  $x +_e z =_{\varepsilon} y +_e z$  where  $e \leq \varepsilon \in \mathbb{Q} \cap [0, 1]$
- The last equation uses one of the new indexed equations in a nontrivial way.
- We call it the *left-invariant* axiom scheme; LIB algebras for short.
- What does this axiomatize?
- The total variation metric on probability distributions.

$$TV(p,q) = \sup_{E \in \Sigma} |p(E) - q(E)|.$$

- It measures the size of the set on which *p*, *q* disagree the most.
- There is a duality theorem that gives it as a minimum rather than a maximum.

- Let B(M, Σ) be the Borel measures on a metric space M with Borel algera Σ.
- We have a product space *M* × *M* with product σ-algebra Σ ⊗ Σ and Borel measures B(*M* × *M*, Σ ⊗ Σ).
- Given probability measures *p*, *q* a *coupling* is a probability measure ω on (*M* × *M*, Σ ⊗ Σ) such that for all *E* ∈ Σ:

 $\omega(E \times M) = p(E)$  and  $\omega(M \times E) = q(E)$ .

•  $\mathcal{C}(p,q)$  is the set of couplings for (p,q).

- Write  $\Delta$  for the diagonal in  $M \times M$ .
- TV duality:  $TV(p,q) = \min \{ \omega(\Delta^c) | \omega \in \mathcal{C}(p,q) \}$ ; min is attained.
- Convex combinations of couplings are couplings.
- Splitting lemma: If p, q are Borel probability measures on M and e = T(p, q). There are p', q', r such that

$$p = ep' + (1 - e)r$$
 and  $q = eq' + (1 - e)r$ .

- We know there is a freely generated LIB algebra from a metric space *M*. What is it concretely?
- Let ∏[M] be the LIB algebra obtained by taking the finitely-supported probability measures on M and interpreting +<sub>e</sub> as convex combination.
- We endow it with the total-variation metric to make it a quantitative algebra.

- Theorem:  $\Pi[M] \in \mathbb{K}(\mathcal{B}, \mathcal{U}^{LI}).$
- Use convexity and splitting lemma to show LI and Nexp.
- Theorem:  $\Pi[M]$  is the free algebra generated by *M*.
- Use the embedding of convex spaces into vector spaces (Stone 49).
- The axioms give rise to the total-variation metric.

## Interpolative barycentric algebras

- Same signature as barycentric algebras.
- Axioms (B1), (B2), (SC), (SA); drop (LI).

• (IB<sub>p</sub>)  $\{x =_{\varepsilon_1} y, x' =_{\varepsilon_2} y'\} \vdash x +_e x' =_{\delta} y +_e y',$ 

where  $(e\varepsilon_1^p + (1-e)\varepsilon_2^p)^{1/p} \leq \delta$ .

- Now we need assumptions in the equation.
- If p = 1 we get

$$\{x =_{\varepsilon_1} y, x' =_{\varepsilon_2} y'\} \vdash x +_e x' =_{\delta} y +_e y',$$

where  $e\varepsilon_1 + (1-e)\varepsilon_2 \leq \delta$ .



## Kantorovich-Wasserstein metric

Let (M, d) be a complete separable metric space and  $p \ge 1$ .

### Wasserstein-*p* metric

$$W_d^p(\mu,\nu) = \inf\left\{\left[\int_{M\times M} d^p(x,y)d\omega\right]^{1/p} \middle| \omega \in \mathcal{C}(\mu,\nu)\right\}$$

### Kantorovich

$$K_d(\mu, \nu) = \sup\left\{\left|\int f d\mu - \int f d\nu\right|\right\}$$

### Duality

$$K_d(\mu, \nu) = \min\left\{ \left[ \int_{M \times M} d(x, y) d\omega \right] \middle| \omega \in \mathcal{C}(\mu, \nu) \right\}$$

Panangaden (McGill)

Quantitative Equational Reasoning

- We take the finitely supported measures on *M* and interpret it as a barycentric algebra as before.
- We give it the Wasserstein metric and show that we get an IB algebra.
- This uses the definition of the  $W_d^p$  metrics as an inf and convexity of couplings.
- We prove a splitting lemma for this case and show that we get the free algebra by similar, but more involved arguments.
- How do we lift it to the continuous case?

- Suppose we have a sequence of measures {µ<sub>i</sub>|i ∈ I}. What does it mean to converge?
- For a "suitable" class of functions:

$$\int f \mathrm{d}\mu_i \to \int f \mathrm{d}\mu.$$

- For Kantorovich use contractive functions; for Wasserstein use a class of functions whose growth is controlled by *d* and *p*.
- The Wasserstein metrics give the topology of weak convergence on measures of finite *p*-moment.
- The finitely supported probability measures are *dense* in the space of all probability measures with weak topology.

- A separable metric space has a countable dense subset.
- Define  $\Delta[M]$  to be the space of all Borel probability measures on a complete separable metric space. We give it the  $W_d^p$  metric and interpret  $+_e$  as convex combination.
- This gives an IB algebra.
- If we construct the term algebra T[M] as before and *complete it* we get an algebra isomorphic to Δ[M].
- In this case we get a monad on **CSMet**<sub>1</sub>: complete separable 1-bounded metric spaces.

- Quantitative equations give a handle on otherwise arcane things like the Wasserstein metrics.
- Other examples: Hausdorff metric, pointed barycentric algebras.
- To do; many more examples:
  - Markov processes
  - Choquet capacities and games
  - quantitative theory of effects
  - quantitative equational axioms for probabilistic programming languages.