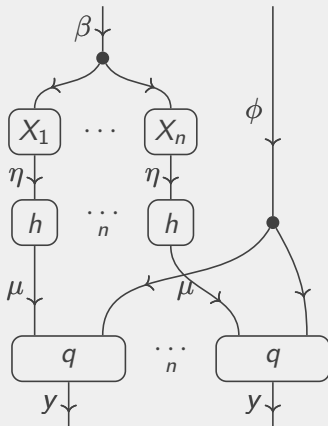


The Algebra of Statistical Theories and Models

MIT Categories Seminar

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Structuralism about statistical models

Statistical models

- (1) are *not* black boxes, but have meaningful **internal structure**
- (2) are *not* uniquely determined, but bear meaningful **relationships** to alternative, competing models
- (3) are sometimes purely phenomenological, but are often derived from, or at least motivated by, more general **scientific theory**

This project aims to understand (1) and (2) via categorical logic.

Statistical models, classically

A **statistical model** is a parameterized family $\{P_\theta\}_{\theta \in \Omega}$ of probability distributions on a common space \mathcal{X} :

- Ω is the **parameter space**
- \mathcal{X} is the **sample space**

Think of a statistical model as a data-generating mechanism

$$P : \Omega \rightarrow \mathcal{X}.$$

Statistical inference aims to approximately invert this mechanism: find an **estimator** $d : \mathcal{X} \rightarrow \Omega$ such that

$$d(X) \approx \theta \quad \text{whenever} \quad X \sim P_\theta.$$

Statistical models, classically

This setup goes back to Wald's [statistical decision theory](#) (Wald 1939; Wald 1950). Within it, one can already:

- define general concepts like *sufficiency* and *ancillarity*
- establish basic results like the *Neyman-Fisher factorization* and *Basu's theorem*

Recently, Fritz has shown that much of this may be reproduced in a purely synthetic setting (Fritz 2020)

However, the classical definition of statistical model abstracts away a large part of statistics:

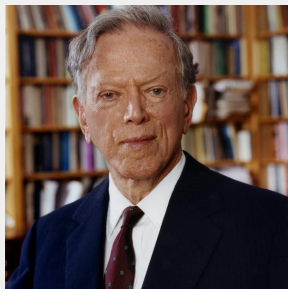
- (1) formalizes models as black boxes
- (2) does not formalize any relationships between different models

Models in logic and in science

Can **logic** help formalize the structure of statistical models?

Not a new idea to connect logical and scientific models.

I claim that the concept of model in the sense of Tarski may be used without distortion and as a fundamental concept in all of the disciplines... In this sense I would assert that the meaning of the concept of model is the same in mathematics and the empirical sciences. The difference to be found in these disciplines is to be found in their use of the concept. (Suppes 1961)



Patrick Suppes
(1922–2014)

The semantic view of scientific theories

Suppes initiated the “**semantic view**” of scientific theories:

- Many different flavors, from different philosophers (van Fraassen, Sneed, Suppe, Suppes, . . .)
- For Suppes, “to axiomatize a theory is to define a set-theoretical predicate” (Suppes 2002)

Difficulties for statistical models and beyond:

- After Suppes, proponents of the semantic view paid little attention to statistics
- Set theory is impractical to implement, esp. with probability
- Hard to make sense of relationships between logical theories

The algebraization of logic

Beginning with Lawvere's thesis (Lawvere 1963), [categorical logic](#) has achieved an *algebraization* of logic:

- Logical theories are replaced by categorical structures
- Distinction between syntax and semantics is blurred

Some consequences:

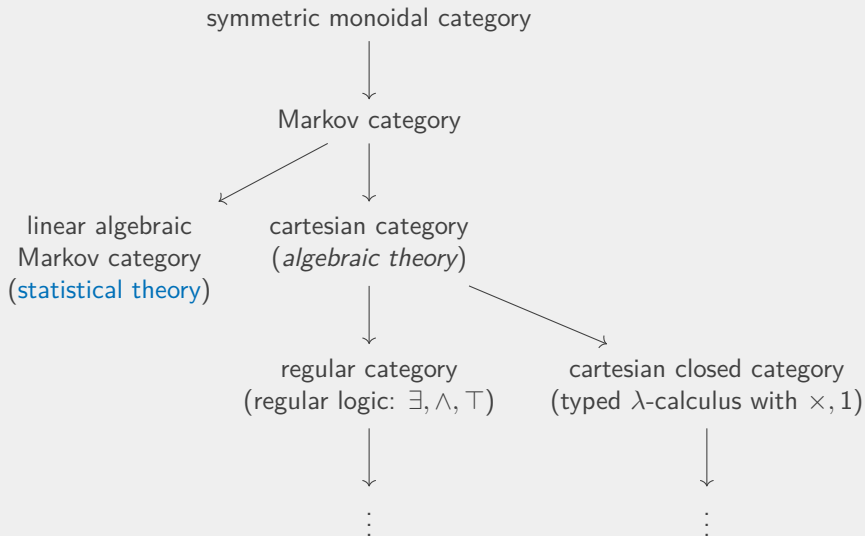
- Theories are *invariant* to presentation
- *Functorial semantics*, especially outside of **Set**
- “Plug-and-play” logical systems, via different categorical gadgets
- Theories have *morphisms*, which formalize relationships

Dictionary between category theory, logic, and statistics

Category theory	Mathematical logic	Statistics
Category T	Theory	Statistical theory [*]
Functor $M : T \rightarrow S$	Model	Statistical model
Natural transformation $\alpha : M \rightarrow M'$	Model homomorphism	Morphism of statistical model

^{*}Statistical theories (T, p) have extra structure, the sampling morphism $p : \theta \rightarrow x$

Statistics in the family tree of categorical logics

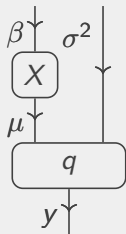


Informal example: linear models

A **linear model** with design matrix $X \in \mathbb{R}^{n \times p}$ has sampling distribution

$$y \sim \mathcal{N}_n(X\beta, \sigma^2 I_n) \quad \text{w/ parameters } \beta \in \mathbb{R}^p, \sigma^2 \in \mathbb{R}_+.$$

A **theory of a linear model** (LM, p) is generated by objects y, β, μ, σ^2 and morphisms $X : \beta \rightarrow \mu$ and $q : \mu \otimes \sigma^2 \rightarrow y$ and has sampling morphism p given by



Then a linear model is a functor $M : \text{LM} \rightarrow \mathbf{Stat}$.

Markov kernels

Statistical theories will have *functorial semantics* in a category of Markov kernels.

Recall: A **Markov kernel** $\mathcal{X} \rightarrow \mathcal{Y}$ between measurable spaces \mathcal{X}, \mathcal{Y} is a measurable map $\mathcal{X} \rightarrow \text{Prob}(\mathcal{Y})$.

Examples:

- A statistical model $(P_\theta)_{\theta \in \Omega}$ is a kernel $P : \Omega \rightarrow \mathcal{X}$ (Čencov 1965; Čencov 1982)
- Parameterized distributions, e.g., the normal family

$$\mathcal{N} : \mathbb{R} \times \mathbb{R}_+ \rightarrow \mathbb{R}, \quad (\mu, \sigma^2) \mapsto \mathcal{N}(\mu, \sigma^2)$$

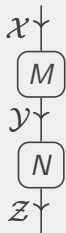
or, more generally, the d -dimensional normal family

$$\mathcal{N}_d : \mathbb{R}^d \times \mathcal{S}_+^d \rightarrow \mathbb{R}^d, \quad (\mu, \Sigma) \mapsto \mathcal{N}_d(\mu, \Sigma).$$

Synthetic reasoning about Markov kernels

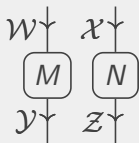
Two fundamental operations on Markov kernels:

1. **Composition**: For kernels $M : \mathcal{X} \rightarrow \mathcal{Y}$ and $N : \mathcal{Y} \rightarrow \mathcal{Z}$,



$$(M \cdot N)(dz | x) := \int_{\mathcal{Y}} N(dz | y)M(dy | x)$$

2. **Independent product**: For kernels $M : \mathcal{W} \rightarrow \mathcal{Y}$ and $N : \mathcal{X} \rightarrow \mathcal{Z}$,

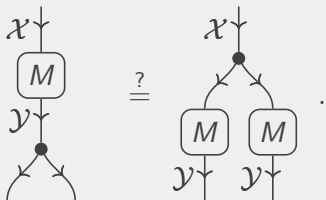


$$(M \otimes N)(w, x) := M(w) \otimes N(x)$$

Synthetic reasoning about Markov kernels

Also a supply of commutative comonoids, for **duplicating** and **discarding** data.

Markov kernels obey all laws of a cartesian category, except one:



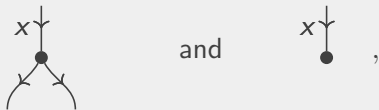
Proposition

Under regularity conditions, a Markov kernel $M : \mathcal{X} \rightarrow \mathcal{Y}$ is **deterministic** if and only if above equation holds.

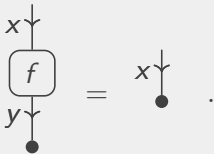
Markov categories

Markov categories are a minimalistic *axiomatization* of categories of Markov kernels (Fong 2012; Cho and Jacobs 2019; Fritz 2020).

Definition: A [Markov category](#) is a symmetric monoidal category with a supply of commutative comonoids

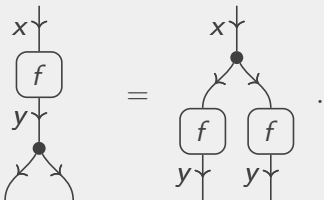


such that every morphism $f : x \rightarrow y$ preserves deleting:



Constructions in Markov categories

Definition: A morphism $f : x \rightarrow y$ in a Markov category is **deterministic** if



Besides (non)determinism, in a Markov category one can express:

- conditional independence and exchangeability
- disintegration, e.g., for Bayesian inference (Cho and Jacobs 2019)
- many notions of statistical decision theory (Fritz 2020)

Linear and other spaces for statistical models

In order to specify most statistical models, more structure is needed.

Much statistics happens in **Euclidean space** or structured subsets thereof:

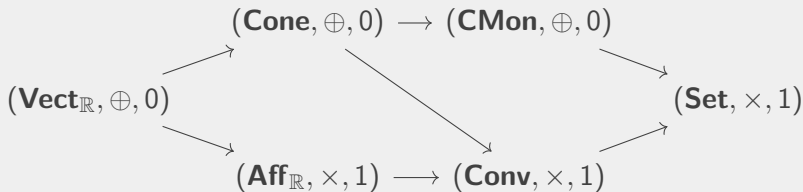
- real vector spaces
- affine spaces
- convex cones, esp. \mathbb{R}_+ or PSD cone $\mathcal{S}_+^d \subset \mathbb{R}^{d \times d}$
- convex sets, esp. $[0, 1]$ or probability simplex $\Delta^d \subset \mathbb{R}^{d+1}$

Also in discrete spaces:

- additive monoids, esp. \mathbb{N} or \mathbb{N}^k
- unstructured sets, say $\{1, 2, \dots, k\}$

Lattice of linear and other spaces

Such spaces belong to a lattice of symmetric monoidal categories:

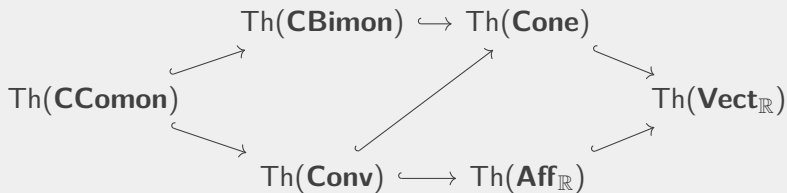


Note:

- **Cone** is category of *conical spaces*, abstracting convex cones
- **Conv** is category of *convex spaces*, abstracting convex sets

Supplying a lattice of PROPs

Dually, there is a lattice of theories (PROPs):



Definition: A **supply** of a meet-semilattice L of PROPs in a symmetric monoidal category (\mathbf{C}, \otimes, I) consists of a monoid homomorphism

$$P : (|\mathbf{C}|, \otimes, I) \rightarrow (L, \wedge, \top), \quad x \mapsto P_x,$$

and for each object $x \in \mathbf{C}$, a strong monoidal functor $s_x : P_x \rightarrow \mathbf{C}$ with $s_x(m) = x^{\otimes m}$, subject to coherence conditions (mildly generalizing Fong and Spivak 2019).

Linear algebraic Markov categories

Definition: A **linear algebraic Markov category** is a symmetric monoidal category supplying the above lattice of PROPs, such that it is a Markov category.

Linear algebraic Markov categories come

- *in the small*, as statistical theories
- *in the large*, as the semantics of statistical theories

Category of statistical semantics

The linear algebraic Markov category **Stat** has

- as objects, the pairs (V, A) , a finite-dimensional real vector space V with a measurable subset $A \subset V$
- as morphisms $(V, A) \rightarrow (W, B)$, the Markov kernels $A \rightarrow B$
- a symmetric monoidal structure, given by

$$(V, A) \otimes (W, B) := (V \oplus W, A \times B), \quad I := (0, \{0\})$$

and by the independent product of Markov kernels

- a supply according to whether the subset A is closed under linear/affine/conical/convex combinations, addition, or nothing.

Linear Markov kernels are deterministic

The linear Markov kernels turn out to be not very interesting:

Theorem

Let $M : V \rightarrow W$ be a Markov kernel between f.d. real vector spaces. If M is **linear**, then M is **deterministic**, hence a linear map.

Proof: By analysis of characteristic functions (Fourier transforms).

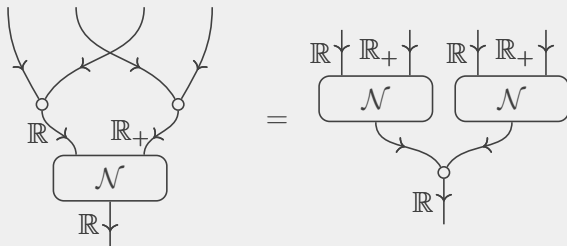
But there are interesting Markov kernels with related properties!

Additivity of normal family

Normal family is **additive**: if $X_i \stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_i, \sigma_i^2)$, then

$$X_1 + X_2 \sim \mathcal{N}(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$$

In **Stat**, additivity is the equation:

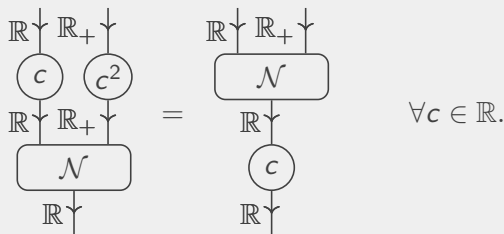


Homogeneity of normal family

Normal family is also “**homogeneous** with exponents 1 and 2”: if $X \sim \mathcal{N}(\mu, \sigma^2)$, then

$$cX \sim \mathcal{N}(c\mu, c^2\sigma^2), \quad \forall c \in \mathbb{R}.$$

In **Stat**, homogeneity is the equation:



Presenting the normal family

In fact, these two properties of being “linear-quadratic” characterize the normal family, up to location and scale.

Theorem

If $M : \mathbb{R}^m \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ is a linear-quadratic Markov kernel, then there exist matrices $A \in \mathbb{R}^{n \times m}$ and $V \in \mathcal{S}_+^n$ such that

$$M(x, \sigma^2) = \mathcal{N}_n(Ax, \sigma^2 V).$$

Remark: Taking other exponents $0 < \alpha \leq 2$ yields presentations of the symmetric α -stable families, with Cauchy ($\alpha = 1$) and normal ($\alpha = 2$) as special cases.

Statistical theories and models

A **statistical theory** (\mathbb{T}, ρ) consists of

- a small linear algebraic Markov category \mathbb{T}
- a morphism $\rho : \theta \rightarrow x$ in \mathbb{T} , the *sampling morphism*

A **model** of a statistical theory (\mathbb{T}, ρ) is a supply preserving functor $M : \mathbb{T} \rightarrow \mathbf{Stat}$.

- $\Omega := M(\theta)$ is the *parameter space*
- $\mathcal{X} := M(x)$ is the *sample space*
- $P := M(\rho) : \Omega \rightarrow \mathcal{X}$ is the *sampling distribution*

Note: Statistical theories generally have many different models.

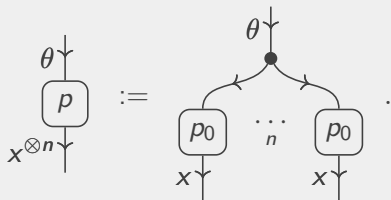
A few simple statistical theories

Example: The **initial statistical theory** (T, p) is freely generated by one morphism $p : \theta \rightarrow x$ on discrete objects θ and x .

Observation

Every statistical model $P : \Omega \rightarrow \mathcal{X}$ is a model of the initial theory.

Example: The **theory of n i.i.d. samples** (T, p) is freely generated by one morphism $p_0 : \theta \rightarrow x$ on discrete objects θ and x , with

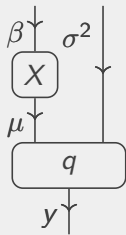


Theory of a linear model

The **theory of a linear model** (LM, ρ) is generated by

- vector space objects β , μ , and y
- conical space object σ^2
- linear map $X : \beta \rightarrow \mu$, i.e., morphism $X : \beta \rightarrow \mu$ subject to equations of linearity and determinism
- linear-quadratic morphism $q : \mu \otimes \sigma^2 \rightarrow y$

with sampling morphism $p : \beta \otimes \sigma^2 \rightarrow y$ given by



Linear models, as models of a theory

The standard models $M : \text{LM} \rightarrow \mathbf{Stat}$ are **linear models**:

- $M(y) = M(\mu) = \mathbb{R}^n$ for some dimension n
- $M(\beta) = \mathbb{R}^p$ for some dimension p
- $M(\sigma^2) = \mathbb{R}_+$
- $M(q) : \mathbb{R}^n \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ is isotropic normal family
- $X_M := M(X) : \mathbb{R}^p \rightarrow \mathbb{R}^n$ is arbitrary linear map

The sampling distribution is then

$$M(p) : \mathbb{R}^p \times \mathbb{R}_+ \rightarrow \mathbb{R}^n \\ (\beta, \sigma^2) \mapsto \mathcal{N}_n(X_M\beta, \sigma^2 I_n)$$

Another model is a **weighted linear model** where, for fixed $V_M \in \mathcal{S}_+^p$,

$$M(p) : (\beta, \sigma^2) \mapsto \mathcal{N}_n(X_M\beta, \sigma^2 V_M).$$

Bayesian statistical theories and models

A **Bayesian statistical theory** (\mathbb{T}, p, π) consists of

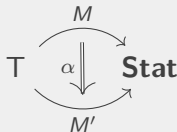
- a statistical theory $(\mathbb{T}, \theta \xrightarrow{p} x)$
- a morphism $I \xrightarrow{\pi} \theta$, the *prior morphism*

A **model** of a Bayesian theory (\mathbb{T}, p, π) is a model $M : \mathbb{T} \rightarrow \mathbf{Stat}$ of the underlying statistical theory.

- $M(p)$ is the *sampling distribution*
- $M(\pi)$ is the *prior*
- $M(\pi \cdot p)$ is the *marginal or prior predictive distribution*

Morphisms of statistical models

A **model homomorphism** between models M and M' of a statistical theory (\mathbb{T}, ρ) is a monoidal natural transformation



Proposition

The components $\alpha_x : M(x) \rightarrow M'(x)$ of model homomorphism are supply homomorphisms. In particular, they are **deterministic**.

Morphisms of linear models

Let M, M' be linear models, as models of (LM, p) , with designs

$$X_M := M(X) \in \mathbb{R}^{n \times p}, \quad X_{M'} := M'(X) \in \mathbb{R}^{n' \times p'}.$$

Proposition

A model homomorphism $\alpha : M \rightarrow M'$ is uniquely determined by linear maps $A := \alpha_Y \in \mathbb{R}^{n' \times n}$ and $B := \alpha_\beta \in \mathbb{R}^{p' \times p}$ such that

$$AA^T \propto I_{n'} \quad \text{and} \quad AX_M = X_{M'}B.$$

Symmetries of statistical models

Corollary

An isomorphism of linear models $\alpha : M \cong M'$, with $n = n'$ and $p = p'$, is uniquely determined by linear maps $A := \alpha_y \in \text{CO}(n)$ and $B := \alpha_\beta \in \text{GL}(p, \mathbb{R})$ such that $X_{M'} = AX_M B^{-1}$.

Symmetry and invariance is a classical topic in statistics. Advantages of our account:

- it does not assume identifiability of model (or loss function)
- it is not restricted to automorphisms or even isomorphisms
- it ensures that transformations preserve *all* structure specified by the theory, not just parameter and sample spaces
- it makes symmetry a **property** of the theory and model, not an extra **structure** added arbitrarily

Equivariance of linear regression

Ordinary-least squares (OLS) linear regression is

- **equivariant** under model isomorphism (a classical result)
- “laxly” **equivariant** under model homomorphism

Theorem

Let $\alpha : M \rightarrow M'$ be a homomorphism of linear models. For any $y \in \mathbb{R}^n$ and $\beta \in \mathbb{R}^p$, if $y' := \alpha_y(y)$ and $\beta' := \alpha_\beta(\beta)$, then

$$\|X_{M'}\beta' - y'\| \leq a\|X_M\beta - y\|,$$

where $a := \sqrt{\alpha_{\sigma^2}} \in \mathbb{R}_+$. In particular, if α is an isomorphism, then

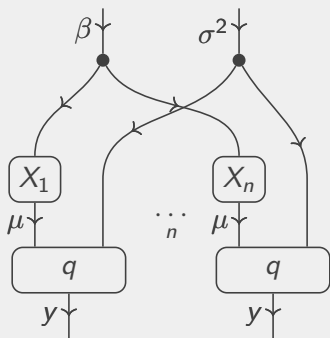
$$\hat{\beta} \in \operatorname{argmin}_{\beta \in \mathbb{R}^p} \|X_M\beta - y\| \quad \text{implies} \quad \hat{\beta}' \in \operatorname{argmin}_{\beta' \in \mathbb{R}^{p'}} \|X_{M'}\beta' - y'\|.$$

Another theory of a linear model

The **theory of a linear model on n samples** (LM_n, p_n) is generated by

- vector spaces β , μ , and y and a conical space σ^2
- linear maps $X_1, \dots, X_n : \beta \rightarrow \mu$,
- a linear-quadratic morphism $q : \mu \otimes \sigma^2 \rightarrow y$

with sampling morphism $p_n : \beta \otimes \sigma^2 \rightarrow y^{\otimes n}$ given by



Linear models on n samples

A **linear model** $M : \text{LM}_n \rightarrow \text{Stat}$ now assigns

- $M(y) = M(\mu) = \mathbb{R}$
- $M(q) = \mathcal{N} : \mathbb{R} \times \mathbb{R}_+ \rightarrow \mathbb{R}$, the univariate normal family

Let M, M' be linear models on n samples, as models of (LM_n, p_n) , with designs $(X_{M,i})_{i=1}^n \in \mathbb{R}^{n \times p}$ and $(X_{M',i})_{i=1}^n \in \mathbb{R}^{n \times p'}$.

Proposition

A model homomorphism $\alpha : M \rightarrow M'$ is uniquely determined by a scalar $a := \alpha_y \in \mathbb{R}$ and a matrix $B := \alpha_\beta \in \mathbb{R}^{p' \times p}$ such that

$$aX_{M,i} = X_{M',i}B, \quad \forall i = 1, \dots, n.$$

More theories of a linear model

Theories of a linear model include

- (LM, p) , of a general linear model
- (LM_n, p_n) , of a LM on n observations
- (LM_p, q_p) , of a LM on p predictors
- $(LM_{n,p}, q_{n,p})$, of a LM on n observations and p predictors

Which theory is the right one? *Wrong question.*

- Different theories allow different models and model homomorphisms
- Yet they are related by [morphisms of theories](#)

Morphisms of statistical theories

Definition: A (strict) morphism of statistical theories

$$F : (T, \rho) \rightarrow (T', \rho')$$

is a supply preserving functor $F : T \rightarrow T'$ such that $F(\rho) = \rho'$.

The theory morphism induces a **model migration functor**

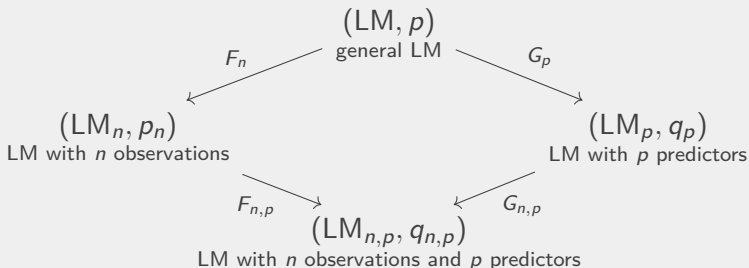
$$F^* : \text{Mod}(T') \rightarrow \text{Mod}(T)$$

(cf. Spivak 2012) by *pre-composition*:

$$\begin{array}{ccc} \begin{array}{c} T' \\ \downarrow M \\ \text{Stat} \end{array} & \xrightarrow{F^*} & \begin{array}{ccc} T & \xrightarrow{F} & T' \\ & \searrow F^*(M) & \downarrow M \\ & & \text{Stat} \end{array} \end{array}$$

Morphisms between theories of linear model

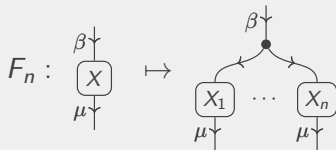
Different theories of linear models are related by theory morphisms:



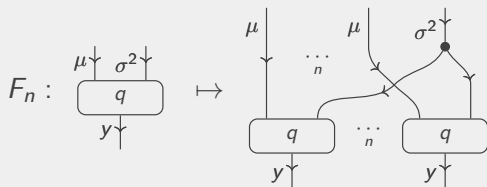
Morphism between two theories of linear model

A theory morphism $F_n : (\text{LM}, \rho) \rightarrow (\text{LM}_n, \rho_n)$

- sends μ to $\mu^{\otimes n}$ and y to $y^{\otimes n}$
- splits the design matrix by rows:



- splits the morphism q accordingly:

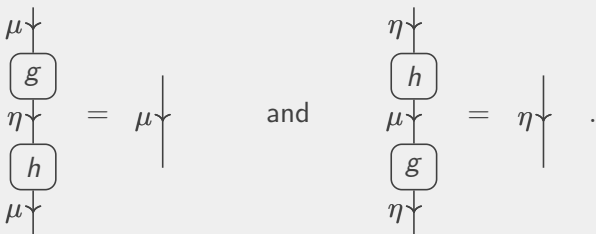


- preserves the other generators

Theory of a generalized linear model

A **theory of a GLM on n samples** (GLM_n, ρ_n) is generated by

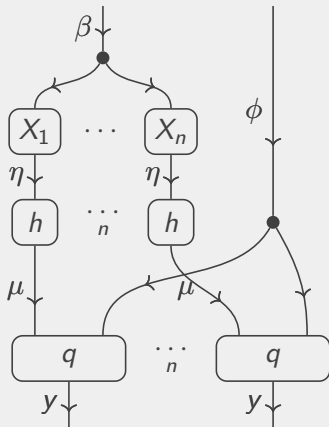
- vector spaces β and η , a convex space μ , and a conical space ϕ
- a discrete object y
- maps $g : \mu \rightarrow \eta$ (**link function**) and $h : \eta \rightarrow \mu$ (**mean function**), which are mutually inverse:



- linear maps $X_1, \dots, X_n : \beta \rightarrow \eta$
- a morphism $q : \mu \otimes \phi \rightarrow y$

Theory of a generalized linear model

The sampling morphism $p_n : \beta \otimes \phi \rightarrow y^{\otimes n}$ is

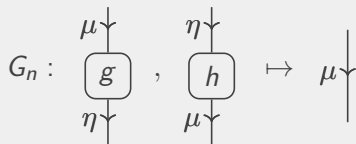


Morphism between theories of GLM and LM

Fact: “A linear model is a special case of a generalized linear model.”

Formally, a theory morphism $G_n : (\text{GLM}_n, \rho_n) \rightarrow (\text{LM}_n, \rho_n)$

- sends both μ and η to μ ,
- sends both g and h to the identity 1_μ :



- sends ϕ to σ^2
- preserves the other generators

Induces a model migration functor $G_n^* : \text{Mod}(\text{LM}_n) \rightarrow \text{Mod}(\text{GLM}_n)$.

Lax morphisms of statistical theories

A weaker notion of theory morphism allows for *expansion* of parameter and sample spaces (cf. McCullagh 2002).

A **lax^{*} morphism of statistical theories** $(T, \theta \xrightarrow{p} x)$ and $(T', \theta' \xrightarrow{p'} x')$ consists of

- a functor $F : T \rightarrow T'$
- a morphism $f_0 : \theta' \rightarrow F(\theta)$ in T'
- a morphism $f_1 : x' \rightarrow F(x)$ in T'

such that the diagram commutes:

$$\begin{array}{ccc} \theta' & \xrightarrow{p'} & x' \\ f_0 \downarrow & & \downarrow f_1 \\ F\theta & \xrightarrow{Fp} & Fx \end{array}$$

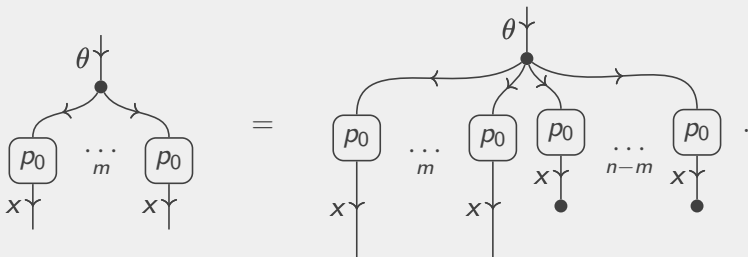
*Called “colax”, not “lax,” in (Patterson 2020)

Samples of different sizes as lax theory morphisms

Recall the [theory of \$n\$ i.i.d. samples](#) (T, p_n) . For any numbers $m \leq n$, projection gives a lax theory morphism

$$(1_T, 1_\theta, \pi_{m,n-m}) : (T, p_m) \rightarrow (T, p_n),$$

where laxness condition is



Conclusion

Summary:

1. introduced *statistical theories* in style of categorical logic
2. recovered *statistical models* as models of statistical theories
3. obtained notion of *statistical model homomorphism*
4. formalized relationships using *morphisms of statistical theories*
5. accompanied by *model migration functors*

Future work: lots!

- mathematical investigation of linear algebraic Markov categories
- *compositionality* of statistical theories and models
- *software* and integration with probabilistic programming

Outlook

How can statistics support **scientific theories and models** broadly?

- Traditionally, statistics has emphasized the formal testing of null hypotheses, as if they exist in isolation
- Rather, science involves an intricate web of interconnected theories, models, experiments, and data

Again, a long precedent in philosophy of science:

[E]xact analysis of the relation between empirical theories and relevant data calls for a hierarchy of models of different logical type. (Suppes 1966)

Suppes' hierarchy of models:

1. theoretical model
2. model of the experiment
3. data model [roughly, a statistical model]

How to make mathematics and statistics out of such ideas?

Thanks!

Main reference is my PhD thesis: *The algebra and machine representation of statistical models* (Patterson 2020)

- Available as arXiv:2006.08945
- Many more examples of statistical theories and models:
 - ▶ contingency tables
 - ▶ simple Bayesian and hierarchical models
 - ▶ linear mixed models
 - ▶ generalized linear (mixed) models
 - ▶ ...

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