Bayesian Model Specification

1: Foundations

David Draper

Department of Applied Mathematics and Statistics University of California, Santa Cruz

and (1 Jul-31 Dec 2013) eBay Research Labs

{draper@ams.ucsc.edu, dadraper@ebay.com} www.ams.ucsc.edu/~draper

SHORT COURSE (DAY 3) UNIVERSITY OF READING (UK)

29 Nov 2013

© 2013 David Draper (all rights reserved)

An Example, to Fix Ideas

Case Study 1. (Krnjajić, Kottas, Draper [KKD] 2008): *In-home* geriatric assessment (IHGA). In an experiment conducted in the **1980s** (Hendriksen et al. 1984), **572 elderly people**, representative of $\mathcal{P} =$ {all non-institutionalized elderly people in Denmark}, were randomized, **287** to a control (*C*) group (who received standard health care) and **285** to a treatment (*T*) group (who received standard care plus IHGA: a kind of preventive medicine in which each person's medical and social needs were assessed and acted upon individually).

One **important outcome** was the **number of hospitalizations** during the **two-year** life of the study:

	Number of Hospitalizations						
Group	0	1		k	n	Mean	SD
Control	<i>n</i> _{C0}	n_{C1}		n _{Ck}	$n_{C} = 287$	ӯс	s _C
Treatment	<i>n</i> _{T0}	n_{T1}		n _{Tk}	$n_T = 285$	Īγ	ST

Let μ_C and μ_T be the **mean hospitalization rates** (per two years) in \mathcal{P} under the *C* and *T* conditions, respectively.

Here are **four statistical questions** that **arose** from **this study**:

The Four Principal Statistical Activities

<u>Q_1:</u> Was the mean number of hospitalizations per two years in the IHGA group different from that in control by an amount that was large in practical terms? $\left[\frac{\text{description}}{\text{description}} \text{ involving } \left(\frac{\bar{y}_{\overline{\gamma}} - \bar{y}_{\overline{C}}}{\bar{y}_{\overline{C}}}\right)\right]$

 Q_2 : Did IHGA (causally) change the mean number of hospitalizations per two years by an amount that was large in statistical terms? [inference about $\left(\frac{\mu_T - \mu_C}{\mu_C}\right)$]

 Q_3 : On the **basis** of **this study**, how **accurately** can You **predict** the **total decrease** in **hospitalizations** over a period of *N* years if **IHGA** were **implemented throughout Denmark**? [prediction]

Q₄: On the **basis** of **this study**, is the **decision** to **implement IHGA** throughout Denmark **optimal** from a **cost-benefit** point of view? [decision-making]

These questions encompass almost all of the discipline of statistics: describing a data set D, generalizing outward inferentially from D, predicting new data D^* , and helping people make decisions in the presence of uncertainty (I include sampling/experimental design under decision-making; omitted: data quality assurance (QA), ...).

An Axiomatization of Statistics

1 (definition) Statistics is the study of uncertainty: how to measure it well, and how to make good choices in the face of it.



3 (axiom) (Your uncertainty about) "Something of interest to You" can always be expressed in terms of propositions: true/false statements A, B, ...

Examples: You may be uncertain about the truth status of

• A = (Hillary Clinton will be elected U.S. President in 2016), or

• B = (the **in-hospital mortality rate** for patients at **hospital** H admitted in **calendar 2010** with a principal diagnosis of **heart attack** was **between 5% and 25%**).

4 (implication) It follows from 1-3 that statistics concerns Your information (NOT Your beliefs) about A, B, ...

Axiomatization (continued)

5 (axiom) But Your information cannot be assessed in a vacuum: all such assessments must be made relative to (conditional on) Your background assumptions and judgments about how the world works vis à vis A, B, \ldots .

6 (axiom) These assumptions and judgments, which are themselves a form of information, can always be expressed in a set B of background propositions, all of which You believe to be true.

Examples of \mathcal{B} :

 \bullet In the IHGA study, based on the experimental design, ${\cal B}$ would include the propositions

(Subjects were representative of [like a random sample from] \mathcal{P}),

(Subjects were randomized into one of two groups, treatment (standard care + IHGA) or control (standard care)).

7 (definition) Call the "something of interest to You" θ ; in applications θ is often a vector (or matrix, or array) of real numbers, but in principle it could be almost anything (a function,

Axiomatization (continued)

an image of the surface of Mars, a phylogenetic tree, ...).

IHGA example: θ = mean relative decrease $\left(\frac{\mu_T - \mu_C}{\mu_C}\right)$ in hospitalization rate in \mathcal{P} .

8 (axiom) There will typically be an information source (data set) D that You judge to be relevant to decreasing Your uncertainty about θ ; in applications D is often again a vector (or matrix, or array) of real numbers, but in principle it too could be almost anything (a movie, the words in a book, ...).

9 (implication) The presence of *D* creates a dichotomy:

• Your information about θ {internal, external} to D.

(People often talk about a different dichotomy: Your information about θ {before, after} D arrives (prior, posterior), but temporal considerations are actually irrelevant.)

- 10 (implication) It follows from 1 9 that statistics concerns itself principally with five things (omitted: description, data QA, ...):
 - (1) Quantifying Your information about θ internal to D (given \mathcal{B}), and doing so well (this term is not yet defined);

(2) Quantifying Your information about θ external to D (given \mathcal{B}), and doing so well;

(3) **Combining** these two **information sources** (and doing so **well**) to create a **summary** of **Your uncertainty** about θ (given \mathcal{B}) that includes **all available information** You judge to be **relevant** (this is **inference**);

and using all Your information about θ (given \mathcal{B}) to make

(4) **Predictions** about **future** data values D^* and

(5) **Decisions** about how to **act sensibly**, even though **Your information** about θ may be **incomplete**.

Foundational question: How should these tasks be accomplished?

This question has two parts: probability and statistics.

The probability foundations (addressed here first), have an interesting and unfortunate history, in which much of the 20th century will (in my view) be seen in the 21st century to have been a series of missed scientific opportunities.

Theory of Probability: Kolmogorov

From the 1650s (Fermat, Pascal) through the 18th century (Bayes, Laplace) to the period 1860–1930 (Venn, Boole, von Mises), three different approaches for how to think about uncertainty quantification — classical, Bayesian, and frequentist probability were put forward in an intuitive way, but no one ever tried to prove a theorem of the form {given these premises, there's only one sensible way to quantify uncertainty} until Kolmogorov, de Finetti, and RT Cox.

— Kolmogorov (1933): following (and rigorizing) Venn, Boole and von Mises, probability is a function on (possibly some of) the subsets of a sample space Ω of uncertain possibilities, constrained to obey some reasonable axioms; this is excellent, as far as it goes, but many types of uncertainty cannot (uniquely, comfortably) be fit into this framework (examples follow).

Kolmogorov was trying to make precise the intuitive notion of repeatedly choosing a point at random in a Venn diagram and asking how frequently the point falls inside a specified set, i.e., his concept of probability had a repeated-sampling, frequentist character:

Frequentist Probability: Kolmogorov

"The basis for the applicability of the results of the mathematical theory of probability to real 'random phenomena' must depend on some form of the frequency concept of probability, the unavoidable nature of which has been established by von Mises in a spirited manner."

* **Example:** You're about to roll a **pair of dice** and **You regard** this dice-rolling as **fair**, by which You mean that (in Your judgment) all $6^2 = 36$ elemental outcomes in $\Omega = \{(1, 1), (1, 2), \dots, (6, 6)\}$ are equally probable; then the Kolomogorov probability of snake eyes ((1, 1)) exists and is unique (from Your fairness judgment), namely $\frac{1}{36}$; but

* **Example:** You're a **doctor**; a **new patient** presents **saying** that he **may** be **HIV positive**; what's the **Kolmogorov probability** that he is?

What's Ω? This patient is not the result of a uniquely-specifiable repeatable "random" process, he's just a guy who walked into Your doctor's office, and — throughout the repetitions of whatever repeatable phenomenon anyone might imagine — his HIV status is not fluctuating "randomly": he's either HIV positive or he's not.

Theory of Probability: de Finetti

The closest You can come to making Kolmogorov's approach work here is to imagine the set Ω of all people {similar to this patient in all relevant ways} and ask how often You'd get an HIV-positive person if You repeatedly chose one person at random from Ω , but to make this operational You have to specify what You mean by "similar to, in all relevant ways," and if You try to do this You'll notice that it's not possible to do so uniquely (in such a way that all other reasonable people would unanimously agree with You).

de Finetti (1937): rigorizing Bayes, probability is a quantification of betting odds about the truth of a proposition, constrained to obey axioms guaranteeing coherence (absence of internal contradictions); this is more general than Kolmogorov — in fact, it's as general as You can get: any statement about sets can be expressed in terms of propositions — but betting odds are not fundamental to science.

de Finetti made many important contributions — in particular, his concept of exchangeability (see AMS 206 or 206B) is crucial in Bayesian modeling — but (in my view) science is about information, not betting.

Theory of Probability: RT Cox

 — RT Cox (1946): following Laplace, probability is a quantification of information about the truth of one or more propositions, constrained to obey axioms guaranteeing internal logical consistency; this is both fundamental to science and as general as You can get.

Cox's goal was to identify what **basic rules** pl(A|B) — the **plausibility** (weight of evidence in favor) of (the truth of) A given B — should follow so that pl(A|B) behaves **sensibly**, where A and B are **propositions** with B assumed by You to be true and the truth status of A unknown to You.

He did this by **identifying** a set of **principles** making **operational** the word **"sensible"** (Jaynes, 2003):

• Suppose You're willing to represent degrees of plausibility by real numbers (i.e., pl(A|B) is a function from propositions A and B to \Re);

- You insist that Your reasoning be logically consistent:
- If a plausibility assessment can be arrived at in more than one way, then every possible way must lead to the same value.

Cox's Principles and Axioms

— You always take into account **all of the evidence** You judge to be **relevant** to the **plausibility assessment** under consideration (this is the **Bayesian** version of **objectivity**).

— You always represent equivalent states of information by equivalent plausibility assignments.

From these principles Cox derived a set of axioms:

• The plausibility of a proposition determines the plausibility of the proposition's negation; each decreases as the other increases.

• The plausibility of the conjunction AB = (A and B) of two propositions A, B depends only on the plausibility of B and that of $\{A \text{ given that } B \text{ is true}\}$ (or equivalently the plausibility of A and that of $\{B \text{ given that } A \text{ is true}\}$).

• Suppose *AB* is **equivalent** to *CD*; then if You acquire **new information** *A* and later acquire **further new information** *B*, and **update** all **plausibilities** each time, the **updated plausibilities** will be the **same** as if You had **first acquired new information** *C* and **then acquired further new information** *D*.

Cox's Theorem

From these axioms Cox proved a theorem showing that uncertainty quantification about propositions behaves in one and only one way:

Theorem: If You accept **Cox's axioms**, then to be **logically consistent** You **must** quantify uncertainty as follows:

Your plausibility operator pl(A|B) — for propositions A and B — can be referred to as Your probability P(A|B) that A is true, given that You regard B as true, and 0 ≤ P(A|B) ≤ 1, with certain truth of A (given B) represented by 1 and certain falsehood by 0.

• (normalization) $P(A|B) + P(\overline{A}|B) = 1$, where $\overline{A} = (\text{not } A)$.

• (the product rule):

 $P(AB|C) = P(A|C) \cdot P(B|AC) = P(B|C) \cdot P(A|BC).$

The proof (see, e.g., Jaynes (2003)) involves deriving two functional equations F[F(x, y), z] = F[x, F(y, z)] and $x S\left[\frac{S(y)}{x}\right] = y S\left[\frac{S(x)}{y}\right]$ that pl(A|B) must satisfy and then solving those equations.

A number of important corollaries arise from Cox's Theorem:

Optimal Reasoning Under Uncertainty

• (the sum rule):

 $P(A \text{ or } B|C) \equiv P(A+B|C) = P(A|C) + P(B|C) - P(AB|C).$

• Extensions of the product and sum rules to an arbitrary finite number of propositions are easy, e.g.,

$$P(A B C|D) = P(A|D) \cdot P(B|AD) \cdot P(C|ABD) \text{ and}$$

$$P(A+B+C|D) = P(A|D) + P(B|D) + P(C|D) - P(AB|D) - P(AC|D) - P(AC|D) - P(BC|D) + P(ABC|D).$$

This framework (obviously) covers optimal reasoning about uncertain quantities θ taking on a finite number of possible values; less obviously, it also handles (equally well) situations in which the set Θ of possible values of θ has infinitely many elements.

- **Example:** You're studying **quality of care** at the **17 Kaiser Permanente (KP) northern California hospitals** in **2003–7**, before the era of **electronic medical records**; during that time there was a **population** \mathcal{P} of N = 8,561 patients at these facilities with a primary admission diagnosis of heart attack. You take a simple random sample of n = 112 of these admissions and record whether or not each patient had an unplanned transfer to the intensive care unit (ICU), observing s = 4 who did; θ is the proportion of such unplanned transfers in all of \mathcal{P} ; here $\Theta = \{\frac{0}{N}, \frac{1}{N}, \dots, \frac{N}{N}\}$, which can be conveniently approximated by $\Theta' = [0, 1]$.

Prior to 2003, the **proportion** of such **unplanned transfers** for heart **attack patients** at **KP** in the **northern California region** was about q = 0.07, so **interest** focuses on P(A|DB), where A is the **proposition** $(\theta \le q)$, D is the **proposition** (s = 4), and B includes (among other things) **details** about the **sampling experiment** (e.g., (n = 112)).

In this setup θ is usually called a (population) parameter, and is not itself the result of any sampling experiment (random or otherwise); for this reason, it's not possible to (directly) quantify uncertainty about θ from the Kolmogorov (set-theoretic) point of view, but it makes perfect sense to do so from the RT Cox (propositional) point of view.

Optimal Reasoning About a Continuous θ

You could now more generally define a function $F_{(\theta|DB)}(q) = P(\theta \le q|DB)$ and call it the cumulative distribution function (CDF) for (not of) $(\theta|DB)$, which is shorthand for

the **CDF** for **Your uncertainty about** θ given D and \mathcal{B} .

If $F_{(\theta|DB)}(q)$ turns out to be **continuous** and **differentiable** in q (I haven't **said yet** how to **calculate** F), it will be **convenient** to write

$$F_{(\theta|D\mathcal{B})}(b) - F_{(\theta|D\mathcal{B})}(a) = P(a < \theta \le b|D\mathcal{B}) = \int_a^b p_{(\theta|D\mathcal{B})}(q) dq, \quad (1)$$

where the (partial) derivative $p_{(\theta|DB)}(q)$ of $F_{(\theta|DB)}$ with respect to q can be called the density for (not of) (Your uncertainty about) θ given D and B.

In a small abuse of notation it's common to write $F(\theta|DB)$ and $p(\theta|DB)$ instead of $F_{(\theta|DB)}(q)$ and $p_{(\theta|DB)}(q)$ (respectively), letting the argument θ of $F(\cdot|DB)$ and $p(\cdot|DB)$ serve as a reminder of the uncertain quantity in question.

Ontology and Epistemology

<u>NB</u> In the Kolmogorov approach a random variable X is a function from Ω to some outcome space O, and if $O = \Re$ You'll often find it useful to summarize X's behavior through the CDF of X: $F_X(x) = P$ (the set of $\omega \in \Omega$ such that $X(\omega) \le x$), usually written in propositional-style shorthand as $F_X(x) = P(X \le x)$.

In the **RT** Cox approach, there are no random variables; there are uncertain things θ whose uncertainty (when $\Theta = \Re^k$, for integer $1 \le k < \infty$) can usefully be summarized with **CDFs** and densities.

Jaynes (2003) makes a worthwhile distinction: the statements

There is noise in the room.

The room is noisy.

Talking about "the density of θ " would be to confuse ontology and epistemology;

The Mind-Projection Fallacy

Jaynes calls this confusion of {the world} (ontology) with {Your uncertainty about the world} (epistemology) the mind-projection fallacy, and it's clearly a mistake worth avoiding.

Returning to the corollaries of Cox's Theorem,

• Given the set \mathcal{B} , of propositions summarizing Your background assumptions and judgments about how the world works as far as θ , D and future data D^* are concerned:

(a) It's **natural** (and indeed **You must be prepared** in this approach) to specify **two conditional probability distributions**:

- $p(\theta|B)$, to quantify **all information** about θ **external** to D that You judge **relevant**; and
 - $p(D|\theta B)$, to quantify Your predictive uncertainty, given θ , about the data set D before it's arrived.

(b) Given the distributions in (a), the distribution $p(\theta|DB)$ quantifies all relevant information about θ , both internal and external to D, and must be computed via Bayes's Theorem:

Optimal Inference, Prediction and Decision

$$p(\theta|DB) = c \, p(\theta|B) \, p(D|\thetaB) \,, \qquad \text{(inference)} \tag{2}$$

where c > 0 is a normalizing constant chosen so that the left-hand side of (2) integrates (or sums) over Θ to 1;

(c) Your predictive distribution $p(D^*|DB)$ for future data D^* given the observed data set D must be expressible as follows:

$$p(D^*|D\mathcal{B}) = \int_{\Theta} p(D^*|\theta D\mathcal{B}) p(\theta|D\mathcal{B}) d\theta;$$

often there's **no information** about D^* contained in D if θ is known, in which case this expression **simplifies** to

$$p(D^*|D\mathcal{B}) = \int_{\Theta} p(D^*|\theta\mathcal{B}) p(\theta|D\mathcal{B}) d\theta; \qquad \text{(prediction)} \qquad (3)$$

(d) to make a sensible **decision** about which **action** *a* You should take in the face of Your **uncertainty** about θ , You **must be prepared to specify**

(i) the set \mathcal{A} of **feasible actions** among which You're **choosing**, and

Bayesian Reasoning

(ii) a utility function $U(a, \theta)$, taking values on \Re and quantifying Your judgments about the rewards (monetary or otherwise) that would ensue if You chose action a and the unknown actually took the value θ ; without loss of generality You can take large values of $U(a, \theta)$ to be better than small values;

then the **optimal decision** is to choose the action a^* that **maximizes** the **expectation** of $U(a, \theta)$ over $p(\theta|DB)$:

$$a^* = \operatorname*{argmax}_{a \in \mathcal{A}} E_{(\theta | D \mathcal{B})} U(a, \theta) = \operatorname*{argmax}_{a \in \mathcal{A}} \int_{\Theta} U(a, \theta) \, p(\theta | D \mathcal{B}) \, d\theta \,. \tag{4}$$

The equation solving the **inference problem** is **traditionally** attributed to **Bayes (1764)**, although it's just an **application** of the **product rule** (page 13), which was **already in use** by **(James) Bernoulli** and **de Moivre** around **1715**, and **Laplace** made **much better use** of this equation from **1774** to **1827** than Bayes did in **1764**; nevertheless the **Laplace/Cox propositional approach** is typically referred to as **Bayesian reasoning**.

Logical Consistency \rightarrow Bayesian Reasoning Justified

Cox's Theorem is equivalent to the assertion

If You wish to quantify Your uncertainty about an unknown θ (and make predictions and decisions in the presence of that uncertainty) in a logically internally consistent manner (as specified through Cox's axioms), on the basis of data D and background assumptions/judgments \mathcal{B} , then You can achieve this goal with Bayesian reasoning, by specifying $p(\theta|\mathcal{B})$, $p(D|\theta \mathcal{B})$, and $\{\mathcal{A}, U(a, \theta)\}$ and using equations (2-4).

This assertion has not rendered Bayesian analyses ubiquitous, although the value of Bayesian reasoning has become increasingly clear to an increasingly large number of people in the last 20 years, now that advances in computing have made the routine use of equations (2-4) feasible.

Advantages include a unified probabilistic framework: e.g., in my earlier ICU example, Kolmogorov's non-Bayesian approach does not permit direct probability statements about a population parameter,

but **Cox's Theorem permits You** to make such statements (summarizing **all relevant available information**) in a natural way.

The Specification Burden

It's worth noting, however, that there really is a theorem here, of the form $A \rightarrow B$, from which $\overline{B} \rightarrow \overline{A}$; this comes close to the assertion

If You employ non-Bayesian reasoning then You're open to the possibility of logical inconsistency,

and indeed there have been some **embarrassing moments** in **non-Bayesian inference** over the past **100 years** (e.g., **negative estimates** for quantities that are **constrained** to be **non-negative**).

Challenges: These **corollaries** to **Cox's theorem** solve problems (3–5) above (page 7) — they leave **no ambiguity** about how to draw **inferences**, and make **predictions** and **decisions**, in the presence of **uncertainty** — but problems (1) and (2) are still **unaddressed**: to **implement** this **logically-consistent approach** in a given application, You have to **specify**

p(θ|B), usually called Your prior information about θ (given B; this is better understood as a summary of all relevant information about θ external to D, rather than by appeal to any temporal (before-after) considerations);

The Specification Burden (continued)

- p(D|θ B), often referred to as Your sampling distribution for D given θ (and B; this is better understood as Your conditional predictive distribution for D given θ, before D has been observed, rather than by appeal to other data sets that might have been observed); and
 - the action space A and the utility function $U(a, \theta)$ for decision-making purposes.

The results of implementing this approach are

- p(θ|D B), often referred to as Your posterior distribution for θ given D (and B; as above, this is better understood as the totality of Your current information about θ, again without appeal to temporal considerations);
- Your posterior predictive distribution $p(D^*|DB)$ for future data D^* given the observed data set D; and
 - the optimal decision a^* given all available information (and \mathcal{B}).

Theory of Applied Statistics

To summarize: Inference and prediction require You to specify $p(\theta|B)$ and $p(D|\theta|B)$; decision-making requires You to specify the same two ingredients plus A and $U(a, \theta)$; how should this be done in a sensible way?

Cox's Theorem and its corollaries provide no constraints on the specification process, apart from the requirement that all probability distributions be proper (integrate or sum to 1).

In my view, in seeking answers to these specification questions, as a profession we're approximately where the discipline of statistics was in arriving at an optimal theory of probability before Cox's work: many people have made ad-hoc suggestions (some of them good), but little formal progress has been made.

Developing (1) principles, (2) axioms and (3) theorems about optimal specification could be regarded as creating a Theory of Applied Statistics, which we need but do not yet have.

Definition. Let's agree to call $\{p(\theta|B), p(D|\theta B), A, U(a, \theta)\}$ Your **model** *M* for **Your uncertainty about** θ , with the **convention** that

Optimal Model Specification

when no decision-making is involved this simplifies to $\{p(\theta|B), p(D|\theta B)\}.$

How should M be **specified**? Where is the **progression**

 $\textbf{Principles} \rightarrow \textbf{Axioms} \rightarrow \textbf{Theorems}$

to guide You, the way Cox's Theorem settled the foundational questions for probability?

In my view this is the **central unsolved foundational problem** in **statistical inference, prediction** and **decision-making**.

Optimal model specification. Can *M* be **specified optimally**?

That depends on what You mean by optimal; here's my definition:

Definition. In model specification, optimal = {conditioning only on propositions rendered true by the context of the problem and the design of the data-gathering process, while at the same time ensuring that the set of conditioning propositions includes all relevant problem context}.

Optimal Model Specification (continued)

Repeat Q: Can this **optimality goal** be **achieved**?

A, Part 1: Yes, sometimes.

Focusing for the moment on inference and prediction, in some special settings, You really don't have any model uncertainty at all — sometimes the prior distribution and/or likelihood/sampling distribution arise directly from problem context (Lecture Notes, Part 2).

Distribution-free well-calibrated Bayesian inferential methods are sometimes also available (Lecture Notes, Part 2A).

References

- Cox RT (1946). Probability, frequency and reasonable expectation. *American Journal of Physics*, **14**, 1–13.
 - De Finetti B (1937). La prévision: ses lois logiques, ses sources subjectives. Annals of the Institute of Henri Poincaré, **7**, 1–68.

References (continued)

• Hendriksen C, Lund E, Stromgard E (1984). Consequences of assessment and intervention among elderly people: a three year randomized controlled trial. *British Medical Journal*, **289**, 1522–1524.

- Jaynes ET (2003). *Probability Theory: The Logic of Science*. Cambridge UK: University Press.
 - Kolmogorov A (1933). *Grundbegriffe der Wahrscheinlichkeitsrechnung*. Berlin: Springer.

• Krnjajić M, Kottas A, Draper D (2008). Parametric and nonparametric Bayesian model specification: a case study involving models for count data. *Computational Statistics and Data Analysis*, **78**, 2110–2128.