SIPTA Summer School: Engineering Day
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## Engineering

- Practical applications
- Get things done, even if not perfectly
- Random variables, not just events
- Logic, arithmetic, FE and ODE models
- Continuous, infinite
- Quick \& dirty is better than elegant \& abstract
- Sloppy with notation, but big on computability


## Installing R

- Locate the latest version by Googling "R" or going to http://www.r-project.org/
- Download and install the base software
- For instance, get version 3.5.0 for Windows from https://cloud.r-project.org/bin/windows/base/R-3.5.0-win.exe
- Install R by executing this self-extracting file and invoke the program by double-clicking on the blue R icon it leaves on your desktop


## Leaving R

- To leave R click File / Exit from the main menu or enter the command quit()
- R may ask whether you want to save your work
- If you do, your variables and functions will be available the next time you invoke R


## Install the pba.r probability box library

- If you left R , invoke it again
- Enter $\mathbf{r m}($ list $=\mathbf{I} \mathbf{s}())$ to clear its memory
- Click File / Source R code on the main menu
- Locate and Open the file pba.r
- You'll get the message ":pba> library loaded"


## Die-hard RStudio users

- If, against advice, you must use RStudio...
- File / Open file pbox.r
- Source (Ctrl+Shift+S) pbox.r
- Enter the instruction RStudio = TRUE 4


## pba.r probability bounds library

## $\mathrm{a}=\operatorname{normal}(5,1)$

a

b = uniform(2, interval(3,4))
b

$a+b$


## Generalized convolutions

## a*b

a \%*\% b
$c=a+$ weibull $(8,1)$ * $\operatorname{beta}(2,3) / b$


C
mean(c)


## Probability bounds analysis in pba.r

- Output
- <enter variable name>, plot, lines, show, summary
- Characterize
- mean, sd, var, median, quantile, fivenum, left, right, prob, cut, percentile, iqr, random, range
- Compute
- exp, log, sqrt, abs, round, trunc, ceiling, floor, sign, sin, cos, tan, asin, acos, atan, atan2, reciprocate, negate, $+,-,{ }^{*}, /$, pmin, pmax, $\wedge$, and, or, not, mixture, smin, smax, complement


## Probability bounds analysis in pba.r

- Construct
- <distribution>
- histogram
- quantiles
- pointlist
- MM <tab> <tab
- ME <tab> <tab>
- ML <tab> <tab>
- CB <tab> <tab>
- NV <tab> <tab>


## Supported named distributions

bernoulli, beta (B), binomial (Bin), cauchy, chi, chisquared, delta, dirac, discreteuniform, exponential, exponentialpower, extremevalue, F, f, fishersnedecor, fishertippett, fisk, frechet, gamma, gaussian, geometric, generalizedextremevalue (GEV), generalizedpareto, gumbel, histogram, inversegamma, laplace, logistic, loglogistic, lognormal (L), logtriangular, loguniform, negativebinomial, normal (N), pareto, pascal, powerfunction, poisson, quantiles, rayleigh, reciprocal, shiftedloglogistic, skewnormal (SN), student, trapezoidal, triangular (T), uniform (U), weibull

## Nonparametric p-boxes

maxmean, minmax, minmaxmean, minmean, meanstd, meanvar, minmaxmode, minmaxmedian, minmaxmedianismode, minmaxpercentile, minmaxmeanismedian, minmaxmeanismode, mmms , mmmv, posmeanstd, symmeanstd, uniminmax, unimmmv, unimmms

# 110 You don't need to test the installation. Just skip to the next slide Testing the pba.r installation 

- Start a new instance of R , and enter the command $\mathbf{r m}(\mathbf{l i s t}=\mathbf{I s}())$
- Click File / Source R code on the main menu; find and Open the file pba.r
- The R Console will display something like

```
> source("C:\\Users\\workshop sra\\pba.r")
:p.ba> library loaded
```

- Enter plot(runif(100)) which will open a plot window with random points
- Click History / Recording on the main (if History is missing, click the plot)
- Click on the R Console, click File/Open script, and find and Open test pba.r
- Press Ctrl-A to select all its text, then press Ctrl-C to copy it to the clipboard, and close the R Editor window
- Click on the R Console, and press Ctrl-V to paste the text into the R Console for execution
- Click on the plot window, and press $\underline{\operatorname{Pg} U p}$ and $\underline{\operatorname{PgDn}}$ to scroll through graphical results of the test calculations
- There should be no error messages on the R Console


## Some help text in the pba.r file

\# Place this file on your computer and, from within R, select File/Source R code... from the main menu. Select this file \# and click the Open button to read it into R. You should see the completion message ":pbox> library loaded". Once the \# library has been loaded, you can define probability distributions
\# $a=\operatorname{normal}(5,1)$
\# $\mathrm{b}=$ uniform $(2,3)$
\# and p-boxes
\# $\mathrm{c}=$ meanvariance $(0,2)$
\# $\mathrm{d}=\operatorname{lognormal}($ interval( 6,7$)$, interval( 1,2 ) $)$
\# $\mathrm{e}=\operatorname{mmms}(0,10,3,1)$
\# and perform mathematical operations on them, including the Frechet convolution such as
\# a \% $\%$ b
\# or a traditional convolution assuming independence
\# a $\%|+| \%$ b
\# If you do not enclose the operator inside percent signs or vertical bars, the software tries to figure out how the
\# arguments are related to one another. Expressions such as
\# $a+b$
\# $\quad a+\log (a) * b$
\# autoselect the convolution to use. If pba.r can't tell what dependence the arguments have, it uses Frechet convolution.
\# Variables containing probability distributions or p-boxes are assumed to be independent of one another unless one \# formally depends on the other, which happens if one was created as a function of the other. Assigning a variable \# containing a probability distribution or a p-box to another variable makes the two variables perfectly dependent. To \# make an independent copy of the distribution or p-box, use the samedistribution function, e.g., $\mathrm{c}=$ samedistribution(a). \# By default, separately constructed distributions such as
\# $a=\operatorname{normal}(5,1)$
\# $\mathrm{b}=$ uniform $(2,3)$
\# will be assumed to be independent (so their convolution $a+b$ will be a precise distribution). You can acknowledge any

Two kinds of uncertainty

## Euclid

Given a line in a plane, how many parallel lines can be drawn through a point not on the line?

For over twenty centuries, the answer was one

## Relax one axiom

- Non-Euclidean geometries say zero or many
- At first, very controversial
- Mathematics richer and wider applications
- Used by Einstein in general relativity


## Crossroads in uncertainty theory

- There is a kind of uncertainty that cannot be handled by traditional Laplacian probability
- Only one axiom changes
- Collision of different views about uncertainty
- Richer math, wider applications
- More reasonable and more reliable results


## Two kinds of uncertainty

- Variability
- Aleatory uncertainty
- Type A uncertainty
- Stochasticity
- Randomness
- Chance
- Risk
- Incertitude
- Epistemic uncertainty
- Type B uncertainty
- Ambiguity
- Ignorance
- Imprecision
- True uncertainty


## Variability $=$ aleatory uncertainty

- Arises from natural stochasticity
- Variability arises from
- spatial variation
- temporal fluctuations
- manufacturing or genetic differences
- Not reducible by empirical effort


## Incertitude $=$ epistemic uncertainty

- Arises from incomplete knowledge
- Incertitude arises from
- limited sample size
- mensurational limits ('measurement uncertainty')
- use of surrogate data
- Reducible with empirical effort


## Propagating incertitude

Suppose

$$
\begin{aligned}
& A \text { is in }[2,4] \\
& B \text { is in }[3,5]
\end{aligned}
$$

What can be said about the sum $A+B$ ?


The right answer for risk analysis is [5,9]

## Must be treated differently

- Variability should be modeled as randomness with the methods of probability theory
- Incertitude should be modeled as ignorance with methods of interval or constraint analysis
- Probability bounding can do both at once


## Probability bounds analysis

## Bounding probability is an old idea

- Boole and de Morgan
- Chebyshev and Markov
- Borel and Fréchet
- Kolmogorov and Keynes
- Berger and Walley


## Why bounding is a good idea

- Often sufficient to specify a decision
- Possible even when estimates are impossible
- Usually easy to compute and simple to combine
- Rigorous, rather than an approximation
- Bounding works with even the crappiest data
(after N.C. Rowe 1988)


## Rigorousness

- The computations can be guaranteed to enclose the true results (if the inputs do)
- "Automatically verified calculations"
- You can still be wrong, but the method won't be the reason if you are


## Closely related to other ideas

- Second-order probability
- PBA is easier to work with and more comprehensive
- Imprecise probabilities
- PBA is somewhat cruder, but a lot easier
- Robust Bayesian analysis

Bounding
approaches
like PBA

- PBA does convolutions rather than updating



## Probability bounds

- Bridge between qualitative and quantitative
- When data are abundant, it works like probability theory
- When data are sparse, it yields both conservative and optimistic results
- Easy to set up, and cheap to implement


## What is a probability box (p-box)?

Interval bounds on a cumulative distribution function (CDF)


## P-box: mathematical definition

$\{\bar{F}, \underline{F}, m, v, \mathbf{F}\}$ where $\bar{F}, \underline{F} \in \mathbb{D}, m, v \in \mathbb{I}, \mathbf{F} \subseteq \mathbb{D}$, denoting a set of distributions $F \in \mathbb{D}$ matching

$$
\begin{aligned}
& \underline{F}(x) \leq F(x) \leq \bar{F}(x), \\
& \int_{-\infty}^{\infty} x \mathrm{~d} F(x) \in m, \\
& \int_{-\infty}^{\infty} x^{2} \mathrm{~d} F(x)-\left(\int_{-\infty}^{\infty} x \mathrm{~d} F(x)\right)^{2} \in v, \text { and } \\
& F \in \mathbf{F}
\end{aligned}
$$

$\mathbb{D}=\{D \mid D: \mathbb{R} \rightarrow[0,1], D(x) \leq D(y)$ whenever $x<y$, for all $x, y \in \mathbb{R}\}$ $\mathbb{I}=\left\{i \mid i=\left[i_{1}, i_{2}\right], i_{1} \leq i_{2}, i_{1}, i_{2} \in \mathbb{F}\right.$,

## Probability bounds analysis

- It's not worst case analysis (distribution tails)
- Marries intervals with probability theory
- Distinguishes variability and incertitude
- Solves many problems in risk analysis
- Input distributions unknown
- Imperfectly known correlation and dependency
- Large measurement error, censoring, small sample sizes
- Model uncertainty


## Calculations

- All standard mathematical operations
- Arithmetic (+,,$- \times, \div, \wedge$, min, max)
- Logical operations (and, or, not, if, etc.)
- Transformations (exp, ln, sin, tan, abs, sqrt, etc.)
- Backcalculation (deconvolutions, updating)
- Magnitude comparisons ( $<, \leq,>, \geq, \subseteq$ )
- Other operations (envelope, mixture, etc.)
- Quicker than Monte Carlo
- Guaranteed to bound the answer
- Optimal solutions often easy to compute


## Example: uncontrolled fire

$$
F=A \& B \& C \& D
$$

Probability of ignition source Probability of abundant fuel presence Probability fire detection not timely Probability of suppression system failure

## Imperfect information

- Calculate $A \star{ }^{\star}{ }^{\star} C \ltimes D$, with partial information:
- A's distribution is known, but not its parameters
- B's parameters known, but not its shape
- C has a small empirical data set
- $D$ is known to be a precise distribution
- Bounds assuming independence?
- Without any assumption about dependence?

```
A={lognormal, mean =[.05,.06], variance = [.0001,.001])
B={\operatorname{min}=0, max = 0.05, mode = 0.03}
C={sample data =0.2,0.5,0.6,0.7,0.75,0.8}
D = uniform(0,1)
```



## Resulting answers



## Summary statistics

## Independent

Range
Median
Mean
Variance
Standard deviation
[0, 0.011]
[0, 0.00113]
[0.00006, 0.00119]
$\left[2.9 \times 10^{-9}, 2.1 \times 10^{-6}\right]$
[0.000054, 0.0014]

No assumptions about dependence
Range
Median
[0, 0.05]

Mean
Variance
[0, 0.04]
[0, 0.04]
[0, 0.00052]
Standard deviation
[0, 0.023]

## How to use the results

When uncertainty makes no difference
(because results are so clear), bounding gives confidence in the reliability of the decision

When uncertainty prevents a decision
(i) use other criteria within probability bounds, or
(ii) use results to identify inputs to study better

## Can uncertainty swamp the answer?

- Sure, if uncertainty is huge
- This should happen (it's not "unhelpful")
- If you think the bounds are too wide, then put in whatever information is missing
- If there isn't any such information... do you want the results to mislead people?


## Using the pba.r library

$A=$ lognormal( $\mathrm{i}(.05, .06), \operatorname{sqrt}(\mathrm{i}(.0001, .001)))$
$B=$ minmaxmode $(0,0.05, .03)$
$C=\operatorname{CBbinomial}(2,4)$
$D=$ uniform $(0,1)$
$\mathrm{fi}=\mathrm{A} \%|\&| \%$ B $\%|\&| \%$ C $\%|\&| \%$ D
$f=A \% \& \% B \% \& \%$ C \% $\%$ D
red(f)
blue(fi)


## Duality

- Bounds on the probability at a value

Chance the value will be 15 or less is between 0 and $25 \%$

- Bounds on the value at a probability
$95^{\text {th }}$ percentile is between 40 and 70



## Breadth (incertitude) v. tilt (variability)



## Probability bounds arithmetic

P-box for random variable $\boldsymbol{A}$


P-box for random variable $B$


What are the bounds on the distribution of the sum of $A+B$ ?

## Cartesian product

| $A+B$ <br> independence | $A \in[1,3]$ <br> $p_{1}=1 / 3$ | $A \in[2,4]$ <br> $p_{2}=1 / 3$ | $A \in[3,5]$ <br> $p_{3}=1 / 3$ |
| :--- | :--- | :--- | :--- |
| $B \in[2,8]$ <br> $q_{1}=1 / 3$ | $A+B \in[3,11]$ <br> prob $=1 / 9$ | $A+B \in[4,12]$ <br> prob $=1 / 9$ | $A+B \in[5,13]$ <br> prob $=1 / 9$ |
| $B \in[6,10]$ <br> $q_{2}=1 / 3$ | $A+B \in[7,13]$ <br> prob $=1 / 9$ | $A+B \in[8,14]$ <br> prob $=1 / 9$ | $A+B \in[9,15]$ <br> prob $=1 / 9$ |
| $B \in[8,12]$ <br> $q_{3}=1 / 3$ | $A+B \in[9,15]$ <br> prob $=1 / 9$ | $A+B \in[10,16]$ <br> prob $=1 / 9$ | $A+B \in[11,17]$ <br> prob $=1 / 9$ |

## $A+B$ under independence



## Where do inputs come from?

## Where do input p-boxes come from?

- Prior modeling
- Uncertainty about dependence
- Robust Bayes analysis
- Constraint information
- Summary publications lacking original data
- Sparse or imprecise data
- Shallow likelihood functions to maximize
- Measurement uncertainty, censoring, missing data
- Inferential (sampling) uncertainty


## Robust Bayes can make a p-box


class of priors, class of likelihoods $\Rightarrow$ class of posteriors

## Constraint propagation






## Comparing p -boxes with maximum entropy distributions



## Maximum entropy's problem

- Depends on the choice of scale
- A solution in terms of degradation rate is incompatible with one based on half life even though the information is equivalent
- P-boxes are the same whichever scale is used

Warner North interprets Ed Jaynes as saying that "two states of information that are judged to be equivalent should lead to the same probability assignments". Maxent doesn't do this! But PBA does.

## Sparse data yield shallow likelihoods



## Treelining likelihood makes a p-box

The p-box encloses all distributions whose
$L \uparrow$ parameters $\theta$ are above some threshold likelihood (not merely maximally likely).


## Sources of incertitude in data

- Periodic observations
- Plus-or-minus measurement uncertainties
- Non-detects and data censoring
- Privacy requirements
- Theoretical constraints
- Bounding studies


## Imprecise sample data

Skinny data
[1.00, 2.00]
[2.68, 2.98]
[7.52, 7.67]
[7.73, 8.35]
[9.44, 9.99]
[3.66, 4.58]

Puffy data
[3.5, 6.4]
[6.9, 8.8]
[6.1, 8.4]
[2.8, 6.7]
[3.5, 9.7]
[6.5, 9.9]
[0.15, 3.8]
[4.5, 4.9]
[7.1, 7.9]


## Empirical distribution of intervals




- Each side is cumulation of respective endpoints
- Represents both uncertainty and variability


## Uncertainty about the EDF



## Fitted to normals



## Distributional uncertainty

- Can we trust the raw data or any distribution fitted to them?
- Should account for sampling uncertainty about a probability distribution given sampled values
- Kolmogorov-Smirnov confidence procedure - 95\% (or whatever) confidence for distribution
- Assumes continuous distribution
- Random samples, which come from random inputs


## Distributional confidence limits



## Confidence band about a p-box



## KS generalizes well

- Works with arbitrary input distribution shapes
- Can handle incertitude too
- Generalizes to multivariate outputs
- Conclusion is distribution-free
- Assuming output shape could tighten bounds


## Distributional confidence limits

(Chen and Iles; Basu)


## Single-sample confidence band

- Rodríguez described confidence intervals for mean and standard deviation assuming normality from only one random sample
- Combine them to get confidence band

```
onepointconfidenceband.normal = function(x, c=0.95) {
    stopifnot(length(x)==1)
    tm}=\textrm{c}(4.83952,9.678851,48.39413)
    ts}=\textrm{c}(8,17,70
    k=which(c==c(0.9, 0.95, 0.99))
                                    confidence band
    normal(x+tm[[k]]*abs(x)*interval(-1,1),interval(0,ts[[k]]*abs(x)))
    }
```


## Very wide, even assuming normality



## Confidence bands aren't rigorous

- Not compatible with interval arithmetic - You can’t intersect or compute with them - Not rigorous...only statistical
- Could artfully use the Fréchet inequality
- Combining two bands at $95 \%$ yields a $90 \%$ band
- Two $97.5 \% \rightarrow 95 \%$, three $95 \% \rightarrow 85 \%$, three $98.35 \% \rightarrow 95 \%$
- Could assume the confidence band is rigorous
- Assumption often used (e.g., EPA uses a UCL as the EPC)


## Every p-box represents assumptions

- Constraint p-boxes assumed you knew those parameters
- Nothing intrinsically different about the assumption that converts a confidence band to a p-box
- You're assuming, given the data, that the distribution is entirely inside the bounds


## Confidence boxes

- Structures that let you infer confidence intervals (at any confidence level) for a parameter
- Extend confidence distributions (like Student's $t$ )
- Different from confidence bands
- Can be propagated as ordinary probability bounds


## Example: binomial rate

- Probability, given $k$ successes out of $n$ trials

$$
\begin{aligned}
& \text { Example } \\
& k=2 \\
& n=10
\end{aligned}
$$


$(\alpha-\beta) 100 \%$ confidence interval for $p$

- Like robust Bayes but no assumption of prior


## Uncertainties expressible with p-boxes

- Sampling uncertainty (from small $N$ )
- Distributional confidence bands, confidence boxes
- Measurement incertitude
- Plus-minus ranges, censoring intervals
- Uncertainty about distribution shape
- Constraints (non-parametric p-boxes)
- Surrogacy uncertainty (have $X$ but want $Y$ )
- Modeling


## Modeling for surrogacy

- Sometimes you correct the best estimate
- Subtract the weight of the dish when they charge for salad in the cafeteria (+)
- Sulfur hexafluoride is worth so much $\mathrm{CO}_{2}(\times)$
- If you're not sure exactly how, then you should widen the uncertainty


## Example: Lobascio's travel time

## $T=\frac{(n+B D \times f o c \times K o c) L}{K \times i}$

Parameter
$L \quad$ source-receptor distance
$i$ hydraulic gradient
$K$ hydraulic conductivity
$n \quad$ effective soil porosity
$B D$ soil bulk density
foc fraction organic carbon Koc organic partition coefficient

| Units | Min | Max | Mean | Stdv |
| :--- | :--- | :--- | :--- | :--- |
| m | 80 | 120 | 100 | 11.55 |
| $\mathrm{~m} / \mathrm{m}$ | 0.0003 | 0.0008 | 0.00055 | 0.0001443 |
| $\mathrm{~m} / \mathrm{yr}$ | 300 | 3000 | 1000 | 750 |
| - | 0.2 | 0.35 | 0.25 | 0.05 |
| $\mathrm{~kg} / \mathrm{m}^{3}$ | 1500 | 1750 | 1650 | 100 |
| - | 0.0001 | 0.005 | 0.00255 | 0.001415 |
| $\mathrm{~m}^{3} / \mathrm{kg}$ | 5 | 20 | 10 | 3 |

## pba.r



## Inputs as mmms p-boxes









## Output p-box



## Detail of left tail



## Example: mercury in wild mink

## Location: Bayou d'Inde, Louisiana

Receptor: generic piscivorous small mammal
Contaminant: mercury
Exposure route: diet (fish and invertebrates)

Based loosely on the assessment described in "Appendix I2: Assessment of Risks to Piscivorus [sic] Mammals in the Calcasieu Estuary", Calcasieu Estuary Remedial Investigation/Feasibility Study (RI/FS): Baseline Ecological Risk Assessment (BERA), prepared October 2002 for the U.S. Environmental Protection Agency. See http://www.epa.gov/earth1r6/6sf/pdffiles/appendixi2.pdf.

## Total daily intake from diet

$T D I=F M R|\times|\left(\frac{C_{\text {fish }}|\times| P_{\text {fish }}}{A E_{\text {fish }} \times G E_{\text {fish }}}+\frac{C_{\text {inverts }}|\times| P_{\text {inverts }}}{A E_{\text {inverts }}|\times| G E_{\text {inverts }}}\right)$

FMR normalized free metabolic rate of the mammal
$A E_{\text {fish }} \quad$ assimilation efficiency of dietary fish in the mammal
$A E_{\text {inverts }}$ assimilation efficiency of dietary invertebrates in the mammal
$G E_{\text {fish }}$ gross energy of fish tissue
$G E_{\text {inverts }}$ gross energy of invertebrate tissue
$C_{\text {fish }} \quad$ mercury concentration in fish tissue
$C_{\text {inverts }}$ mercury concentration in invertebrate tissue
$P_{\text {fish }} \quad$ proportion of fish in the mammal's diet
$P_{\text {inverts }}$ proportion of invertebrates in the mammal's diet

## What is known about the variables

$F M R$, free metabolic rate
Studied in terms of mammal body mass; $F M R=a B W^{b}$, regression intervals $a, b$
$B W$, body mass of the mammal
Empirically well studied; Normal with highly precise mean and dispersion
$A E_{\text {fish }}, A E_{\text {inverts }}$, assimilation efficiencies for different diet components
A few field measurements; Mean and upper and lower values
$G E_{\text {fish }}, G E_{\text {inverts }}$, gross energy of fish and invertebrate tissues
Many measurements; Normal distribution with precise mean and dispersion
$C_{\text {fish }}, C_{\text {inverts }}$, mercury concentration in fish or invertebrate tissue Dictated by EPA policy; Range between sample mean and 95\% UCL
$P_{\text {fish }}, P_{\text {inverts }}$, proportions of fish and invertebrates in the mammal's diet Assumed by analyst; Constant

## Input assignments

$B W=\operatorname{normal}(608$ gram, 66.9 gram $)$
$F M R=[0.412 \pm 0.058]^{*} \operatorname{mag}(B W)^{\wedge}[0.862 \pm 0.026]^{*} 1$ Kcal over kg day
AEfish $=\operatorname{minmaxmean}(0.77,0.98,0.91)$
AEinverts $=\operatorname{minmaxmean}(0.72,0.96,0.87)$
GEfish $=$ normal $(1200 \mathrm{Kcal}$ per kg, 240 Kcal per kg)
GEinverts $=$ normal $(1050$ Kcal per kg, 225 Kcal per kg $)$
$C$ fish $=[0.1,0.3] \mathrm{mg}$ per kg
Cinverts $=[0.02,0.06] \mathrm{mg}$ per kg
$P$ fish $=0.9$
Pinverts $=0.1$

## pba.r

$B W=$ normal $(608,66.9)$
pmi $=$ function(m, pm) pbox(interval(m-pm, $m+p m))$
$F M R=\operatorname{pmi}(0.412,0.058) * B W^{\wedge} \operatorname{pmi}(0.862,0.026)$
AEfish $=\operatorname{minmaxmean}(0.77,0.98,0.91)$
AEinverts $=$ minmaxmean $(0.72,0.96,0.87)$
GEfish $=$ normal $(1200,240)$
GEinverts = normal $(1050,225)$
Cfish = interval $(0.1,0.3)$
Cinverts $=$ interval $(0.02,0.06)$
Pfish $=0.9$
Pinverts $=0.1$
TDI $=$ FMR * (Cfish\%*\%Pfish\%/\%(AEfish*GEfish) $\%+\%$ Cinverts\%*\% Pinverts\%/\%(AEinverts*GEinverts))

## Input p-boxes



Subscript 1 denotes fish, 2 denotes inverts

## Results



## 2 MC simulations may not fill p-boxes

- $2^{\text {nd }}$ order Monte Carlo is not comprehensive
- Inadequate model of ignorance
- Dependence among parameters of a distribution
- Uncertainty about dependence (Fréchet)
- Non-denumerable model uncertainty
- Probability bounds analysis is not optimal
- Independence between parameters of a distribution
- Ternary (and higher) Fréchet operations


## Probability bounds analysis

- Combines interval and probability methods
- Shows when uncertainty is (or isn't) important
- Won't underestimate risks of extremes, yet isn't hyperconservative like worst case
- Solves many risk analysis problems

Input distributions unknown
Large measurement error, censored data, and small samples
Correlation and dependency ignored
Model uncertainty

## Advantages

- Fewer assumptions
- Not just different assumptions, fewer of them
- Distribution-free methods
- Rigorous results
- Built-in quality assurance
- Automatically verified calculation


## What p-boxes can't do

- Show what's most likely within a p-box
- Express second-order information
- Get best-possible bounds on non-tail risks
- Get best-possible bounds for any data set
- When dependencies are intricate
- When information about modes are availabe


## Don't know the ingy

- Don't have to specify the distributions
- Shouldn't use a distribution without evidence
- Maximum entropy criterion erases uncertainty rather than propagates it
- Sensitivity analysis is very hard since it's an infinite-dimensional problem
- P-boxes easy, but should use all information


## Probability bounds analysis in pba.r

- Output
- <enter variable name>, plot, lines, show, summary
- Characterize
- mean, sd, var, median, quantile, fivenum, left, right, prob, cut, percentile, iqr, random, range
- Compute
- exp, log, sqrt, abs, round, trunc, ceiling, floor, sign, sin, cos, tan, asin, acos, atan, atan2, reciprocate, negate, $+,-,{ }^{*}, /$, pmin, pmax, $\wedge$, and, or, not, mixture, smin, smax, complement


## Probability bounds analysis in pba.r

- Construct
- <named distribution>
- histogram
- quantiles
- pointlist
- MM <tab> <tab>
- ME <tab> <tab>
- ML <tab> <tab>
$-\mathrm{CB}<t a b><t a b>$
Supported named distributions
bernoulli, beta (B), binomial (Bin), cauchy, chi, chisquared, delta, dirac, discreteuniform, exponential, exponentialpower, extremevalue, F, f, fishersnedecor, fishertippett, fisk, frechet, gamma, gaussian, geometric, generalizedextremevalue (GEV), generalizedpareto, gumbel, histogram, inversegamma, laplace, logistic, loglogistic, lognormal (L), logtriangular, loguniform, negativebinomial, normal ( N ), pareto, pascal, powerfunction, poisson, quantiles, rayleigh, reciprocal, shiftedloglogistic, skewnormal (SN), student, trapezoidal, triangular ( T ), uniform (U), weibull


## Computing with confidence

## Many ways to fit distributions to data

- Maximum entropy
- Maximum likelihood
- Bayesian inference
- Method of matching moments
- Goodness of fit (KS, AD, $\chi^{2}$, etc.)
- PERT
- Regression techniques
- Empirical distribution functions


## Little coherence in practice

- Disparate methods used across risk analysis
- Common to mix and match distributions with different justifications
- Analyses are thus based on no clear criterion or standard of performance
- Is this okay?


## Frequentist confidence intervals

- Favored by many engineers
- Guarantees statistical performance over time
- But difficult to employ consistently in analyses
- Not clear how to propagate them through mathematical calculations


## Bayesian approaches

- Permit mathematical calculations
- But lack guarantees ensuring long-run statistical performance
- Many engineers are reluctant to use Bayesian methods


## Confidence distributions

- Not widely used in statistics
- Introduced by Cox in the 1950s
- Closely related to well known ideas
- Student's $t$-distribution
- Bootstrap distributions


## Confidence distributions

- Distributional estimators of (fixed) parameters
- Give confidence interval at any confidence level



## Confidence interval

- A confidence interval with coverage $\alpha$

In replicate problems, a proportion $\alpha$ of computed confidence intervals will enclose the true value

- Using methods to compute confidence intervals thus ensures statistical performance


## Confidence distributions

- Have the shape of a distribution
- But correspond to no random variables
- Not supposed to compute with them
- Don't always exist (e.g., for the binomial rate)


## Confidence structures (c-boxes)

- Generalization of confidence distributions
- Reflect inferential uncertainty about parameter
- Known for many cases
- binomial rate and other discrete parameters
- normals, and many other problems
- non-parametric case
- Still have performance/confidence interpretation


## Confidence interpretation



## Estimators

- Point estimates (e.g., sample mean)
- Interval estimates (e.g., confidence intervals)
- Distributional estimates (Bayesian posteriors)
- P-box estimates (e.g., c-boxes)


## Binomial rate $p$ for $k$ of $n$ trials

$p \sim \operatorname{env}(\operatorname{beta}(k, n-k+1), \operatorname{beta}(k+1, n-k))$


If $1-\alpha=\beta$, result is identical to classical Clopper-Pearson interval

## How does the Bayes analysis compare?

- No such thing as the Bayes analysis
- There are always many possible analyses - Different priors, which yield different answers - When data sets are small, the differences are big
- For binomial rate there are four or five priors Bayesians have not been able to chose among





## C-boxes partition the vacuous square



## Example: normal mean

$$
\mu \sim \bar{x}+s \cdot \mathrm{~T}_{n-1} / \sqrt{n}
$$

Data

$$
\begin{array}{r}
8 \\
5.5 \\
-1.3 \\
3.5 \\
0.8 \\
2.8 \\
1.8 \\
2.2 \\
3.5 \\
5.3
\end{array}
$$



## Example: normal mean

$$
\mu \sim \bar{x}+s \cdot \mathrm{~T}_{n-1} / \sqrt{n}
$$

Data
$[8,11]$
$[5.5,6.9]$
$[-1.3,0.3]$
$[3.5,7.5]$
$[0.8,1]$
$[2.8,4.2]$
$[1.8,5.2]$
$[2.2,5.2]$
$[3.5,5.7]$
$[5.3,6.1]$


## Deriving c-boxes

- Have to be derived for each special case
- Traditional approaches based on pivots
- Many solutions have been worked out $\operatorname{binomial}(p, n)$, given $n \quad \operatorname{normal}(\mu, \sigma)$ $\operatorname{binomial}(p, n)$, given $p \quad \operatorname{lognormal}(\mu, \sigma)$ $\operatorname{binomial}(p, n)$
Poisson(p)
$\operatorname{gamma}(a, b)$
exponential( $\lambda$ )


## Example: non-parametric problem

Data
140.2
121.2
154
162.6
136.9
215.9
117.5
166.7
165.2
128.9
150.6
214.3 $X \sim[(1+C(x)) /(1+n), C(x) /(1+n)]$ where $C(x)=\#\left(X_{i} \leq x\right)$


## Captured uncertainties

- Uncertainty about distribution shape
- Sampling uncertainty (from small $n$ )
- Measurement incertitude ( $\pm$, censoring)
- Demographic stochsticity (integrality of data)


## Propagated as probability boxes

- C-boxes can be combined in mathematical expressions using the p-box technology
- Results also have performance interpretations
- C-boxes can also make predictive p-boxes - Analogous to frequentist prediction distiva - Or Bayesian posterior predictive distriNtions


## Prediction structures

- C-boxes can model the uncertainty about the underlying distribution that generated the data
- Stochastic mixture of p-boxes from interval parameters specified by slices from the c-box
- This is a composition of the c-box through the probability model


## Example: Bernoulli distribution




Each interval slice defines a p-box for the underlying distribution (rather than a precise distribution)

Average all such p-boxes


## Predictive p-boxes for observables

Bernoulli trials $b_{i} \sim \mathrm{~B}(p), i=1, \ldots, n$
$b_{n+1} \sim \operatorname{Bernoulli}([k, k+1] /(n+1)), k=\Sigma_{i} b_{i}$
Random binomial sample $k \sim \operatorname{binomial}(p, n)$ $k_{2} \sim[\mathrm{BB}(k, n N-k+1, N), \mathrm{BB}(k+1, n N-k, N)]$

Random normal samples $X_{i} \sim \mathrm{~N}(\mu, \sigma), i=1, \ldots, n$ $X_{n+1} \sim \operatorname{mean}\left(X_{i}\right)+\operatorname{stdev}\left(X_{i}\right) \cdot \operatorname{sqrt}(1+1 / n) \cdot \mathrm{T}(n-1)$

## Example: Binomial distribution



## Prediction structures are p-boxes

- Results also have the confidence interpretation, but the intervals are prediction intervals rather than confidence intervals
- Prediction intervals enclose a specified percentage of observable values, on average
- It is also possible to derive analogous tolerance structures, which encode tolerance intervals ( $X \%$ sure to enclose $Y \%$ of the population)


## Computing with c-boxes



What if we used all three plans independently?

## Conjunction (AND)



## C-boxes are fully Bayesian

- Under robust Bayes approach, c-boxes can be thought of as Bayesian posteriors
- Don't require specification of a unique prior
- Have added feature of statistical performance
- Imply posterior predictive distributions
- Compatible with specifying a robust or precise prior when that's desirable


## C-boxes are fully frequentist too

- Frequentists like confidence intervals but cannot use them in subsequent calculations
- Bayesians can compute with posteriors, but they don't guarantee statistical performance
- C-boxes take the best from both worlds


## Summary for c-boxes

- Confidence boxes carry inferential uncertainties through mathematical operations
- Give confidence intervals on results at any $\alpha$ level
- Defined by performance, so not unique - Just as confidence intervals are not unique - May create some flexibility
- Don't seem to be overly conservative
- Elaborate simulation studies have so far not found this


## Conclusions

- C-boxes characterize risk analysis inputs given limited sample or constraint information
- Reasonable answers when data and tenable assumptions don't justify particular distributions
- C-boxes don't optimize; they perform
- C-boxes could serve as the lexicon in a language of risk analysis


## More information

https://sites.google.com/site/confidenceboxes/

- Papers
- Slide presentations
- Free software

Google "confidence boxes" [plural. . . singular is a
blog on teenage self-esteem \& self-empowerment]

Little data, or none at all

## Dramatic technocratic failures

- Shuttle risk estimated at $1 / 10,000$ per flight, it was actually 1 per 70 flights
- 100-year flood risks underestimated and uncertainties not communicated
- Grossly understating risks in the financial industry precipitated the 2008 recession
- Failure cascades in electricity distribution systems are more common than they are forecasted to be (RAWG 2005; USCPSOTF 2006)


## Dramatic technocratic failures

- Kansai International Airport
- Diablo Canyon Nuclear Power Plant
- Vioxx withdrawal
- Fukushima
- Mars Climate Orbiter
- Google Flu
- Ariane 5
- Minneapolis bridge collapse


## These are not noble failures

- They are not simply the unfortunate but expected extreme tail events
- They occur more often than our risk estimates predict
- Analysts are doing risk estimations wrong
- Managers never see the problems coming


## Engineers cannot always get data

- New systems may have no performance history
- spacecraft of new design or in a new environment
- biological control strategies using novel genetic constructs that have never existed before
- Two ways to estimate probabilities without data
- disaggregation into parts whose probabilities are easier to estimate (i.e., breaking it into subproblems)
- expert elicitation (i.e., guessing)


## Rare event probabilities

- Hardly ever any actual data
- Sometimes we have experts
- But how should we model bald assertions:
- "1 in 10 million"
- "about 1 in 1000"
- "never been seen in 100 years"


## In my experience

People using expert elicitation often take the pronouncements made by their informants exactly as they are specified

- Sometimes even as point values
(If your experience is different, I'd like to chat)


## Is there no uncertainty?

- What is the uncertainty in estimates like
- "1 in $10{ }^{7}$ ",
- "about 1 in 1000", or
- "never been seen in over 100 years of observation"?
- How should this uncertainty be captured and projected in computations?


## Rare events

- Often the driving concern in analyses
- Typically big consequences
- Hardly ever characterized by good data
- Perhaps never seen, or seen only once


## Random sample data

- ML says $p$ is zero for never-seen events
- Nobody believes this is a reasonable estimate
- Bayesian estimator is more reasonable...




## Random sample data

- ML says $p$ is zero for never-seen events
- Nobody believes this is a reasonable estimate
- The Bayesian estimator is many things
- 'Reasonable' only in that it's whatever you want
- Modern estimators
- Imprecise beta (Dirichlet) models
- Confidence structures


## Confidence structure (c-box)

- P-box-shaped estimator of a (fixed) parameter
- Gives confidence interval at any confidence level
- Can be propagated just like p-boxes
- Allow us to compute with confidence


## Probability of rare event

- Inference about probability from binary data, $k$ successes out of $n$ trials

$$
p \sim[\operatorname{beta}(k, n-k+1), \operatorname{beta}(k+1, n-k)]
$$

- Identical to Walley's Imprecise Beta Model with $s=1$, but needs no prior



## Zero out of $10^{k}$ trials

$-\sqrt{(\sqrt{6} \text { zero corner' }}$

## One out of $10^{k}$ trials



## Vesely's tank

What's the chance the tank ruptures under pumping?


Vesely et al. 1981

## Fault tree


$\mathrm{E} 1=\mathrm{T} \vee(\mathrm{K} 2 \vee(\mathrm{~S} \&(\mathrm{~S} 1 \vee(\mathrm{~K} 1 \vee \mathrm{R}))))$

## Vesely's pressurized tank





Top event tank rupture under pressurization $E 1$


## Try it in pba.r

## T = CBbinomial(0, 2000)

 K2 $=$ CBbinomial $(3,500)$E1 = T \%|\% (K2 \%|\% (S \%\&\% (S1 \%|\% (K1 \%|\% R))))

## Overconfidence

- People, including scientists and engineers, systematically understate their uncertainty
- $90 \%$ confidence intervals ought to enclose the true value $90 \%$ of the time, but do only about $40 \%$ of time
- Overconfidence "has been found to be almost universal in all measurements of physical quantities"
- Likely to be at least as important in expert elicitation when nothing is being measured



## We need an elicitation penalty

- Expert opinions aren't like random data
- Their uncertainty should be inflated
- The penalty size should be derived empirically from validation studies of prior elicitations

Who's doing such studies?

## Here's a placeholder for the penalty

- The numbers in " 1 in 300 " are not counts but estimates with imprecision implied by sigdigs

$$
\begin{aligned}
" 1 \text { in } 300 " & =[0.5,1.5] /[250,350] \\
& =[0.5 / 350,1.5 / 250]
\end{aligned}
$$

- The envelope of all corresponding c-boxes


## Significant-digit intervals

- Significant digits imply an interval ( $\pm$ half the magnitude of the last significant decimal place)

| $x$ | $s(x)$ |
| :--- | :--- |
| 0 | $[0,0.5]$ |
| 1 | $[0.5,1.5]$ |
| 9 | $[8.5,9.5]$ |
| 10 | $[5,15]$ |
| 300 | $[250,350]$ |
| 8150 | $[8145,8155]$ |
| $1 \times 10^{7}$ | $\left[5 \times 10^{6}, 1.5 \times 10^{7}\right]$ |

## Examples for elicitations " $k$ in $n$ "



Gray c-boxes $\mathrm{B}(k, n)$, and black c-box envelopes $\mathrm{E}(k, n)=\mathrm{B}(\mathrm{s}(k), \mathrm{s}(n))$

## More uncertainty for round numbers

- Doubles (or more than doubles) the uncertainty
- Why more than doubles?

$$
\begin{array}{ll}
s(9)=[8.5,9.5] & \text { unit width } \\
s(10)=[5,15] & \text { width of } 10
\end{array}
$$

- Presumes greater uncertainty when round numbers are used to characterize a probability

Maximum
likelihood

Maximum
entropy

Bayesian inference

## Estimation

Expert elicitation

"the great frontier of
making things up"

Method of
PERT moments

## C-boxes

- Don't optimize anything; they perform
- Characterize inputs from limited or even no data
- With an uncertainty penalty, seems to capture some uncertainty in experts' bald assertions like
" 1 in 1000"
"1 in ten million"
"never been seen in 100 years"


## C-boxes are compatible p-boxes

- P-boxes have a performance interpretation too
- If constraints are known that specify a rigorous p-box, then it encodes prediction intervals
- So our performance interpretation applies for - Parametric problems
- Nonparametric problems
- No data problems
- Constraint problems



## Topics

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- Dependence 35
- Sensitivity analysis 30
- Validation 30
- Backcalculation 25
- Spacecraft design at NASA 20
- Statistics for interval data 35
- Neuroscience of uncertainty 40
- Model uncertainty 20


# Imprecise probabilities 

## Probability of an event

- Imagine a gamble that pays one dollar if an event occurs (but nothing otherwise)
- How much would you pay to buy this gamble?
- How much would you be willing to sell it for?
- Probability theory requires the same price for both
- By asserting the probability of the event, you agree to buy any such gamble offered for this amount or less, and to sell the same gamble for any amount equal to or more than this 'fair' price... and to do so for every event!
- IP just says, sometimes, your highest buying price might be smaller than your lowest selling price


## Why is yet another method needed?

- Some statements of uncertainty can't be expressed with p-boxes or interval probability
- Need to express uncertainty of all kinds
- Sometimes mere bounding isn't good enough


## What bounding probability can't do

- Represent comparative probability judgments, e.g., event $A$ is at least as likely as event $B$
- Give unique expectations needed for making decisions
- Give unique conditional probabilities needed for making inferences
- Maintain best possible bounds through updating


## Imprecise probabilities

- Generic term for any theory that doesn't assume a unique underlying probability
- Often expressed in terms of closed, convex sets of probability distributions (not the same as a p-box)
- General case v. special case set v . interval imprecise probabilities v. p-boxes, probability intervals


## Sets of distribution functions

- Consider the set of all Bernoulli distributions (which are discrete with mass at only 0 and 1)

- Clearly, there's a one-dimensional family of such distributions, parameterized by how the mass is distributed between the two points


## Space of distributions

- This one-dimensional family constitutes a space of distributions in which each point represents a distribution



## Three-dimensional case

- When the distributions have 3 point masses, the space becomes two-dimensional and has a triangular shape
- The points on this surface are those whose coordinates add to one



## Simplex

- For discrete distributions with $n$ masses, the space, called a simplex, has ( $n-1$ )-dimensions
- One degree of freedom is lost to the constraint that probabilities sum to one
- For the continuous case, the space becomes infinite-dimensional, or you could be content to use discrete approximations



## Walley's (2000) football game

- 3 possibilities for our team: win, draw, loss
- Suppose we have qualitative judgments:
'Not win' is at least as probable as win
Win is at least as probable as draw
Draw is at least as probable as loss
- These constrain the probability distribution $P$

$$
\begin{aligned}
& P(\text { win }) \leq 1 / 2 \\
& P(\text { win }) \geq P(\text { draw }) \\
& P(\text { draw }) \geq P(\text { loss })
\end{aligned}
$$




## So what?

- The closed, convex set of probability distributions (the red triangular region) expresses the uncertainty
- This set of distributions is smaller than the set implied by bounds on the three probabilities (the green area enclosing the triangle)
- This difference can affect expectations of functions that depend on the events, and conditional probabilities


## Credal set

- Knowledge and judgments can be used to define a set of possible probability measures
. - All distributions within bounds are possible
- Only distributions having a given shape
- Probability of an event is within some interval
- Event $A$ is at least as probable as event $B$
- Nothing is known about the probability of $C$
- Computing with credal sets usually requires mathematical programming


## Correlation and dependency

## Dependence

- Most variables assumed independent
- But some variables clearly aren't
- Density and porosity
- Rainfall and temperature
- Body size and skin surface area


## Dependence can be complex



## Dependence for fixed correlation








Every scattergram has (Pearson) correlation 0.816


## Dependencies

- Independence (knowing $X \sim F$ tells nothing about $Y \sim G$ )
- Perfect dependence
- Opposite dependence
- Complete dependence
- Linearly correlated

- Ranks linearly correlated
- Functional modeling

- Complex dependence


Uncorrelatedness is not independence

## Scattergrams with zero correlation




## $X+Y$ depends on dependence

All these come from uncorrelated variables


## Can't always assume independence

- If you know the mechanism of dependence, you can model it
- Else, have to reproduce the statistical patterns
- If dependence unknown, can't use either way
- Even small correlations can have a big effect on convolutions


## What about other dependencies?

- Independent
- Perfectly positive (comonotonic)
- Opposite (countermonotonic)
- Positively or negatively associated
- Specified correlation coefficient
- Nonlinear dependence (copula)
- Unknown dependence


## Perfect dependence

| $A+B$ <br> perfect positive | $A \in[1,3]$ <br> $p_{1}=1 / 3$ | $A \in[2,4]$ <br> $p_{2}=1 / 3$ | $A \in[3,5]$ <br> $p_{3}=1 / 3$ |
| :--- | :--- | :--- | :--- |
| $B \in[2,8]$ <br> $q_{1}=1 / 3$ | $A+B \in[3,11]$ <br> prob $=1 / 3$ | $A+B \in[4,12]$ <br> prob $=0$ | $A+B \in[5,13]$ <br> prob $=0$ |
| $B \in[6,10]$ <br> $q_{2}=1 / 3$ | $A+B \in[7,13]$ <br> prob $=0$ | $A+B \in[8,14]$ <br> prob $=1 / 3$ | $A+B \in[9,15]$ <br> prob $=0$ |
| $B \in[8,12]$ <br> $q_{3}=1 / 3$ | $A+B \in[9,15]$ <br> prob $=0$ | $A+B \in[10,16]$ <br> prob $=0$ | $A+B \in[11,17]$ <br> prob $=1 / 3$ |

## Opposite dependence

| $A+B$ | $A \in[1,3]$ <br> $p_{1}=1 / 3$ | $A \in[2,4]$ <br> $p_{2}=1 / 3$ | $A \in[3,5]$ <br> $p_{3}=1 / 3$ |
| :--- | :--- | :--- | :--- |
| opposite positive |  |  |  |
| $B \in[2,8]$ | $A+B \in[3,11]$ <br> $q_{1}=1 / 3$ | $A+B \in[4,12]$ <br> prob $=0$ | $A+B \in[5,13]$ <br> prob $=0$ |
| $B \in[6,10]$ <br> $q_{2}=1 / 3$ | $A+B \in[7,13]$ <br> prob $=0$ | $A+B \in[8,14]$ <br> prob $=1 / 3$ | $A+B \in[9,15]$ <br> prob $=0$ |
| $B \in[8,12]$ <br> $q_{3}=1 / 3$ | $A+B \in[9,15]$ <br> prob $=1 / 3$ | $A+B \in[10,16]$ <br> prob $=0$ | $A+B \in[11,17]$ <br> prob $=0$ |

## Perfect and opposite dependencies



## Uncertainty about dependence

- Sensitivity analyses usually used
- Vary correlation coefficient between -1 and +1
- But this underestimates the true uncertainty
- Example: suppose $X, Y \sim$ uniform $(0,24)$ but we don't know the dependence between $X$ and $Y$


## Varying the correlation coefficient



## Counterexample: outside the cone!




## Fréchet inequalities

They make no assumption about dependence (Fréchet 1935) $\max (0, \mathrm{P}(A)+\mathrm{P}(B)-1) \leq \mathrm{P}(A \& B) \leq \min (\mathrm{P}(A), \mathrm{P}(B))$ $\max (\mathrm{P}(A), \mathrm{P}(B)) \leq \mathrm{P}(A \vee B) \leq \min (1, \mathrm{P}(A)+\mathrm{P}(B))$


## Fréchet case (no assumption)

| $A+B$ | $A \in[1,3]$ <br> $p_{1}=1 / 3$ | $A \in[2,4]$ <br> $p_{2}=1 / 3$ | $A \in[3,5]$ <br> $p_{3}=1 / 3$ |
| :--- | :--- | :--- | :--- |
| Fréchet case |  |  |  |

## Naïve Fréchet case



## Fréchet can be improved

- Interval estimates of probabilities don't reflect the fact that the sum must equal one
- Resulting p-box is too fat
- Linear programming needed to get the optimal answer using this approach
- Frank, Nelsen and Sklar (1987) gave a way to compute the optimal answer directly


## Frank, Nelsen and Sklar (1987)

Suppose $X \sim F$ and $Y \sim G$.
If $X$ and $Y$ are independent, then the distribution of $X+Y$ is

$$
\sigma_{+, C}(F, G)(z)=\int_{x+y<z} d C(F(x), G(y))
$$

In any case, and irrespective of their dependence, this distribution is bounded by
$\left[\sup _{z=x+y} \max (F(x)+G(y)-1,0), \inf _{z=x+y} \min (F(x)+G(y), 1)\right]$
This formula can be generalized to work with bounds on $F$ and $G$.

## Best possible bounds



## Unknown dependence



## Fréchet dependence bounds

- Cannot be obtained by sensitivity studies
- Guaranteed to enclose results no matter what correlation or dependence there may be between the variables
- Best possible (couldn't be any tighter without saying more about the dependence)
- Can be combined with independence assumptions between other variables


## Between independence and Fréchet

- Some information may be available by which the p-boxes could be tightened over the Fréchet case without specifying the dependence perfectly, e.g.,
- Dependence is positive (PQD)
$\mathrm{P}(X \leq x, Y \leq y) \geq \mathrm{P}(X \leq x) \mathrm{P}(Y \leq y)$ for all $x$ and $y$
- Variables are uncorrelated

Pearson correlation $r$ is zero

## Unknown but positive dependence



## Uncorrelated variables



## "Linear" correlation



## Can model dependence exactly too



No assumptions

## 



Perfect


Uncorrelated


Positive dependence


Independence


Opposite


## Example: dioxin inhalation

Location: Superfund site in California
Receptor: adults in neighboring community
Contaminant: dioxin
Exposure route: inhalation of windborne soil

Modified from Table II and IV in Copeland, T.L., A.M. Holbrow, J.M Otani, K.T. Conner and D.J. Paustenbach 1994. Use of probabilistic methods to understand the conservativism in California's approach to assessing health risks posed by air contaminant. Journal of the Air and Waste Management Association 44: 1399-1413.

## Total daily intake from inhalation

$$
T D I=\left(\frac{R \times C_{\mathrm{GL}} \times F_{\mathrm{inh}} \times E D \times E F}{B W \times A T}\right)
$$

$R=\operatorname{normal}(20,2)$
$C_{\text {GL }}=2$
$F_{\text {inh }}=$ uniform $(0.46,1)$
$E D=\operatorname{exponential(11)}$
$E F=$ uniform $(0.58,1)$
$B W=\operatorname{normal}(64.2,13.19)$
$A T=\operatorname{gumbel}(70,8)$
respiration rate, $\mathrm{m}^{3} /$ day
concentration at ground level, $\mathrm{mg} / \mathrm{m}^{3}$ fraction of particulates retained in lung, [unitless]
exposure duration, years exposure frequency, fraction of a year receptor body weight, kg averaging time, years

## Input distributions







## Results



## Uncertainty about depender be $\leftrightarrows D$ DIT

- Impossible with sensitivity analysis since it's an infinite-dimensional problem
- Kolmogorov-Fréchet bounding lets you be sure
- Sometimes there's a big difference, sometimes it's negligible


## Try it in pba.r

## Auto Frechet Perfect Opposite Independent

Plus $+\quad \%+\% \quad \% /+/ \% \quad \% \mathrm{o}+0 \% \quad \%|+| \%$
Minus - $\%-\% \quad \% /-/ \% \quad \% \mathrm{o}-0 \% \quad \%|-| \%$
etc.

## Independence

- In the context of precise probabilities, there was a unique notion of independence
- In the context of imprecise probabilities, however, this notion radiates into several distinct ideas
- The different kinds of independence behave differently in computations


## Imprecise probability independence

- Random-set independence
- Epistemic irrelevance (asymmetric)
- Epistemic independence
- Strong independence
- Repetition independence
- Others?


## Interesting example

- $X=[-1,+1], \quad Y=\{([-1,0], 1 / 2),([0,1], 1 / 2)\}$


- If $X$ and $Y$ are "independent", what is $Z=X Y$ ?


## Compute via Yager's convolution

Y<br>$([-1,0], 1 / 2) \quad([0,1], 1 / 2)$<br>$X([-1,+1], 1) \quad([-1,+1], 1 / 2) \quad([-1,+1], 1 / 2)$

The Cartesian product with one row and two columns produces this p-box


## But consider the means

- Clearly, $\mathrm{E} X=[-1,+1]$ and $\mathrm{E} Y=[-1 / 2,+1 / 2]$
- Therefore, $\mathrm{E}(X Y)=[-1 / 2,+1 / 2]$
- But if this is the mean of the product, and its range is $[-1,+1]$, then we know better bounds on the CDF



## And consider the quantity signs

- What's the probability $\mathrm{P}_{Z}$ that $Z<0$ ?
- $Z<0$ only if $X<0$ or $Y<0$ (but not both)
- $\mathrm{P}_{Z}=\mathrm{P}_{X}\left(1-\mathrm{P}_{Y}\right)+\mathrm{P}_{Y}\left(1-\mathrm{P}_{X}\right)$, where

$$
\mathrm{P}_{X}=\mathrm{P}(X<0), \mathrm{P}_{Y}=\mathrm{P}(Y<0)
$$

- But $\mathrm{P}_{Y}$ is $1 / 2$ by construction
- So $\mathrm{P}_{Z}=1 / 2 \mathrm{P}_{X}+1 / 2\left(1-\mathrm{P}_{X}\right)=1 / 2$
- Thus, zero is the median of $Z$

- Knowing median and range improves bounds


## Best possible

- These bounds are realized by solutions If $X=0$, then $Z=0$ If $X=Y=\mathrm{B}=\{(-1,1 / 2),(+1,1 / 2)\}$, then $Z=\mathrm{B}$



- So these bounds are also best possible


## So which is correct?



Moment independence


Strong independence


The answer depends on what one meant by "independent"

## So what?

- The example illustrates a practical difference between random-set independence and strong independence
- It disproves the conjecture that the convolution of uncertain numbers is not affected by dependence assumptions if at least one of them is an interval
- It tempers the claim about the best-possible nature of convolutions with probability boxes and DempsterShafer structures


## Strategy for risk analysts

- Random-set independence is conservative
- Using the Cartesian product approach is always rigorous, though may not be optimal
- Convenient methods to obtain tighter bounds under stronger kinds of independence await discovery


Sensitivity analysis

## When to break down and get more data

## Justifying further empirical effort

- If the incertitude associated with the results of an analysis is too broad to make practical decisions, and the bounds are best possible, more data is needed
- Strong argument for collecting more data
- Planning empirical efforts can be improved by doing sensitivity analysis of the model


## Sensitivity analysis of p-boxes

- Quantifies the reduction in uncertainty of a result when an input is pinched
- Pinching is hypothetically replacing it by a less uncertain characterization


## Pinching sensitivity analyses

- Model the possible contraction of incertitude in each input p-box from additional data to be collected
- Recompute analysis with this tighter p-box
- Others inputs held in their original form
- Or possibly tighten several if appropriate for planned data
- Estimate improvement in results
- breadth(tighter input) / breadth(base)
- Repeat for all inputs or data collection strategies
- Don't omit variables from sensitivity study or "shortlist"
- Allocate empirical effort by the magnitude of the potential improvement in uncertainty


## Pinching to a precise distribution




## Examples



Uses no assumption about dependence between $A$ and $B$

## Pinching to a point value




## Examples



## Pinching dependence

- An uncertain dependence can also be pinched to a more specific dependence positive $\rightarrow$ independence positive $\rightarrow$ perfect positive $\rightarrow$ normal copula with correlation 0.3 Fréchet $\rightarrow$ independence etc.


## Example




Pinch the
dependence to independence

## Pinching to a zero-variance interval



Assumes value is constant, but unknown
There's no analog of this in Monte Carlo

## Pinching to a zero-variance interval



## Pinching to other targets

- Pinchings need not be to particular targets, e.g., a single point or a precise distribution
- Traditionally, the results of pinching to various targets were averaged (called "freezing"), but that approach erases the effect of uncertainty
- Instead, we ask: what is the range of observed reductions in uncertainty as the pinching target is varied over many different possibilities?


## Case study: dike reliability



## The inputs

Relative density of the revetment blocks
$\Delta=[1.60,1.65]$
Block thickness
$D=[0.68,0.72]$ meters
Slope of the revetment
$\alpha=\operatorname{atan}([0.32,0.34])=[0.309,0.328]$ radians
Analysts' "model uncertainty" factor
$M=$ [3.0, 5.2]
Significant wave height (average of the highest third of waves) $H=$ weibull([1.2, 1.5] meters, [10, 12])

Offshore peak wave steepness
$s=\operatorname{normal}([0.039,0.041],[0.005,0.006])$

## Analysis








Probability of negative $Z$ (i.e., dike failure) is less than 0.05

Nominal pinching targets are dotted

## Percent reduction of uncertainty

| Input | Nominal <br> pinching | All possible <br> pinchings |  |
| :---: | :---: | :---: | ---: |
| $\Delta$ | 5.5 | $\left[\begin{array}{r}{[4.7,}\end{array} 5.7\right]$ |  |
| $D$ | 10.0 | $[9.2$, | $11.0]$ |
| $M$ | 53.0 | $[41.0$, | $60.0]$ |
| $\alpha$ | 6.5 | $[3.8$, | $9.1]$ |
| $H$ | 23.0 | $[15.0$, | $30.0]$ |
| $S$ | 3.6 | $[2.0$, | $5.2]$ |

Empirical study rank order: $M H D \alpha \Delta s$

## On the same axis

(intervals depicted as triangles)


Empirical study rank order: $M H D \alpha \Delta s$

## Caveat

Omitting some variables from a sensitivity analysis ("shortlisting") because their uncertainties are small is a bad idea.

Doing this reduces dimensionality, but it also erases uncertainty.

What about engineering control?

## Sensitivity analysis with p-boxes

- Local sensitivity via derivatives
- Explored macroscopically over the uncertainty in the input
- Describes the ensemble of tangent slopes to the function over the range of uncertainty

Monotone function


Nonlinear function


## Local derivatives

$$
\begin{aligned}
& \frac{\partial Z}{\partial \Delta}=D \\
& \frac{\partial Z}{\partial D}=\Delta \\
& \frac{\partial Z}{\partial \alpha}=\frac{-H\left(1+\sin ^{2}(\alpha)\right)}{\cos ^{3}(\alpha) M \sqrt{s}} \\
& \frac{\partial Z}{\partial M}=\frac{H \tan (\alpha)}{\cos (\alpha) M^{2} \sqrt{s}} \\
& \frac{\partial Z}{\partial H}=\frac{-\tan (\alpha)}{\cos (\alpha) M \sqrt{s}} \\
& \frac{\partial Z}{\partial s}=\frac{H \tan (\alpha)}{2 \cos (\alpha) M s^{3 / 2}}
\end{aligned}
$$








## On the same axis



Engineering control rank order: $s \alpha D \Delta H M$

## Completely different rankings

- The uncertainty reduction in hypothetical pinching assesses the possible effect of more or better data
- Evaluating local derivates as p-boxes tells how effective control or management can be

Empirical study:
Best for study Engineering control: MHD $\alpha \Delta s$


Best for control

## Different 'sensitivity' questions

Empirical planning

- What variables need study to reduce uncertainty?

Engineering control

- What variables can be modified to change the result?
$\checkmark$ Robustness analysis
- How robust are the results of the assessment?
$\mathbf{x}^{\mathbf{T}}$ Tracking analysis
- Which input combinations yield extreme results?


## Validation

## Goals

- Objectively measure the conformance of predictions with empirical data
- Use this measure to characterize the reliability of other predictions


## Initial setting

- The model is fixed, at least for the time being - No changing it on the fly during validation
- A prediction is a probability distribution - Expressing stochastic uncertainty
- Observations are precise (scalar) numbers
- Measurement uncertainty is negligible


## Validation metric

- A measure of the mismatch between the observed data and the model's predictions
- Low value means a good match
- High value means they disagree
- Distance between prediction and data


## Desirable properties of a metric

- Expressed in physical units
- Generalizes deterministic comparisons
- Reflects full distribution
- Not too sensitive to long tails
- Mathematical metric
- Unbounded (you can be really off)



## How the data come



## How we look at them



## One suggestion for a validation metric



## Area metric

- "Distance" between two distributions
- Smallest mean absolute difference of deviates


## Reflects full distribution



## Single observation



## When the prediction is really bad



- The metric degenerates to simple distance
- Probability is dimensionless, so units are the same


## Depends on the local scale



## Why physical units?




- Distributions in the left graph don't even overlap but they seem closer than those on the right


## Why an unbounded metric?




- Neither overlaps, but left is better fit than right
- Smirnov's metric $D_{\text {max }}$ considers these two cases indistinguishable (they're both just 'far')


## The model says different things



Time [seconds]



## Pooling data comparisons

- When data are to be compared against a single distribution, they're pooled into $S_{n}$
- When data are compared against different distributions, this isn't possible
- Conformance must be expressed on some universal scale


## Universal scale


$u_{i}=F_{i}\left(x_{i}\right)$ where $x_{i}$ are the data and $F_{i}$ are their respective predictions

## $u$-pooling



## Statistical test for model accuracy

- Kolmogorov-Smirnov test of distribution of $u_{i}$ 's against uniform over [0,1]
- Tests whether the data were drawn from the respective prediction distributions
Probability integral transform theorem (Angus 1994) says the $u$ 's will be distributed as uniform $(0,1)$ if $x_{i} \sim F_{i}$
- Assumes the empirical data are independent of each other


## Extends to correlated multivariate case

- Li, et al. (2014) say $u$-pooling doesn't generalise to multivariate predictions with correlations
- But they just misunderstood how to do it
- Two kinds of $u$-pooling:
$\boldsymbol{\square}$ Are not predicting (or don't know) dependencies
$\boldsymbol{\rightarrow}$ Are making predictions about dependencies
Small $d$ means match in distributions and dependencies


# Epistemic uncertainty 

## How should we compare intervals?



## Validation for intervals

- Validation measure is the smallest difference
- Overlapping intervals match perfectly
- Validity is distinct from precision
- Otherwise no value in an uncertainty analysis



## Epistemic uncertainty in predictions





- In left, the datum evidences no discrepancy at all
- In middle, the discrepancy is relative to the edge
- In right, the discrepancy is even smaller


## Epistemic uncertainty in both



Predictions in red
Observations in blue 280

## Predictive capability

## Predictive capability

- Not a measure of how good the model is
- A characterization of how much we should trust its predictions


## Predictive capability

- Additional uncertainty (estimate of possible error) that is recognized by comparing a model's predictions against available data
- On top of introspective model uncertainty estimates already embodied in the analysis
- How should we characterize this uncertainty?
- Let's consider three possible approaches


## Plus or minus $d$ (area metric)



## All distributions that are $d$-close



## Area versus distribution of differences









Area between distributions Distribution (or p-box) of differences

## Signed difference and bias



## Research topic

- Difference interval, distribution, or p-box
- Sign
- Signed differences to account for model bias
- Plus-or-minus absolute differences
- Extrapolation by regression analysis
- From conditions for which data are available to conditions at which the prediction is to be made
- Interpolation by regression analysis
- Sampling uncertainty about the differences


## Extrapolate to 2000 degrees



## Interpolating at 800 degrees



## Sampling uncertainty about data

- Regression methods account for the trends and scatter (variation over some axis) of the data
- But, for predictive capability, the blue data p-box should reflect sampling uncertainty too
- May be important when sample size is small
- Can use confidence or tolerance band to form the blue p-box summarizing the data


## Predictive capability

- Turns on epistemic and aleatory uncertainty
- Post-hoc measure of model uncertainty
- Distinct from validation
- Clearly crucial to any sort of modeling
- Still the subject of broad discussion and debate


## Assessment versus reliability

## Validation

- Discrepancy between prediction and data
- Absolute value
- May neglect sampling uncertainty of data
- Summarizes across predictions and even dimensions

Predictive capability

- Distribution of differences between prediction and data
- May have sign
- Must account for sampling uncertainty about data
- Uses regression across predictions, but limited to one dimension


## Summary

- Both assessment and reliability of extrapolation - How good is the model? Validation
- Should we trust its pronouncements? Predictive capability
- Calibration and updating are separate activities
- Validation measure must be bespoke but universal; predictive capability is still part of modeling
- Epistemic uncertainty introduces some wrinkles - Full credit for being modest about predictions


## Backcalculation

## Backcalculation

- Engineering design requires backcalculation
- How can we untangle the expression

$$
A+B=C
$$

when we know $A$ and $C$, and need $B$ ?

## Can't just invert the equation

prescribed

Concentration $=$ Dose $\times$ Bodymass $/$ Intake

When concentration is put back into the forward equation, the resulting dose is wider than planned



## Normal approximation

- If $A+B=C$, compute $B$ as $C-A$ under the assumption the correlation between $A$ and $C$ is $r=\operatorname{sd}(A) / \operatorname{sd}(C)$

To simulate normal deviates with correlation $r$, compute

$$
\begin{aligned}
& Y_{1}=Z_{1} \times \sigma_{1}+\mu_{1} \\
& Y_{2}=\left(r Z_{1}+Z_{2} \sqrt{ }\left(1-r^{2}\right)\right) \times \sigma_{2}+\mu_{2}
\end{aligned}
$$

where $Z_{1}$ and $Z_{2}$ are independent standard normal deviates, and $\mu$ and $\sigma$ denote the respective desired means and standard deviations

- Uses Pearson correlation (not rank correlation)
- Good for multivariate normal, and maybe more

Normal approximation with non-normal distributions





## Iterative (trial \& error) approach

- Initialize $B$ with $C-A$
- This distribution is too wide
- Transform density $p(x)$ to $p(x)^{m}$
- Rescale so that area remains one
- Whenever $m>1$ dispersion decreases
- Vary $m$ until you get an acceptable fit



## Backcalculation with intervals

- Backcalculation is well understood for intervals
- Each interval operation has multiple modes:

Shell (or "united") solution is forward projection

The shell contains every solution
Kernel (or "tolerance") solution is backward
Every element of the kernel is a solution

## Kernel versus shell

$A=[1,2] \quad C=[2,6] \quad C=A+B$
There are different ways to solve for $B$
Shell

$$
\begin{aligned}
B & =C-A \\
& =\left[C_{1}-A_{2}, C_{2}-A_{1}\right] \\
& =[0,5]
\end{aligned}
$$

Kernel

$$
\begin{aligned}
B & =\operatorname{backcalc}(A, C) \\
& =\left[C_{1}-A_{1}, C_{2}-A_{2}\right] \\
& =[1,4]
\end{aligned}
$$



| When you And need for est | And you have estimates for | Use this formula to find the unknown |
| :---: | :---: | :---: |
| $A+B \subseteq C$ | $A, B$ | $C=A+B$ |
|  | A, C | $B=\operatorname{backcalc}(A, C)$ |
|  | et of" $B, C$ | $A=\operatorname{backcalc}(B, C)$ |
| $A-B \subseteq C$ | A, B | $C=A-B$ |
|  | A, C | $B=-\operatorname{backcalc}(A, C)$ |
|  | $B, C$ | $A=\operatorname{backcalc}(-B, C)$ |
| $A \times B \subseteq C$ | A, B | $C=A * B$ |
|  | A, C | $B=$ factor $(A, C)$ |
|  | $B$, $C$ | $A=\operatorname{factor}(B, C)$ |
| $A / B \subseteq C$ | A, B | $C=A / B$ |
|  | $A, C$ | $B=1 /$ factor $(A, C)$ |
|  | $B$, $C$ | $A=$ factor $(1 / B, C)$ |
| $A^{\wedge} B \subseteq C$ | A, B | $C=A^{\wedge} B$ |
|  | $A, C$ | $B=$ factor $(\log A, \log C)$ |
|  | $B, C$ | $A=\exp (\operatorname{factor}(B, \log C))$ |
| $2 A \subseteq C$ | A | $C=2 * A$ |
|  | C | $A=C / 2$ |
| $A^{2} \subseteq C$ | A | $C=A^{\wedge} 2$ |
|  | C | $A=\operatorname{sqrt}(C)$ |

## Backcalculation with p-boxes

Suppose $A+B=C$, where
$A=\operatorname{normal}(5,1)$
$C=\left\{0 \leq C\right.$, median $\leq 1.5,90^{\text {th }} \%$ ile $\left.\leq 35, \max \leq 50\right\}$



## Backcalc algorithm for p-boxes

Additive untangling of the kernel for $B$ from the equation $C=A+B$, where p-boxes for $A$ and $C$ are known. Only the algorithm for the left bound is shown; the right bound is similar.
$\mathrm{N}=$ number of percentiles (\%ile) used in the representation;
left limit on B at lowest \%ile $=$ left limit on C at lowest $\%$ ile - left limit on A at lowest $\%$ ile; for $\mathrm{i}=1$ to N do begin
set flag to "not done";
for $\mathrm{j}=0$ to $\mathrm{i}-1$ do begin
if (left limit on C at $\mathrm{i}^{\text {th }} \%$ ile $) \leq\left(\right.$ left limit on A at $\left.[\mathrm{i}-\mathrm{j}]^{\text {th }} \% i l e\right)+\left(\right.$ left limit on B at the $\mathrm{j}^{\text {th }} \%$ ile $)$ then set flag to "done";
if flag is "done"
then left limit on B at $\mathrm{i}^{\text {th }} \% \mathrm{ile}=$ left limit on B at $[\mathrm{i}-1]^{\text {th }} \%$ ile $\{$ the one right below it$\}$
else left limit on B at $\mathrm{i}^{\text {th }} \% \mathrm{ile}=$ left limit on C at $\mathrm{i}^{\text {th }} \% \mathrm{ile}-$ left limit on A at $0^{\text {th }} \%$ ile; end; \{for j$\}$
end; \{for i, left bound $\}$

## Getting the answer

- The backcalculation algorithm basically reverses the forward convolution
- Any distribution totally inside $B$ is sure to satisfy the constraint ... it's a "kernel"



## Check it by plugging it back in

## $A+\boldsymbol{B}=C^{*} \subseteq C$



## Precise distributions don't work

- Precise distributions can't express the target
- A concentration distribution giving a prescribed distribution of doses seems to say we want some doses to be high
- But any distribution to the left would be better
- A p-box on the dose target expresses this idea


## Backcalculation algebra

- Can define untanglings for all basic operations e.g., if $A \times B=C$, then $B=\exp ($ backcalc $(\ln A, \ln C))$
- Can chain them together for big problems
- Assuming independence widens the result
- Repeated terms need special strategies


## Se concentration in SF Bay mussels

San Francisco Bay blue mussels Mytilus edulis are contaminated with the heavy metal selenium (Se)

What concentration [Se] in the bay is safe for humans given that it concentrates in food chains


## Tolerable Se doses for humans

NOAEL $=15 \mathrm{mg} / \mathrm{kg} / \mathrm{d}_{\text {(ATSDR 1996) }}$

- Median exposures no greater than $5 \mathrm{mg} / \mathrm{kg} / \mathrm{d}$
- 95th \%tile exposure no greater than $10 \mathrm{mg} / \mathrm{kg} / \mathrm{d}$
- Maximum exposure of $15 \mathrm{mg} / \mathrm{kg} / \mathrm{d}$


Any dose distribution entirely in this box meets the constraints

## Mussel consumption

- Data on mussel consumption by Americans were collected by the U.S. National Marine Fisheries Service in a nationwide survey between 1973 and 1974 (Rupp et al. 1980). These data were re-analyzed by Ruffle et al. (1994) and fit to lognormal distributions. Genders are combined for adults aged 19-98, and the consumption data is divided into U.S. regions. We chose the data for the Pacific region (WA, OR, CA, AK, and HI)
- The data are very old, but the best available. Ruffle et al. suggest adding 0.22 to the mean intake rate to account for increased shellfish consumption since 1974, and the intake distribution is then lognormal with mean $(1.177+0.22)$ and standard deviation $0.938 \mathrm{~g} / \mathrm{d}$.


Should this have been a p-box too?

## Human body mass

- Brainard and Burmaster (1992) provide body weight distributions for men and women aged 18-74 using data in the NHANES II data set (collected between 1976 and 1980).

|  |  |  |
| :---: | :---: | :---: |
| 30 | $\begin{array}{cc} 60 & 90 \\ \text { Body weight (kg) } \end{array}$ | 120 |

## Use "factor" to backcalculate

$$
\begin{gathered}
\text { Dose }=\text { WConc } \frac{(k+h \times B \times g \times p)}{(l+f \times N \times g \times p)} \times \frac{\text { Intake }}{B W} \\
\text { WConc }=\text { factor }\left(\frac{(k+h \times B \times g \times p)}{(l+f \times N \times g \times p)} \times \frac{\text { Intake }}{B W}, \text { Dose }\right)
\end{gathered}
$$

The factor algorithm untangles the convolutions

- Finds bounds on WConc distributions leading to safe doses
- Repeated terms ( $g$ and $p$ ) need "region-growing" strategy
- Result has thickest possible tails


## Factor algorithm

Multiplicative untangling of the kernel for $B$ from the equation $C=A B$, where p-boxes for $A$ and $C$ are known. Only the algorithm for the left bound is shown; the right bound is similar.
$\mathrm{N}=$ number of percentiles (\%ile) used in the representation;
left limit on B at lowest \%ile $=$ left limit on C at lowest $\%$ ile $/$ left limit on A at lowest \%ile; for $\mathrm{i}=1$ to N do begin
set flag to "not done";
for $\mathrm{j}=0$ to $\mathrm{i}-1$ do begin
if $\left(\right.$ left limit on C at $\mathrm{i}^{\text {th }} \%$ ile $) \leq\left(\right.$ left limit on A at $[\mathrm{i}-\mathrm{j}]^{\text {th }} \%$ ile $) \times\left(\right.$ left limit on B at the $\mathrm{j}^{\text {th }} \%$ ile $)$ then set flag to "done";
if flag is "done"
then left limit on B at $\mathrm{i}^{\text {th }} \% \mathrm{ile}=$ left limit on B at $[\mathrm{i}-1]^{\text {th }} \%$ ile $\{$ the one right below it$\}$
else left limit on B at $\mathrm{i}^{\text {th }} \%$ ile $=$ left limit on C at $\mathrm{i}^{\text {th }} \% \mathrm{ile} /$ left limit on A at $0^{\text {th }} \%$ ile; end; \{for j$\}$
end; \{for i, left bound $\}$

## Results



## Check



## Now what?

- So we know how low the Se concentrations in mussels have to be to be safe
- What does that imply about concentrations for the water in the bay?


## Multiple pathways



## Untangling the trophic chain

- Steady-state model for the trophic chain (Spencer et al. 2001)
- Assumes all parameters, including [Se] in water, are at equilibrium
- Needs two backcalculations
- First determines the p-box around the set of Se concentration distributions in edible mussel tissue that are protective of human health
- Second derives the p-box around the set of distributions of Se concentration in water that result in concentrations of Se in edible mussel tissue meeting the constraint


## Steady-state fate/transport model

Dose $=M$ Conc $\times \frac{\text { Intake }}{B W} \quad$ MConc $=W \operatorname{Conc} \frac{(k+h \times B \times g \times p)}{(l+f \times N \times g \times p)}$
Mconc $=$ Se concentration in mussels $(\mu \mathrm{g} / \mathrm{g})$
Wconc $=$ Se concentration in bay water $(\mu \mathrm{g} / \mathrm{L})$
Intake $=$ mussel intake rate (g/d)
$B W=$ adult body weight ( kg )
We want to
$k=$ mussel Se uptake rate from the dissolved phase ( $\mathrm{L} / \mathrm{g} / \mathrm{d}$ )
$h=$ mussel Se assimilation from phytoplankton (unitless)
$B=$ Se bioconcentration factor in phytoplankton ( $\mathrm{L} / \mathrm{g}$ )
$g=$ mussel water filtration rate ( $\mathrm{L} / \mathrm{g} / \mathrm{d}$ )
$p=$ phytoplankton concentration $(\mathrm{g} / \mathrm{L})$
$l=$ mussel selenium elimination rate $\left(\mathrm{d}^{-1}\right)$
$f=$ mussel carbon assimilation efficiency (unitless)
$N=$ mussel net growth efficiency (unitless)

## Steady-state parameters










Why is it that $P$ is a precise distribution?


Backcalculated allowable concentration of Se in water.


Concentration of Se in mussels given Se in water (at left). Allowable concentration in green.


Se in mussels, San Francisco Bay

## So what?

- Many distributions drawn from the shell are not protective of human health
- Algorithms can backcalculate the kernel for both simple and complex exposure models
- The bioavailable Se concentration in San Francisco Bay is well within the kernel of tolerable concentration distributions, as is the Se concentration in edible mussel tissue


## Conclusion

- Engineering design requires backcalculation
- Monte Carlo methods don't generally work except in a trial-and-error approach
- Can express the constraint target as a p-box, although this is awkward in a precise distribution


## Not the same as deconvolution

Deconvolution is a related procedure for equations involving uncertainty

Deconvolution is used, for instance, to improve the estimate of the distribution of $X$ given a distributions of measurements $Y$ and measurement error $\varepsilon$

$$
Y=X+\varepsilon
$$

Deconvolution doesn't satisfy a constraint like backcalculation does

## Se/mussel references

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Case studies

## Case study:

## Spacecraft design under mission uncertainty

## Integrated concurrent engineering

- Real-time collaborative, interactive process - Implemented at JPL, LaRC, and others
- Reduces design time by an order of magnitude - But quantitative risk assessment is difficult
- Design solutions are iterative
- So a Monte Carlo approach may not be practical


## Mission

## Deploy satellite carrying a large optical sensor




Wertz and Larson (1999) Space Mission Analysis and Design (SMAD). Kluwer.


## Typical subsystems



Moments of inertia determine
Torque needed determines
Power requirements determines
Solar panel size determines
Moments of inertia

## Demonstration system



- Calculations within a single subsystem ${ }_{\text {(aCS) }}$
- Calculations within linked subsystems


## Attitude control subsystem (ACS)

- 3 reaction wheels
- Design problem: solve for $h$
- Required angular momentum
- Needed to choose reaction wheels
- Mission constraints
$-\Delta t_{\text {orbit }}=1 / 4$ orbit time
$-\theta_{\text {slew }}=$ max slew angle
$-\Delta t_{\text {slew }}=\min$ maneuver time
- Inputs from other subsystems
$-I, I_{\max }, I_{\min }=$ inertial moment
- Depend on solar panel size, which depends on power needed, so on $h$

$$
\begin{gathered}
h=\tau_{\text {tot }} \times \Delta t_{\text {orbit }} \\
\tau_{\text {tot }}=\tau_{\text {slew }}+\tau_{\text {dist }} \\
\tau_{\text {slew }}=\frac{4 \theta_{\text {slew }}}{\Delta t_{\text {slew }}} I \\
\tau_{\text {dist }}=\tau_{g}+\tau_{s p}+\tau_{m}+\tau_{a} \\
\tau_{\mathrm{g}}=\frac{3 \mu}{2\left(R_{\mathrm{E}}+H\right)^{3} I_{\text {max }}-I_{\text {min }} \mid \sin (2 \theta)} \\
\tau_{\text {sp }}=L_{\mathrm{sp}} \frac{F_{\mathrm{s}}}{c} A_{\mathrm{s}}(1+q) \cos (i) \\
\tau_{\mathrm{m}}=\frac{2 M D}{\left(R_{\mathrm{E}}+H\right)^{3}} \\
\tau_{\mathrm{a}}=\frac{1}{2} L_{\mathrm{a}} \rho C_{\mathrm{d}} A V^{2}
\end{gathered}
$$

## Attitude control input variables

| Symbol | Unit | Variable | Type | Value | SMAD |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $C_{\text {d }}$ | unitless | Drag coefficient | p-box | $\begin{gathered} \text { range }=[2,4] \\ \text { mean }=3.13 \end{gathered}$ | 3.13 |
| $L_{\text {a }}$ | m | Aerodynamic drag torque moment | p-box | $\begin{gathered} \text { range }=[0,3.75] \\ \text { mean }=0.25 \\ \hline \end{gathered}$ | 0.25 |
| $L_{\text {sp }}$ | m | Solar radiation torque moment | p-box | $\begin{gathered} \text { range }=[0,3.75] \\ \text { mean }=[0.25] \end{gathered}$ | 0.25 |
| D | $\mathrm{A} \mathrm{m}^{2}$ | Residual dipole | interval | [0,1] | 1 |
| $i$ | degrees | Sun incidence angle | interval | [0,90] | 0 |
| $\rho$ | $\mathrm{kg} \mathrm{m}{ }^{3}$ | Atmospheric density | interval | $\begin{gathered} {[3.96 \mathrm{e}-12,} \\ 9.9 \mathrm{e}-11] \end{gathered}$ | 1.98e-11 |
| $\theta$ | degrees | Major moment axis deviation from nadir | interval | [10,19] | 10 |
| $q$ | unitless | Surface reflectivity | interval | [0.1,0.99] | 0.6 |
| $I_{\text {min }}$ | $\mathrm{kg} \mathrm{m}^{2}$ | Minimum moment of inertia | interval | [4655] | 4655 |
| $I_{\text {max }}$ | $\mathrm{kg} \mathrm{m}^{2}$ | Maximum moment of inertia | interval | [7315] | 7315 |
| $\mu$ | $\mathrm{m}^{3} \mathrm{~s}^{-2}$ | Earth gravity constant | point | 3.98 e 14 | 3.98 e 14 |
| A | $\mathrm{m}^{2}$ | Area in the direction of flight | point | $3.75{ }^{2}$ | $3.75{ }^{2}$ |
| RE | km | Earth radius | point | 6378.14 | 6378.14 |
| H | km | Orbit altitude | point | 340 | 340 |
| $F_{\text {s }}$ | W m ${ }^{-2}$ | Average solar flux | point | 1367 | 1367 |
| $\theta_{\text {slew }}$ | degrees | Maximum slewing angle | point | 38 | 38 |
| $c$ | $\mathrm{m} \mathrm{s}^{-1}$ | Light speed | point | 2.9979 e 8 | 2.9979 e 8 |
| M | $\mathrm{A} \mathrm{m}^{2}$ | Earth magnetic moment | point | 7.96e22 | 7.96 e 22 |
| $\Delta t_{\text {slew }}$ | s | Minimum maneuver time | point | 760 | 760 |
| $A_{\text {s }}$ | $\mathrm{m}^{2}$ | Area reflecting solar radiation | point | $3.75{ }^{2}$ | $3.75{ }^{2}$ |
| $\Delta t_{\text {orbit }}$ | S | Quarter orbit period | point | 1370 | 1370 |

## Coefficient of drag, $C_{\mathrm{d}}$



Aerodynamic drag torque moment, $L_{\mathrm{a}}$
SMAD


## Interval inputs and $S M A D$ points









## Required angular momentum, $h$



$$
h=\Delta t_{\text {orbit }} \times\left(\tau_{\text {slew }}+\tau_{\text {dist }}\right)
$$

## Value of information: pinching $\rho$




## Linked subsystems

- Minimum moment of inertia $I_{\text {min }}$
- Maximum moment of inertia $I_{\max }$
- Total torque $\tau_{\text {tot }}$
- Total power $P_{\text {tot }}$
- Solar panel area $A_{\text {sa }}$

Iteratively calculated

## Solar Attitude

 determines
Power requirements determines
Solar panel size
determines
Moments of inertia
Power

## Analysis of calculations

- Do p-boxes enclose Monte Carlo and SMAD?
- Does iteration through links cause runaway uncertainty growth (or contraction)?
- Four parallel analyses
- SMAD's point estimates
- Monte Carlo simulation
- P-boxes but without linkage among subsystems
- P-boxes with fully linked subsystems


## Ranges of results



## Findings

- Calculations workable
- No runaway inflation (or loss) of uncertainty
- Comprehensive bounds easier than via Monte Carlo
- Practical and useful results
- Uncertainty influences engineering decisions
- Reducing uncertainty about $\rho$ (by picking a launch date) strongly reduces design uncertainty


## Attitude control subsystem

| Symbol | Unit | Type | Value | SMAD |
| :---: | :---: | :---: | :---: | :---: |
| $C_{\mathrm{d}}$ | unitless | p-box | range $=[2,4]$ <br> mean=3.13 | 3.13 |
| $L_{\mathrm{a}}$ | m | p-box | range $=[0,3.75]$ <br> mean $=0.25$ | 0.25 |
| $L_{\mathrm{sp}}$ | m | p -box | range $=[0,3.75]$ <br> mean $=[0.25]$ | 0.25 |
| $D$ | $\mathrm{~A} \mathrm{~m}^{2}$ | interval | $[0,1]$ | 1 |
| $i$ | degrees | interval | $[0,90]$ | 0 |
| $\rho$ | $\mathrm{~kg} \mathrm{~m}^{3}$ | interval | $[3.96 \mathrm{e}-12$, <br> $9.9 \mathrm{e}-11]$ | $1.98 \mathrm{e}-11$ |
| $\theta$ | degrees | interval | $[10,19]$ | 10 |
| $q$ | unitless | interval | $[0.1,0.99]$ | 0.6 |
| $I_{\text {min }}$ | $\mathrm{kg} \mathrm{m}^{2}$ | interval | $[4655]$ | 4655 |
| $I_{\text {max }}$ | $\mathrm{kg} \mathrm{m}^{2}$ | interval | $[7315]$ | 7315 |
| $\mu$ | $\mathrm{~m}^{3} \mathrm{~s}^{-2}$ | point | 3.98 e 14 | 3.98 e 14 |
| $A$ | $\mathrm{~m}^{2}$ | point | $3.75^{2}$ | $3.75^{2}$ |
| $R E$ | $\mathrm{~km}_{2}$ | point | 6378.14 | 6378.14 |
| $H$ | $\mathrm{~km}^{2}$ | point | 340 | 340 |
| $F_{\mathrm{s}}$ | $\mathrm{W} \mathrm{m}^{-2}$ | point | 1367 | 1367 |
| $\theta_{\text {slew }}$ | degrees | point | 38 | 38 |
| $c$ | $\mathrm{~m} \mathrm{~s}^{-1}$ | point | 2.9979 e 8 | 2.9979 e 8 |
| $M$ | $\mathrm{~A} \mathrm{~m}^{2}$ | point | 7.96 e 22 | 7.96 e 22 |
| $\Delta t_{\text {slew }}$ | s | point | 760 | 760 |
| $A_{\mathrm{s}}$ | $\mathrm{m}^{2}$ | point | $3.75^{2}$ | $3.75^{2}$ |
| $\Delta t_{\text {orbit }}$ | s | point | 1370 | 1370 |

$$
\begin{gathered}
h=\tau_{\text {tot }} \times \Delta t_{\text {orbit }} \\
\tau_{\text {tot }}=\tau_{\text {slew }}+\tau_{\text {dist }} \\
\tau_{\text {slew }}=\frac{4 \theta_{\text {slew }}}{\Delta t_{\text {slew }}} I \\
\tau_{\text {dist }}=\tau_{g}+\tau_{s p}+\tau_{m}+\tau_{a} \\
\tau_{\mathrm{g}}=\frac{3 \mu}{2\left(R_{\mathrm{E}}+H\right)^{3}}\left|I_{\max }-I_{\min }\right| \sin (2 \theta) \\
\tau_{\mathrm{sp}}=L_{\mathrm{sp}} \frac{F_{\mathrm{s}}}{c} A_{\mathrm{s}}(1+q) \cos (i) \\
\tau_{\mathrm{m}}=\frac{2 M D}{\left(R_{\mathrm{E}}+H\right)^{3}} \\
\tau_{\mathrm{a}}=\frac{1}{2} L_{\mathrm{a}} \rho C_{\mathrm{d}} A V^{2}
\end{gathered}
$$

Be careful with units!

Neuroscience of risk

## Psychometry

- Probability and decision theory are rife with paradoxes that no other areas in math have
- Cottage industry in documenting ways in which humans mess up probabilities


## Paradoxes \& biases

- Ellsberg paradox
- St. Petersburg paradox
- Two-envelopes problem
- Monty Hall problem
- Simpson's paradox
- Risk aversion
- Loss aversion


## Risk aversion

- Suppose you can get $\$ 100$ if a randomly drawn ball is red from an urn with half red and half blue balls...or you can just get $\$ 50$
- Which prize do you want?


EU is the same, but most people take the sure $\$ 50$

## Ambiguity aversion

Keynes; Dempster

- Balls can be either red or blue
- Two urns, both with 36 balls
- Get $\$ 100$ if a randomly drawn ball is red
- Which urn do you wanna draw from?



## Ellsberg Paradox

- Balls can be red, blue or yellow
- A well-mixed urn has 30 red balls and 60 other balls
- Don't know how many are blue or how many are yellow

Gamble $\mathbf{A} \quad R>B$
Get $\$ 100$ if draw red

## Gamble C

Get $\$ 100$ if red or yellow

Gamble B
Get $\$ 100$ if draw blue

## Gamble D



Get $\$ 100$ if blue or yellow

## Persistent paradox

- People always prefer unambiguous outcomes
- Doesn't depend on your utility function or payoff
- Not related to risk aversion
- We simply don't like ambiguity
- Not explained by probability theory, or by prospect theory


## Ambiguity (incertitude)

- Ambiguity aversion is ubiquitous in human decision making, and is utterly incompatible with Bayesian norms
- Humans are wired to process incertitude separately and differently from variability


## Neuroscience of risk perception

## (Marr 1982; Barkow et al. 1992; Pinker 1997, 2002)

Instead of being divided into rational and emotional sides, the human brain has many special-purpose calculators

$\overline{1 \mathrm{~cm}}$

## Partial list of mental calculators

- Language (grammar and memorized dictionary)
- Practical physics (pre-Newtonian)
- Intuitive biology (animate differs from inanimate)
- Intuitive engineering (tools designed for a purpose)
- Spatial sense (dead reckoner and mental maps)
- Number sense (1, 2, 3, many)
- Probability sense (frequentist Bayes)
- Uncertainty detector (procrastination)
- Intuitive economics (reciprocity, trust, equity, fairness)
- Intuitive psychology (theory of mind, deception)

What's the evidence for an 'uncertainty detector' in humans?

## fMRI

- Hsu et al. (2005) found localized regions of activity in the brain under situations of ambiguity (incertitude)
- Amygdala associated with processing fear and threat

$y=35$



## Ambiguity/incertitude detector

- Humans have an incertitude processor
- Triggered by situations with ambiguity
- Especially focused on the worst case
- Common response is procrastination
- Functional organ
- Normal feature of the human brain, also apes, rats
- Not a product of learning
- Visible in fMRI
- Brain lesions can make people insensitive to incertitude...so they behave as Bayesians


## Other species

- Chimpanzees and bonobos preferred peanuts (which they like less than bananas) when they don't know the probability of getting bananas


What's the evidence for a 'probability sense' in humans?

## Probability sense

- One of the ways we know there is a probability calculator is that we can watch it turn on
- Platt and Glimcher (NYU) found particular neurons in the lateral intraparietal cortex in rhesus monkeys encode both the probability of an outcome and its magnitude
- We can also see it in reasoning behaviors


## Bayesian reasoning (poor)

If a test to detect a disease whose prevalence is $0.1 \%$ has a false positive rate of $5 \%$, what is the chance that a person found to have a positive result actually has the disease, assuming that you know nothing about the person's symptoms or signs? $\qquad$
$12-18 \%$ of medical students get this correct

## Bayesian reasoning (good)

If a test to detect a disease whose prevalence is $1 / 1000$ has a false positive rate of $50 / 1000$, what is the chance that a person found to have a positive result actually has the disease, assuming that you know nothing about the person's symptoms or signs? _1 out of $\mathbf{5 1}$.
$76-92 \%$ of medical students get this correct. That it's so easy to solve suggests hardwiring.

## Calculators must be triggered

- Humans have an innate probability sense, but it is triggered by natural frequencies
- This calculator kicked in for the medical students who got the question in terms of natural frequencies, and they mostly solved it
- The mere presence of the percent signs in the question hobbled the other group


## Multiple calculators may fire

- There are distinct calculators associated with
- Probabilities and risk (variability)
- Ambiguity and uncertainty (incertitude) Hsu et al.
- Trust and fairness
- Brain processes them differently
- Different brain regions
- Different chemical systems
- They can give conflicting answers


## Conflict explains Ellsberg paradox

- Ambiguity detector countermands any risk estimate that might be produced by the probability sense
- What matters most, and perhaps exclusively, is how bad it could be...not how likely or unlikely that outcome is


## Biological basis for Ellsberg

Hsu et al. 2005

- Probability sense and the ambiguity detector interfere with each other
- Humans do not make decisions based purely on probability in such cases
- Probabilists use equiprobability to model incertitude which confounds it with variability


## Conflict may explain other biases too

- Ambiguity aversion
- Loss aversion
- Hyperbolic discounting
- Base rate fallacy
- Neglect of probability
- Pseudocertainty

People just seem downright stupid
about risks and
uncertainty

[^0]
## Loss aversion

(asymmetry in perceptions about losses and gains)

## Loss aversion



Prospect theory adopts (but does not explain) loss aversion

## But why?

- Prospect theory is the state of the art
- Purely descriptive
- Doesn't say why loss aversion should exist
- What is the biological basis for loss aversion?
- How could it have arisen in human evolution?

Let's make a simpler symmetry assumption

Pessimism in uncertainty

Loss aversion

## If uncertainty <br> is massive...

...the bottom falls out of the market

## Loss aversion disappears with certainty

- Loss aversion disappears
- with a person you trust, or
- after the gamble has been realized
- Gilbert et al. 2004
- Kermer et al. 2006
- Yechiam \& Ert 2007
- Erev, Ert, \& Yechiam 2008
- Ert \& Erev 2008
- When losses and gains are surely exchangeable, the uncertainty contracts to the symmetric utility


## Direct experimental evidence

- Ellsberg made the probabilities ambiguous
- Psychologist Christian Luhmann (Stony Brook) made rewards ambiguous
- Visually obscured the promised payoffs
- "I'll pay you between 1 and 10 bucks"
- Loss aversion varies with the size of uncertainty
- Disappears with certainty


## Clinical evidence

- Amygdala damage eliminates loss aversion
- But doesn't affect a person's ability to gamble and respond to changing values and risk $(n=2)$

Still normal in
risk aversion

- Amygdalectomied rhesus monkeys approach stimuli that healthy monkeys avoid


## But why pessimism?

- Pessimism is often advantageous evolutionarily
- Natural selection can favor pessimism
- Death is 'hard selection'
- Animal foraging strategies
- Programmed plant behaviors
- Being wrong often has asymmetric consequences
- Foraging: Finding dinner versus being dinner
- Competition: Preemption versus being preempted


## And even in plants!



## Pessimism is not inevitable

- Pessimism is not the only reaction to uncertainty
- Normal people in stressful situations
- Pathological gamblers
- Maniacs
- Ambiguity aversion decreases with optimism (Pulford 2009)


## Third calculator: intuitive economics

- Computes fairness of situations
- Detects cheaters who are getting more than their share, or not shouldering their responsibility

Ultimatum Game: a scientist offers money to two players

- One player proposes how the money should be divided between the two players
- The other player can accept (and both get their share) or reject the division (and neither gets anything)


## How should you play?

- Economists say the rational behavior is
- Responder: always accept any deal (it's free money!)
- Proposer: always offer the smallest possible amount
- Actual plays are much closer to fair
- Proposer offers a split much closer to 50:50
- Responder accepts only if the split is closer to 50:50


## Universal in humans

- Ultimatum Game is only surprising to economists
- The pattern may be universal in human behavior - Over 100 papers in 25 western societies
- 15 non-western societies
- Exceptions
- Sociopaths - Kids under 5
- Chimpanzees - People playing against machines
- Chimps are more rational that humans


## Why do humans do this?

- Adaptation for reciprocal altruism
- Cares about fairness and reciprocity
- Alters outcomes of others at a personal cost
- Rewards those who act in a prosocial manner
- Punishes those who act selfishly, even when punishment is costly
- Mediated by the fairness calculator
- Pattern absent when fairness is not an issue


## "Irrationality"

- Irrationality is a hallmark of human decisions
- Why are humans biased, irrational, stupid?
- Using the wrong mental calculator (optical illusion)
- Disagreement among mental calculators
- Concerned with issues outside the risk analysis
- Fairness, justice
- Outcomes not treated in the analysis
- Chance the risk analyst is lying

Different

- Chance the risk analyst is inept


## Currently, confusion is guaranteed

- Neuroimagery and clinical psychology show humans distinguish incertitude and variability
- Probabilists traditionally use equiprobability to model incertitude, which confounds the two
- Risk analysts report their findings in ways that we know will create misunderstandings


## Import for risk assessment

- Risk analyses woefully incomplete
- Neglect or misunderstand incertitude
- Omit important issues and thus understate risks
- Presentations use very misleading formatting
- Percentages, relative frequencies, conditionals, etc.
- Both problems can be fixed
- By changing analysts' behavior (not the public's)


## Risk communication

- Informed consent in medicine
- Effective communication to decision makers
- If you want people to understand your risk calculations, you have to speak their language


## Take-home messages

- Evolution has wired humans to see incertitude distinctly, and differently, from variability
- Conflict between the two seems to explain many probability and decision paradoxes
- There is a proper calculus that handles both although it is incompatible with current norms


# Statistics for the next century 

## Small sample size

- Student's $t$ statistic introduced in 1908
- Statistics has spent a century developing analyses in which sample size is limiting
- But sample sizes are not so small anymore
- Financial data
- Continuous mechanized sampling
- Satellite imagery and other mass collections
- Commercial data
- Social media
- Internet of Things (30 trillion sensors feeding the web)


## Other uncertainties

- Sample size will always be an issue
- But it may not always be the only issue anymore
- Other issues become important as sample sizes grow
- Measurement imprecision (mensurational uncertainty)
- Missingness and censoring
- Model uncertainty, non-stationarity, etc.
- Many believe it's always better to collect more samples than to improve the precision of samples
- This is not true
- Believing this creates suboptimal experimental designs


## Measurements aren't reals

- Real line is a poor model for measurements
- "Measure" by comparing readings against a scale
- Almost all real values cannot be measurements
- All real measurements have uncertainties
- A real value cannot express this
- Real values have infinitely many zeros after the last decimal place
- Such precision is never achievable in the real world
- The real line is totally ordered


## Missing data

- Traditional methods assume MCAR or MAR
- These assumptions are not always reasonable
- Assuming them anyway leads to wrong answers
- Correctly accounting for missingness can yield dilation, in which your uncertainty increases even when you increase sample size
- If a temperature sensor fails from extremes in either direction, a missing value may mean the temperature is much higher or much lower than you thought


## Censoring

- Traditional methods are decidedly bad and can be grossly misleading
- Likelihood strategies make assumptions that may not be tenable
- Can produce unreasonable results


## Interval data

- Calculating variances, $t$-statistics, etc. for data sets that contain intervals are NP-hard problems
- But various special cases are quite easy
- Censored
- Binned
- Same precision
- Nested
- These let us compute variance in $O(n)$ time
- Can compute variance for 500,000 samples in less than 0.5 second on a laptop


## Intervndentituedteainty

- Intermittent observations
- Plus-minus intervals
- Non-detects and data censoring
- Missing values
- Blurring for privacy or security reasons
- Bounding studies


## Two approaches

- Model each interval as uniform distribution
- Presumes different values are equally likely
- Laplace's principle of insufficient reason
- Calculations relatively easy, but interpretation subtle
- Model each interval as a set of possible values - Specifies no single distribution within the range - Theory of imprecise probabilities
- Calculations often NP-hard, but interpretation easy


## A tale of two data sets

Skinny data
[1.00, 2.00]
[2.68, 2.98]
[7.52, 7.67]
[7.73, 8.35]
[9.44, 9.99]
[3.66, 4.58]

Puffy data
[3.5, 6.4]
[6.9, 8.8]
[6.1, 8.4]
[2.8, 6.7]
[3.5, 9.7]
[6.5, 9.9]
[0.15, 3.8]
[4.5, 4.9]
[7.1, 7.9]


## Empirical distribution

- Summary of the data themselves
- No distributional assumptions
- Uniforms approach yields a single distribution
- Intervals approach yields a probability box (i.e., a class of distributions)


## Intervals approach




- Each side is cumulation of respective endpoints
- Represents both incertitude and variability


## Uncertainty about the EDF



## Uniforms approach




- Mixture (vertical average) of uniforms
- Conflates incertitude and variability


## What's the difference?

- Might be advisable to propagate the two kinds of uncertainty separately and differently
- Example: suppose we're interested in the product of Skinny and Puffy...


## Uniforms versus intervals approach



## Randomness self-cancels



## Fitted distribution

- Assumes some shape for the distributions
- Uniforms approach yields a single distribution
- Intervals approach yields a probability box


## Interval approach

- Creates a class of maximum likelihood solutions
- Every one solves a ML problem for a set of scalar values within the respective intervals
- Example: let's fit exponential distributions


$$
x_{1} \in[1,2] \quad x_{2} \in[3,4]
$$



## Results from intervals approach




## Maximum likelihood for censored data

Given a datum $\boldsymbol{x}=[\underline{x}, \bar{x}]$,

$$
\begin{aligned}
L(\boldsymbol{x}) & =\operatorname{Pr}(\underline{x} \leq X \leq \bar{x}) \\
& =\operatorname{Pr}(\bar{x} \leq X)-\operatorname{Pr}(\underline{x} \leq X) \\
& =F(\bar{x} ; \lambda)-F(\underline{x} ; \lambda)
\end{aligned}
$$

where, for an exponential distribution,

$$
F(x ; \lambda)=1-\exp (-\lambda x)
$$

and $1 / \lambda$ is the mean

## Single datum $x \in[1,2]$

$$
L(\lambda)=\exp (-\lambda)-\exp (-2 \lambda)
$$



## Maximum likelihood for multiple data



## Results from uniforms approach




## Negligible difference



## Are these answers reasonable?

- Picking a single exponential to fit interval data
- Essentially no difference between Skinny and Puffy data sets, despite disparity of uncertainties
- Confidence bands actually smaller for Puffy, even though its uncertainty is much larger
- No guarantee that the answer approaches the true distribution even if asymptotically many data are collected


## Descriptive statistics

- Practical algorithms for all common statistics
- Mean, variance, skewness, etc., but not mode
- Empirical and fitted distributions
- Confidence limits, outlier statistics, etc.
- Some are simple to compute
- Many are NP-hard to compute, e.g., variance
- Feasible algorithms exist for many special cases - Variance can be computed in linear time with $n$ - In practice, interval data is computationally easy


## Central tendency



## Dispersion

Skinny
Variance
Sample variance
Standard deviation [2.81, 3.29]
Interquartile range [2.68, 8.35]
[9.50, 12.92]

Puffy
[7.91, 10.77] [0.91, 10.98]
[1.03, 12.35]
$[0.95,3.32]$
[3.50, 8.80]


## Take-home messages

- Intervals generalise real-valued measurements
- Handle $\pm$ measurement precision, data censoring and missingness as special cases
- We can mix good and bad data in a consistent way
- Interval approach yields more robust results than methods that depend on subtle assumptions such as missing at random, or the 'uniforms' model

Model uncertainty

## Model uncertainty

- Doubt about the structural form of the model

- Usually incertitude rather than variability
- Usually considerable in ecosystems models
- Often the elephant in the middle of the room


## Uncertainty in probabilistic analyses

- Parameters
- Data surrogacy
already $\{$ - Distribution shape
- Intervariable dependence
- Arithmetic expression
- Level of abstraction


## Monte Carlo strategy

- Introduce a new discrete variable
- Let the value of the variable dictate which model will be used in each rep
- Wiggle the value from rep to rep
- Only works for short, explicit list of models (you have to list the models)
- Many theorists object to this strategy

Model uncertainty as a mixture If $u>0.5$ then model=I else model=II


## General strategies

- Sensitivity (what-if) studies
- Probabilistic mixture
- Bayesian model averaging
- Enveloping and bounding analyses


## Sensitivity (what-if) studies

- Simply re-compute the analysis with alternative assumptions
- Intergovernmental Panel on Climate Change
- No theory required to use or understand


## Drawbacks of what-if

- Consider a long-term model of the economy under global warming stress

3 baseline weather trends
3 emission scenarios
3 population models
3 mitigation plans

81 analyses to compute, and to document

- Combinatorially complex as more model components are considered
- Cumbersome to summarize results


## Probabilistic mixture

- Identify all possible models
- Introduce a new discrete random variable whose value says which model to use; let it vary in MC
- This averages probability distributions
- Use weights to account for different credibility (or assume equiprobability)


## Drawbacks of mixture

- If you cannot enumerate the possible models, you can't use this approach
- Averages together incompatible theories and yields an answer that neither theory supports
- Can underestimate tail risks


## Bayesian model averaging

- Similar to the probabilistic mixture
- Updates prior probabilities to get weights
- Takes account of available data


## Drawbacks of Bayesian averaging

- Requires priors and can be computationally challenging
- Must be able to enumerate the possible models
- Averages together incompatible theories and yields an answer that neither theory supports
- Can underestimate tail risks


## Bounding probabilities

- Translate model uncertainties to a choice among distributions
- Envelope the cumulative distributions
- Treat resulting p-box as single object


## Drawbacks of bounding

- Cannot account for different model credibilities
- Can't make use of data
- Doesn't account for 'holes'


## Numerical example

The function $f$ is one of two possibilities. Either

$$
f(A, B)=f_{\mathrm{Plus}}(A, B)=\mathrm{A}+\mathrm{B}
$$

or

$$
f(A, B)=f_{\text {Times }}(A, B)=\mathrm{A} \times \mathrm{B}
$$

is the correct model, but the analyst does not know which. Suppose that
$A \sim \operatorname{triangular}(-2.6,0,2.6)$
$B \sim$ triangular(2.4, 5, 7.6).
$f_{\text {Plus }}$ is twice as likely as $f_{\text {Times }} ; \quad$ datum: $f(A, B)=7.59$



## When you can enumerate the models

- What-if analysis isn't feasible in big problems
- Probabilistic mixture is, at best, ad hoc
- For abundant data, Bayesian approach is best
- Otherwise, it's probably just wishful thinking
- Bounding is reliable, but may be too wide


## When you can't list the models

- If you cannot enumerate all the models, bounding is often the only tenable strategy
- Shape of input distributions
- Dependence
- Functional form
- Laminar versus turbulent flow
- Linear or nonlinear low-dose extrapolation
- Ricker versus Beverton-Holt density dependence


## Synopsis of the four approaches

- What-if
- Straightforward, doesn't conflate uncertainties
- Must enumerate, combinatorial
- Probabilistic mixture, Bayesian model averaging
- Single distribution, accounts for data (and priors)
- Must enumerate, averages incompatible theories
- Can underestimate tail risks
- Bounding
- Yields one object; doesn't conflate or understate risk
- Cannot account for data or differential credibility

Conclusions

## Probability theory isn't good enough

- Probability theory, as its commonly used, doesn't cumulate gross uncertainty correctly
- Precision of the answer (measured as cv) depends strongly on the number inputs and not so strongly on their distribution shapes, even if they are uniforms or flat priors
- The more inputs, the tighter the answer


## A few grossly uncertain inputs



A lot of grossly uncertain inputs．．．


Where does this surety come from？ What justifies it？

## Smoke and mirrors certainty

- Conventional probability theory, at least as it's naively applied, seems to manufacture certainty out of nothing
- This is why some critics say probabilistic analyses are "smoke and mirrors"
- P-boxes give a vacuous answer if all you give them are vacuous inputs


## The problem is wishful thinking

In practice, probabilists often use conventions and make assumptions that may be convenient but are not really justified:

1. Variables are independent of one another
2. Uniform distributions capture incertitude
3. Distributions are stationary (unchanging)
4. Specifications are perfectly precise

## Untenable assumptions

- Distributions normal
- Uncertainties are small
- Sources of variation are independent
- Uncertainties can cancel each other out
- Linearized models good enough
- Most of the physics is known and modeled


## Need ways to relax assumptions

- Possibly large, non-normal uncertainties
- Non-independent, or unknown dependencies
- Uncertainties that may not cancel
- Arbitrary mathematical operations
- Model uncertainty


## Everyone makes assumptions

- But not all sets of assumptions are equal!

Point value<br>Interval range<br>Entire real line<br>Normal distribution<br>Unimodal distribution<br>Any distribution

- Like to discharge unwarranted assumptions "Certainties lead to doubt; doubts lead to certainty"


## Take-home messages

- Monte Carlo will always be useful, like Euclidean geometry
- Using bounding, you don't have to pretend you know a lot to get quantitative answers
- Approximation and bounding are often complementary
- Paying attention to measurement imprecision, censoring, and missingness requires new approaches
- Integrating them with small- and no-data problems, with model uncertainty, yields a non-Laplacian theory

| What is known <br> empirically | Monte Carlo analysis | Probability bounds <br> analysis |
| :--- | :--- | :--- |
| Know only range <br> of variable | Assume uniform <br> distribution | Assume interval |
| Know some <br> constraints about <br> random variable | Select largest entropy <br> distribution from all thus <br> constrained distributions | Form envelope around <br> class of distributions <br> matching constraints |
| Uncertainty about <br> distribution <br> family or shape | Repeat analysis for other <br> plausible distribution <br> shapes | Form distribution-free p- <br> box as envelope of all <br> plausible distributions |
| Sample data | Form empirical distribution <br> function (EDF) | Form nonparametric c-box <br> or KS confidence limits <br> around EDF |
| Variable follows <br> known marginal <br> distribution | Sample from particular <br> distribution | Use particular distribution |
| Measurement <br> uncertainty | Ignore it (usually), or <br> perform sensitivity analysis | Express it in intervals and <br> incorporate it into analysis |


| What is known empirically | Monte Carlo analysis | Probability bounds analysis |
| :---: | :---: | :---: |
| Non-detects | Replace non-detect with 12 DL (detection limit) | Replace non-detect with interval [0, DL] |
| Know variables are independent | Assume independence | Assume (random-set) independence |
| Know magnitude of correlation | Simulate correlation from particular (but usually arbitrary) copula | Bound result from possible copulas with correlation, or use known copula |
| Know only the general sign (+ or <br> -) of dependence | Assume some correlation of appropriate sign, or repeat analysis for different correlations | Bound result assuming only the sign of the dependence and specific or all possible copulas |
| Do not know the nature of the dependence | Assume independence (usually), or repeat analysis for different correlations | Bound result for all possible dependencies (Fréchet case) |
| Model uncertainty | Form stochastic mixture (vertical average) of distribution functions | Form envelope of distribution functions |

## Cheat sheet for the pba.r library

- plot, lines, show, summary
- mean, sd, var, median, quantile, left, right, prob, cut, percentile, iqr, random, range
- exp, log, sqrt, abs, round, trunc, ceiling, floor, sign, $\sin$, cos, tan, asin, acos, atan, atan2, reciprocate, negate, $+,-, *, /$, pmin, pmax, $\wedge$, and, or, not, mixture, smin, smax


## Supported named distributions

bernoulli, beta, binomial, cauchy, chi, chisquared, delta, dirac, discreteuniform, exponential, exponentialpower, extremevalue, f, fishersnedecor, fishertippett, fisk, frechet, gamma, gaussian,
normal, etc.
histogram
quantiles
pointlist
MM <tab><tab>
ME<tab><tab>
ML〈tab><tab>
CB <tab><tab>
NV <tab><tab> geometric, generalizedextremevalue, generalizedpareto, gumbel, histogram, inversegamma, laplace, logistic, loglogistic, lognormal, logtriangular, loguniform, negativebinomial, normal, pareto, pascal, powerfunction, poisson, quantiles, rayleigh, reciprocal, shiftedloglogistic, skewnormal, student, trapezoidal, triangular, uniform, Weibull

## Nonparametric p-boxes

maxmean, minmax, minmaxmean, minmean, meanstd, meanvar, minmaxmode, minmaxmedian, minmaxmedianismode, minmaxpercentile, minmaxmeanismedian, minmaxmeanismode, mmms, mmmv, posmeanstd, symmeanstd, uniminmax, unimmmv, unimmms

## Synopsis: probability bounds analysis

How?

- specify what you are sure about
- establish bounds on probability distributions
- pick dependencies (no assumption, indep., perfect, etc.)

Why?

- account for uncertainty better than maximum entropy, etc.
- puts bounds on Monte Carlo results
- bounds get narrower with better empirical information

Why not?

- does not yield second-order probabilities
- best-possible results can sometimes be expensive to compute


## Synopsis: imprecise probabilities

## How?

- avoid sure loss, $\underline{\mathrm{P}}(A) \leq \overline{\mathrm{P}}(A)$
- be coherent, $\underline{\mathrm{P}}(A)+\underline{\mathrm{P}}(B) \leq \underline{\mathrm{P}}(A \cup B)$
- use natural extension (mathematical programming) to find consequences


## Why?

- most expressive language for uncertainty of all kinds
- can provide expectations and conditional probabilities
- provides best possible results that do not lose information

Why not?

- requires mathematical programming
- can strain mathematical ability of the analyst


## Software for probability bounds

- R libraries pbox.r and pba.r
- Add-in for Excel (NASA, beta version)
- RAMAS Risk Calc 4.0 (NIH, commercial)
- StatTool (Dan Berleant, freeware)
- PBDemo (NIH, freeware)
- Constructor (Sandia and NIH, freeware)
- Williamson and Downs (1990)


## Web presentations and documents

Introduction to probability bounds analysis written for Monte Carlo users http://www.ramas.com/pbawhite.pdf
Introduction of probability bounds analysis to interval researchers http://www2.imm.dtu.dk/~km/int-05/Slides/ferson.ppt

Gert de Cooman's gentle introduction to imprecise probabilities http://maths.dur.ac.uk/~dma31jm/durham-intro.pdf
Fabio's Cozman's introduction to imprecise probabilities http://www.cs.cmu.edu/~qbayes/Tutorial/quasi-bayesian.html
Notes from a week-long summer school on imprecise probabilities http://idsia.ch/~zaffalon/events/school2004/school.htm
Introduction to p-boxes and related structures
http://www.sandia.gov/epistemic/Reports/SAND2002-4015.pdf
Handling dependencies in uncertainty modeling
http://www.ramas.com/depend.zip
Introduction to Bayesian and robust Bayesian methods in risk analysis
http://www.ramas.com/bayes.pdf
Statistics for data that may contain interval uncertainty
http://www.ramas.com/intstats.pdf

## Topical websites

- Intervals and Probability Distributions http://class.ee.iastate.edu/berleant/home/ServeInfo/Interval/intprob.html
- Imprecise Probabilities Project http://ippserv.rug.ac.be/home/ipp.html
- Sandia National Laboratory's Epistemic Uncertainty Project http://www.sandia.gov/epistemic/
- R software for confidence boxes https://sites.google.com/site/confidenceboxes/
- Applied Biomathematics’ Risk Calc website http://www.ramas.com/riskcalc.htm
- Society for Imprecise Probabilities Theory and Applications http://www.sipta.org/


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[^0]:    Making risk-averse choices for positive outcomes, but risk-seeking for negative

