

Backcalculating Cleanup Targets Across Trophic Levels in a Probabilistic Assessment

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Why Conduct Risk Assessments?

Two primary goals:

- To determine if hazardous exposure is occurring or may occur.
- To determine whether and how much remediation will be necessary.

The second goal requires backcalculation.

Backcalculation

Simple forward dose equation: $Dose = Concentration \times Intake$.
mandated → unknown → known

With point estimates, invert the equation to backcalculate and find the target *Concentration*:

$$Concentration = Dose / Intake.$$

This is the *Concentration* target required for cleanup and remediation planning.

Deconvolution

Deconvolution is a procedure for backcalculating from expressions containing probability distributions and uncertain numbers.

How can we untangle (deconvolve) the expression:

$$Dose = Concentration \times Intake ?$$

- Cannot simply invert the equation.
- No general Monte Carlo method solution.
- Special methods are required.

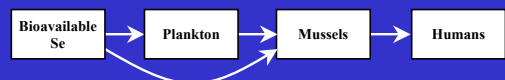
Probability Bounds Analysis

- Allows operations between and among point estimates, intervals, probability distributions and probability boxes.
- Models variability and uncertainty without confounding them.
- Produces forward convolutions that are often best-possible.
- Solutions rigorously bound the answer.
- Allows deconvolution of expressions containing probability distributions and/or uncertain numbers.

Selenium (Se) in San Francisco Bay Mussels (*Mytilus edulis*)

Objective: We want to solve a cleanup target for bay water Se concentration.

Scenario: Bay water is contaminated with Se. People eat mussels harvested from the bay. Se moves through trophic levels to reach humans.



Steady State Fate and Transport Model (Spencer et al. 2001)

$$Dose = MConc \times \frac{Intake}{BW}$$

$$MConc = WConc \frac{(k + h \times B \times g \times p)}{(l + f \times N \times g \times p)}$$

Where:

- Mconc = Se concentration in mussels (µg/g)
- Mconc = Se concentration in bay water (µg/L)
- Intake = mussel intake rate (g/d)
- BW = adult body weight (kg)
- k = mussel Se uptake rate from the dissolved phase (L/g/d)
- h = mussel Se assimilation from phytoplankton (unitless)
- B = Se bioconcentration factor in phytoplankton (L/g)
- P = phytoplankton concentration (g/L)
- l = mussel selenium elimination rate (d⁻¹)
- f = mussel carbon assimilation efficiency (unitless)
- N = mussel net growth efficiency (unitless)

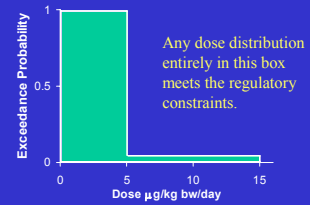
We want to backcalculate this

Allowable Se Dose for Humans

NOAEL = 15 µg/kg/d (ATSDR 1996).

Maximum safe level of intake = NOAEL / 3.

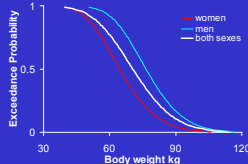
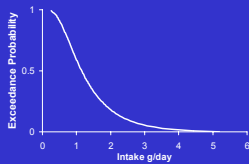
Modeled as a p-box with 95% of doses < 5 µg/kg/d.



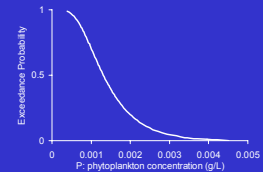
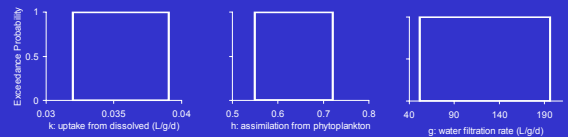
Intake Rate and Body Weight

Intake for adults in pacific states, Ruffle et al. 1994.

Body weight for men and women combined assuming an even sex ratio, Brainard and Burmaster 1992.



Steady State Equation Variables



How to Do the Backcalculation?

$$Dose = WConc \frac{(k + h \times B \times g \times p)}{(l + f \times N \times g \times p)} \times \frac{Intake}{BW}$$

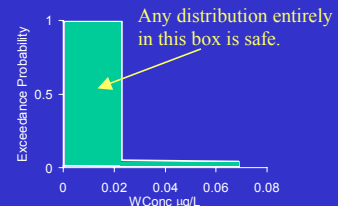
$$WConc = factor \left(\frac{(k + h \times B \times g \times p)}{(l + f \times N \times g \times p)} \times \frac{Intake}{BW}, Dose \right)$$

Algorithm untangles the forward convolutions.

- Finds rigorous bounds around water concentration distributions leading to safe doses.
- Bounds are around thickest possible tails.
- Repeated variables (g and p) require a numerical "region-growing" algorithm.

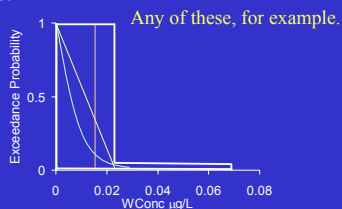
The Answer

Bounds around concentration distributions leading only to safe doses for mussel consumers.



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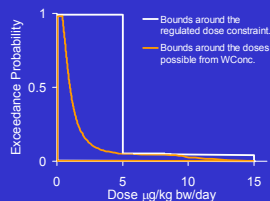


Forward Calculation

Forward calculation checks the results.

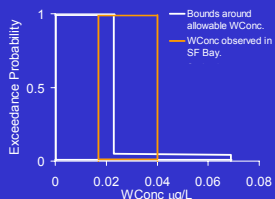
Plug the answer back into the Dose equation.

These bounds are rigorous and best-possible.



Actual Se Concentration in San Francisco Bay

Remediation may be necessary.



Conclusions

- Rigorous methods are now available to calculate cleanup targets in probabilistic assessment.
- These methods require deconvolution.
- Efficient deconvolution algorithms are available with probability bounds analysis.
- San Francisco Bay may need remediation.

Acknowledgments

- National Cancer Institute
- National Institute of Environmental Health Sciences

Subinterval Resection

`sir(int, #)`

Subinterval resection bounds the space of possibilities implied by the input interval *int* and the function you specified in *map1*. This routine partitions the input interval into # subintervals. The value of # could be 5 or higher. The result is guaranteed to enclose the true answer, so it cannot ever be too small or leave out any possibilities.

The result can be wider than necessary when the *map1* function is non-monotonic. However, the error can be made arbitrarily small by increasing the value of #. (See Corliss, G.F. 1988 "How can you apply interval techniques in an industrial setting?" Technical Report #301 (December 1988), Department of Mathematics, Statistics and Computer Science, Marquette University, Milwaukee.)

```
func map1() _begin; _return $1; _end;
```

```
_func sir() _begin; //arguments: input interval, number of subintervals
```

```
  sir1 = _left $1;  
  sire = map1(sir1);  
  sirw = width($1)/$2;  
  sirk := 1;  
  _while (sir1 <= sire) _do _begin;  
    sir2 = [ (sir1-1), sirk] * sirw + sire;  
    sir3 = map1(sir2);  
    sire = _env(sire, sir3);  
    sirk = sirk + 1;  
  _end;  
  _return sire;  
_end;
```