Validated Numerics
a short introduction to rigorous computations

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Are floating point computations reliable?

Computing with the `C/C++` `single` format

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Example 1: Repeated addition

$$\sum_{i=1}^{10^3} \langle 10^{-3} \rangle = 0.999990701675415,$$

$$\sum_{i=1}^{10^4} \langle 10^{-4} \rangle = 1.000053524971008.$$

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Example 2: Order of summation

$$1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{10^6} = 14.357357,$$

$$\frac{1}{10^6} + \cdots + \frac{1}{3} + \frac{1}{2} + 1 = 14.392651.$$

Are floating point computations reliable?

Given the point $(x, y) = (77617, 33096)$, evaluate the function

$$f(x, y) = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$$

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IBM S/370 ($\beta = 16$) with FORTRAN:

type	p	$f(x, y)$
`REAL*4`	24	$1.172603\ldots$
`REAL*8`	53	$1.1726039400531\ldots$
`REAL*10`	64	$1.172603940053178\ldots$

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type	p	$f(x, y)$
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Correct answer: $-0.8273960599\ldots$

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How do we control rounding errors?

Round each partial result both ways

If $x, y \in \mathbb{F}$ and $\star \in \{+, -, \times, \div\}$, we can enclose the exact result in an *interval*:

$$x \star y \in [\bigtriangledown(x \star y), \bigtriangleup(x \star y)].$$

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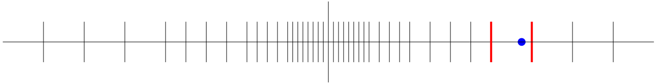
$$x \star y \in [\nabla(x \star y), \Delta(x \star y)].$$

Since all (modern) computers round with *maximal quality*, the interval is the smallest one that contains the exact result.



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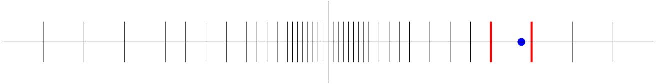

Question

How do we compute with intervals? And why, really?

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Arithmetic over $\mathbb{IR}$

Definition

If $\star$ is one of the operators $+, -, \times, \div$, and if $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{IR}$, then

$$\boldsymbol{a} \star \boldsymbol{b} = \{a \star b \colon a \in \boldsymbol{a}, b \in \boldsymbol{b}\},$$

except that $\boldsymbol{a} \div \boldsymbol{b}$ is undefined if $0 \in \boldsymbol{b}$.

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Simple arithmetic

$$\begin{aligned}
\boldsymbol{a} + \boldsymbol{b} &= [\underline{\boldsymbol{a}} + \underline{\boldsymbol{b}}, \overline{\boldsymbol{a}} + \overline{\boldsymbol{b}}] \\
\boldsymbol{a} - \boldsymbol{b} &= [\underline{\boldsymbol{a}} - \overline{\boldsymbol{b}}, \overline{\boldsymbol{a}} - \underline{\boldsymbol{b}}] \\
\boldsymbol{a} \times \boldsymbol{b} &= [\min\{\underline{\boldsymbol{a}}\underline{\boldsymbol{b}}, \underline{\boldsymbol{a}}\overline{\boldsymbol{b}}, \overline{\boldsymbol{a}}\underline{\boldsymbol{b}}, \overline{\boldsymbol{a}}\overline{\boldsymbol{b}}\}, \max\{\underline{\boldsymbol{a}}\underline{\boldsymbol{b}}, \underline{\boldsymbol{a}}\overline{\boldsymbol{b}}, \overline{\boldsymbol{a}}\underline{\boldsymbol{b}}, \overline{\boldsymbol{a}}\overline{\boldsymbol{b}}\}] \\
\boldsymbol{a} \div \boldsymbol{b} &= \boldsymbol{a} \times [1/\overline{\boldsymbol{b}}, 1/\underline{\boldsymbol{b}}], \quad \text{if } 0 \notin \boldsymbol{b}.
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\end{aligned}$$

On a computer we use *directed rounding*, e.g.

$$\boldsymbol{a} + \boldsymbol{b} = [\bigtriangledown(\underline{\boldsymbol{a}} \oplus \underline{\boldsymbol{b}}), \bigtriangleup(\overline{\boldsymbol{a}} \oplus \overline{\boldsymbol{b}})].$$

Interval-valued functions

Range enclosure

Extend a real-valued function f to an interval-valued F:

$$R(f;\boldsymbol{x}) = \{f(x) \colon x \in \boldsymbol{x}\} \subseteq F(\boldsymbol{x})$$

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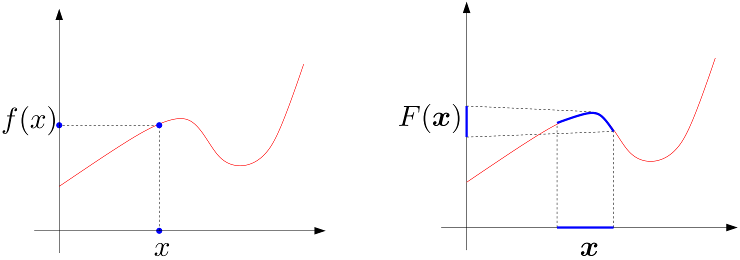

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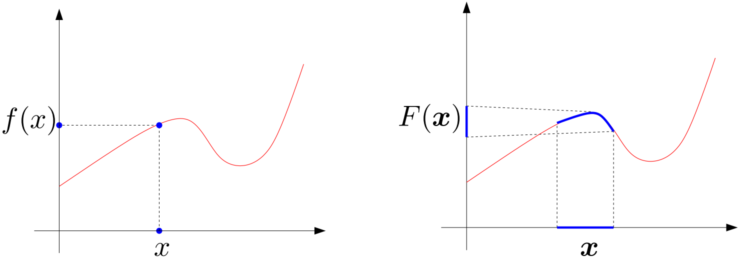

$y \notin F(\boldsymbol{x})$ implies that $f(x) \neq y$ for all $x \in \boldsymbol{x}$.

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\begin{array}{lcll}
e^{\boldsymbol{x}} & = & [e^{\underline{\boldsymbol{x}}}, e^{\overline{\boldsymbol{x}}}] & \\
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\log \boldsymbol{x} & = & [\log \underline{\boldsymbol{x}}, \log \overline{\boldsymbol{x}}] & \text{if } 0 < \underline{\boldsymbol{x}} \\
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Set $S^+ = \{2k\pi + \pi/2 \colon k \in \mathbb{Z}\}$ and $S^- = \{2k\pi - \pi/2 \colon k \in \mathbb{Z}\}$.
Then $\sin \boldsymbol{x}$ is given by

$$\begin{cases} [-1, 1] & : \text{ if } \boldsymbol{x} \cap S^- \neq \emptyset \text{ and } \boldsymbol{x} \cap S^+ \neq \emptyset, \\ [-1, \max\{\sin \underline{\boldsymbol{x}}, \sin \overline{\boldsymbol{x}}\}] & : \text{ if } \boldsymbol{x} \cap S^- \neq \emptyset \text{ and } \boldsymbol{x} \cap S^+ = \emptyset, \\ [\min\{\sin \underline{\boldsymbol{x}}, \sin \overline{\boldsymbol{x}}\}, 1] & : \text{ if } \boldsymbol{x} \cap S^- = \emptyset \text{ and } \boldsymbol{x} \cap S^+ \neq \emptyset, \\ [\min\{\sin \underline{\boldsymbol{x}}, \sin \overline{\boldsymbol{x}}\}, \max\{\sin \underline{\boldsymbol{x}}, \sin \overline{\boldsymbol{x}}\}] & : \text{ if } \boldsymbol{x} \cap S^- = \emptyset \text{ and } \boldsymbol{x} \cap S^+ = \emptyset. \end{cases}$$

A controlled discretization

We can now select and adapt the level of discretization

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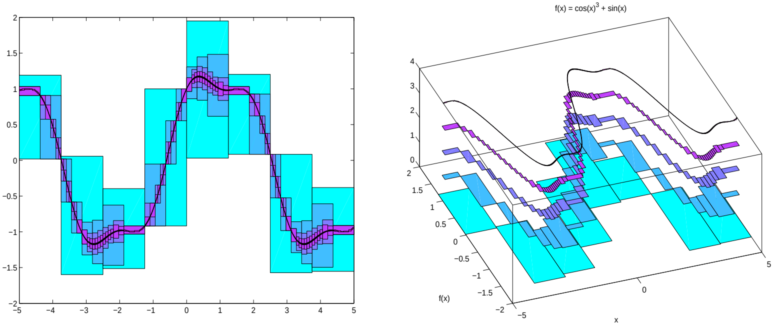
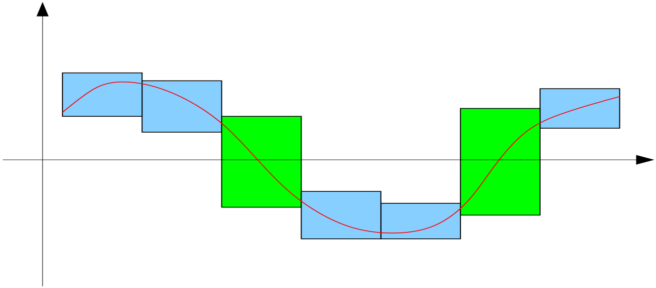


Various levels of discretization of $f(x) = \cos^3 x + \sin x$.

Solving non-linear equations



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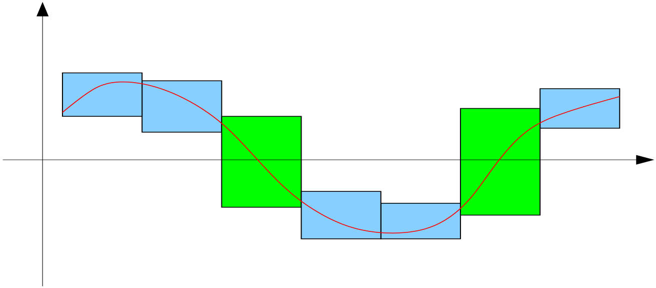

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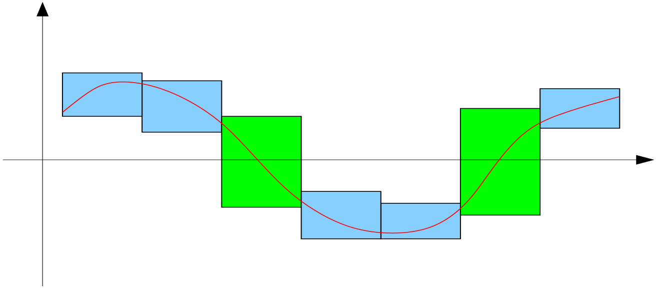

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No solutions can be missed!

Solving non-linear equation

The code is transparent and natural

```
function bisect(fcnName, X, tol)
f = inline(fcnName);
if ( 0 <= f(X) )              % If f(X) contains zero...
    if Diam(X) < tol          % and the tolerance is met...
        X                     % print the interval X.
    else                      % Otherwise, divide and conquer.
        bisect(fcnName, interval(Inf(X), Mid(X)), tol);
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Nice property

If F is well-defined on the domain, the algorithm produces an enclosure of *all* zeros of f. [No existence is established, however.]

Existence and uniqueness

Existence and uniqueness require *fixed point* theorems.

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Brouwer's fixed point theorem

Let B be homeomorhpic to the closed unit ball in $\mathbb{R}^n$. Then given any continuous mapping $f: B \to B$ there exists $x \in B$ such that $f(x) = x$.

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Let X be a normed vector space, and let $K \subset X$ be a non-empty, compact, and convex set. Then given any continuous mapping $f: K \to K$ there exists $x \in K$ such that $f(x) = x$.

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Banach's fixed point theorem

If f is a contraction defined on a complete metric space X, then there exists a unique $x \in X$ such that $f(x) = x$.

Newton's method in $\mathbb{IR}$

Theorem

Let $f \in C^1(\mathbb{R}, \mathbb{R})$, *and set* $\check{x} = \mathrm{mid}(\boldsymbol{x})$. *We define*

$$N_f(\boldsymbol{x}) \stackrel{\text{def}}{=} N_f(\boldsymbol{x}, \check{x}) = \check{x} - [DF(\boldsymbol{x})]^{-1} f(\check{x}).$$

If $N_f(\boldsymbol{x})$ *is well-defined, then the following statements hold:*

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Similar statements hold for the *Krawczyk operator*

$$K_f(\boldsymbol{x}) \stackrel{\text{def}}{=} \check{x} - [Df(\check{x})]^{-1} f(\check{x}) - \left(1 - [Df(\check{x})]^{-1} F'(\boldsymbol{x})\right)[-r, r],$$

where we use the notation $r = \mathrm{rad}(\boldsymbol{x})$.

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Newton's method in $\mathbb{IR}$

Algorithm

Starting from an initial search region $\boldsymbol{x}_0$, we form the sequence

$$\boldsymbol{x}_{i+1} = N_f(\boldsymbol{x}_i) \cap \boldsymbol{x}_i \qquad i = 0, 1, \ldots.$$

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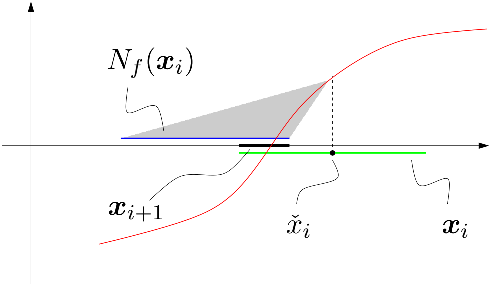

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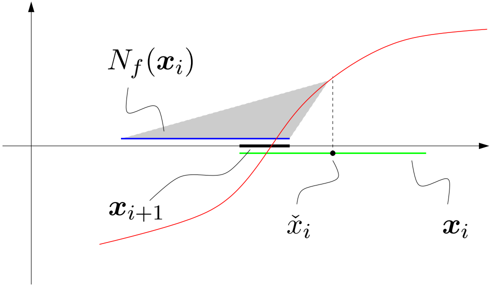

Performance

If well-defined, this method is never worse than bisection, and it converges quadratically fast under mild conditions.

Example

Take $f(x) = -2.001 + 3x - x^3$ and start with $\boldsymbol{x}_0 = [-3, -3/2]$.

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X(0) = [-3.000000000000000,-1.500000000000000]; rad = 7.50000e-01
X(1) = [-2.140015625000001,-1.546099999999996]; rad = 2.96958e-01
X(2) = [-2.140015625000001,-1.961277398284108]; rad = 8.93691e-02
X(3) = [-2.006849239640351,-1.995570580247208]; rad = 5.63933e-03
X(4) = [-2.000120104486270,-2.000103608530276]; rad = 8.24798e-06
X(5) = [-2.000111102890393,-2.000111102873815]; rad = 8.28893e-12
X(6) = [-2.000111102881727,-2.000111102881724]; rad = 1.55431e-15
X(7) = [-2.000111102881727,-2.000111102881724]; rad = 1.55431e-15
Finite convergence!
Unique root in -2.00011110288172 +- 1.555e-15
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Stopping condition

Stop when no further improvement takes place.

The Krawczyk method with bisection

When we have several zeros, we must bisect to isolate the zeros.

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Take $f(x) = \sin(e^x + 1)$ and start with $\boldsymbol{x}_0 = [0, 3]$.

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Domain          : [0, 3]
Tolerance       : 1e-10
Function calls  : 71
 Unique zero in the interval 0.761549782880[8890,9006]
 Unique zero in the interval 1.664529193[6825445,7060436]
 Unique zero in the interval 2.131177121086[2673,3558]
 Unique zero in the interval 2.4481018026567[773,801]
 Unique zero in the interval 2.68838906601606[36,68]
 Unique zero in the interval 2.8819786295709[728,1555]
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 Unique zero in the interval 2.131177121086[2673,3558]
 Unique zero in the interval 2.4481018026567[773,801]
 Unique zero in the interval 2.68838906601606[36,68]
 Unique zero in the interval 2.8819786295709[728,1555]
```

Applications

Counting short periodic orbits for ODEs [Z. Galias]
Measuring the stable regions of the quadratic map [D. Wilczak]

Implicit curves (level sets)

Example

Draw the level-set defined by

$$f(x,y) = \sin\left(\cos x^2 + 10 \sin y^2\right) - y \cos x = 0;$$

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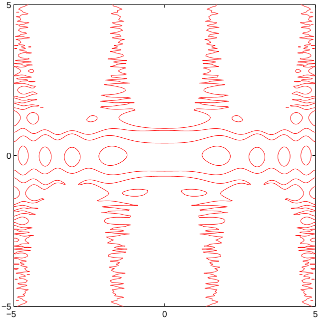

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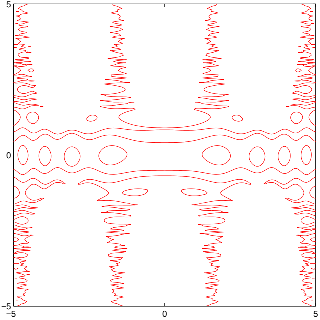

According to the same m-file, the level set defined by $|f(x,y)| = 0$, however, appears to be empty.

But this is the same set!!!

Implicit curves

The (increasingly tight) set-valued enclosures in both cases are

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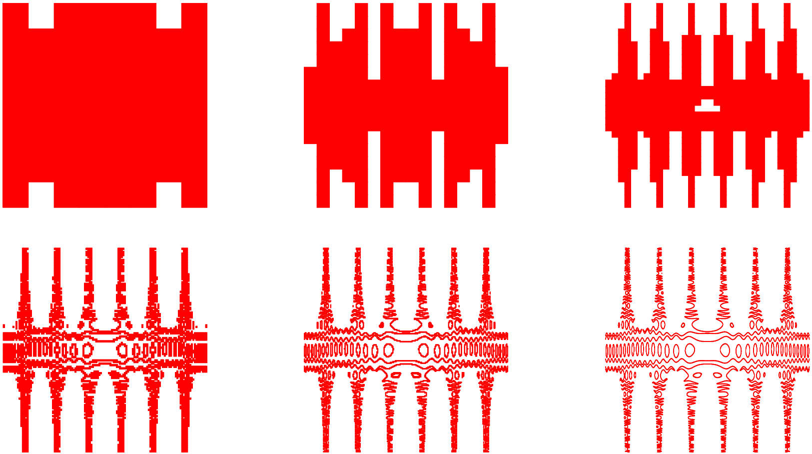

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Quadrature

Example (A bonus problem)

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$$ ./adQuad 0 8 20 1e-10
Partitions: 874
CPU time   : 0.45 seconds
Integral   : 0.3474001726[492276,652638]
```

Parameter estimation

Problem formulation

Given a finitely parametrized model function together with some (noisy) data, and a search region $\mathcal{P}$ in parameter space:

$$\underbrace{y = f(x; p)}_{\text{model}} \qquad \underbrace{\{(x_i, y_i)\}_{i=1}^{N}}_{\text{data}} \qquad \underbrace{p \in \mathcal{P}}_{\text{space}}$$

try to find parameters that give a *good agreement* between the data and the model. [A classic inverse problem]

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- **Instability:** inverse problems can be extremely ill-conditioned.

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A statistical approach

Use a (weighted) least-squares approach to find the best parameter:

$$\operatorname*{argmin}_{p\in\mathcal{P}} \sum_{i=1}^{N} w_i |f(x_i;p) - y_i|^2.$$

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A set-valued approach

Locate nearby models that are *consistent* with nearby data:

$$f(x;p) \longrightarrow f(x;\boldsymbol{p}) \qquad\qquad (x_i, y_i) \longrightarrow (x_i, \boldsymbol{y}_i).$$

Set-valued computations

Points versus sets in parameter space

We move from the *point-valued* model function $f(x; p)$ to the *set-valued* version $f(x; \boldsymbol{p})$.

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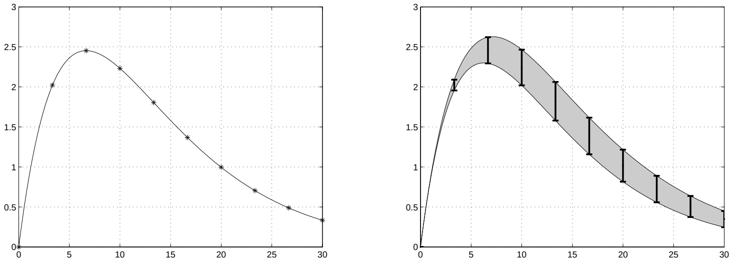

Figure: (a) $p = 0.15$, a point in $\mathcal{P}$. (b) $\boldsymbol{p} = [0.14, 0.16]$, a subset of $\mathcal{P}$. The model function is $f(x;p) = xe^{-px}$, and 10 samples are shown.

Parameter estimation

Strategy

Adaptively bisect the parameter space into sub-boxes: $\mathcal{P} = \cup_{j=1}^{K} \boldsymbol{p}_j$ and examine each $\boldsymbol{p}_j$ separately. [Good for parallelisation]

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(3) undetermined

not (1), but $f(x_i; \boldsymbol{p}) \cap \boldsymbol{y}_i \neq \emptyset$ for all $i = 0, \ldots, N$. SPLIT

Parameter estimation

Example

Consider the model function

$$f(x; p_1, p_2) = 5e^{-p_1 x} - 4 \times 10^{-6} e^{-p_2 x}$$

with samples taken at $x = 0, 5 \ldots, 40$ using $p^\sharp = (0.11, -0.32)$. Accepting a relative noise level of 90%, we get the following set of consistent parameters:

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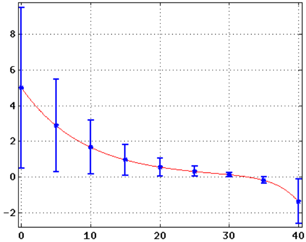

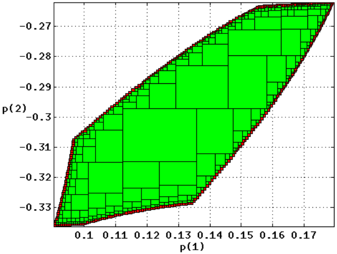

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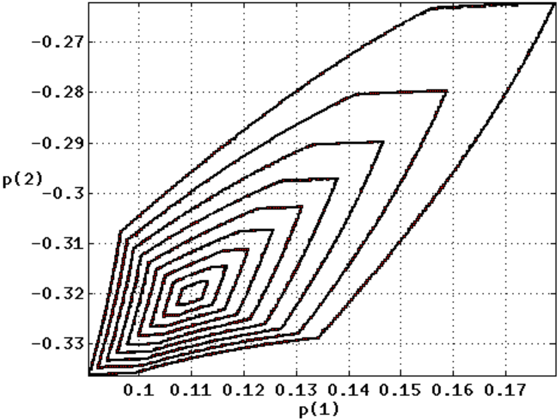
Parameter estimation

Varying the relative noise levels between $10, 20 \ldots, 90\%$, we get the following indeterminate sets.



Constraint propagation

Constraining the parameter/data space

We use set-valued constraint propagation to quickly discard inconsistent regions in the data and the parameter space.

This is done without bisection!

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$$f(2; [0, 1]) = 2e^{-2[0,1]} = 2e^{[-2,0]} = 2[e^{-2}, 1] = [2e^{-2}, 2].$$

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This allows us to contract the data range according to

$$\boldsymbol{y} \mapsto \boldsymbol{y} \cap f(x; \boldsymbol{p}) = [1,3] \cap [2e^{-2}, 2] = [1,2].$$

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Directed Acyclic Graphs (DAGs)

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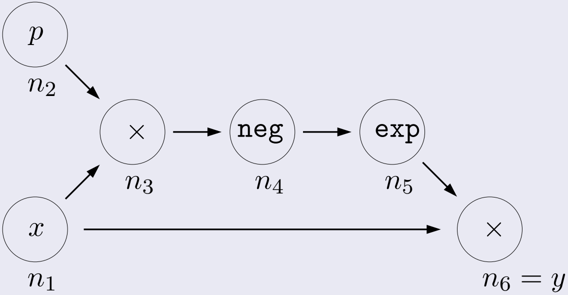

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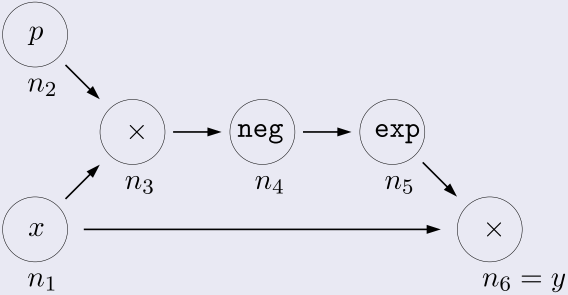

$$
\begin{aligned}
n_1 &= x \\
n_2 &= p \\
n_3 &= n_1 \times n_2 \\
n_4 &= -n_3 \\
n_5 &= e^{n_4} \\
n_6 &= n_1 \times n_5.
\end{aligned}
$$

Figure: The DAG representation of a forward sweep of $y = xe^{-px}$, together with the corresponding code list.

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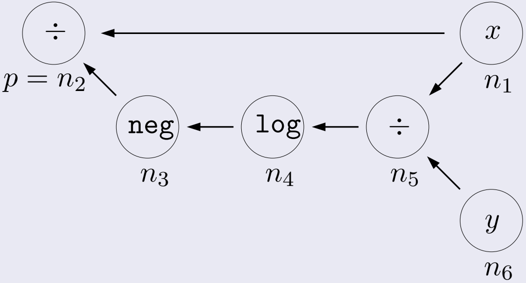

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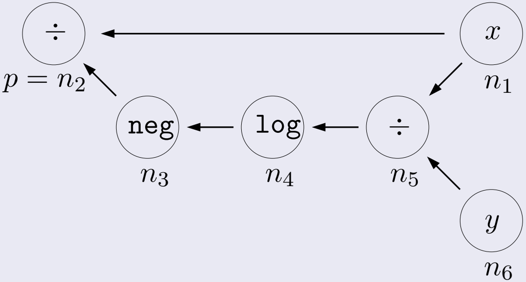

$$
\begin{aligned}
n_5 &= n_6 \div n_1 \\
n_4 &= \log n_5 \\
n_3 &= -n_4 \\
n_2 &= n_3 \div n_1.
\end{aligned}
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Figure: The DAG representation of a backward sweep of $y = xe^{-px}$, together with the corresponding code list.

Example

Again, we work on the model function $y = f(x; p) = xe^{-px}$, but now with the data $(x, \boldsymbol{y}) = (2, [1, 3])$, together with the parameter domain $\boldsymbol{p} = [0, 1]$.

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$$
\begin{array}{rcccccc}
n_5 & = & n_6 \div n_1 & = & [1,2] \div 2 & = & [\frac{1}{2}, 1] \\
n_4 & = & \log n_5 & = & \log [\frac{1}{2}, 1] & = & [-\log 2, 0] \\
n_3 & = & -n_4 & = & [0, \log 2] & & \\
n_2 & = & n_3 \div n_1 & = & [0, \log 2] \div 2 & \approx & [0, 0.34657359].
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Note that, in one forward/backward sweep, we managed to exclude over 65% of the parameter domain, at the same time reducing the data uncertainty by 50%.

Mixed-effects models

Mixed-effects models

We are given several data sets (trajectories) corresponding to k different "individuals":

$$
\begin{aligned}
\text{individual}_1 : &\quad (x_{11}, y_{11}), (x_{12}, y_{12}), \dots, (x_{1N}, y_{1N_1}) \\
\text{individual}_2 : &\quad (x_{21}, y_{21}), (x_{22}, y_{22}), \dots, (x_{2N}, y_{2N_2}) \\
&\qquad \vdots \qquad\qquad \vdots \qquad\qquad\qquad \vdots \\
\text{individual}_k : &\quad (x_{k1}, y_{k1}), (x_{k2}, y_{k2}), \dots, (x_{kN}, y_{kN_k}).
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Some model parameters are equal (shared) for all individuals, and some are distinct.

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- We need to consider all individuals simultaneously. Otherwise the number of unknown parameters may be too large.

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A mixed-effects model for orange tree truncs

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We will apply our method to the following scenario:

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Model function: $$f(x;p) = \frac{p_1}{1 + p_2 e^{p_3 x}}$$

Individual parameter: $$p_{i1} = p_1^\sharp + \eta_i, \quad \eta_i \sim N(0, \sigma^2)$$

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For this specific example, we will use $N_p \in \{1, 2, 5, 50\}$ subjects, sampled at $N_d = 10$ data sites, evenly spaced within $[100, 1600]$.

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Target parameters:

$p^\sharp = (191.84, 8.153, -0.0029)$, $\sigma = 20$, $\epsilon \in \{0.01, 0.1, 0.2, 0.5\}$.

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Search region:

$$\mathcal{P} = ([0,300],[0,9],[-1,0]).$$

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A mixed-effects model for orange tree truncs

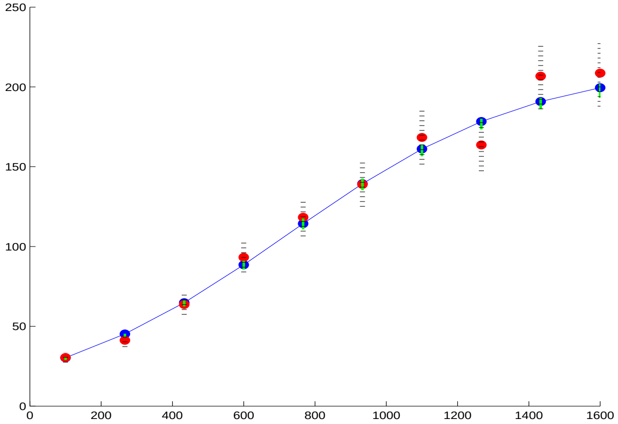

Figure: Data inflation and contraction for the example. The graph of the model function for one subject (blue line). The data points are marked with red dots. The inflated data sets are shown as striped bars, and the re-contracted data as green bars.

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Numerical results

	$N_p = 1$	$N_p = 2$
$\epsilon = 0.01$	190.639 (– –) (0.010)	193.141 (19.6) (0.013)
$\epsilon = 0.1$	194.139 (– –) (0.092)	195.233 (21.1) (0.097)
$\epsilon = 0.2$	189.139 (– –) (0.190)	193.437 (20.3) (0.192)
$\epsilon = 0.5$	167.226 (– –) (0.604)	167.770 (26.6) (0.589)

	$N_p = 5$	$N_p = 50$
$\epsilon = 0.01$	191.675 (20.1) (0.014)	191.239 (20.1) (0.012)
$\epsilon = 0.1$	192.954 (21.4) (0.099)	198.428 (22.2) (0.110)
$\epsilon = 0.2$	191.773 (20.3) (0.203)	197.580 (23.6) (0.214)
$\epsilon = 0.5$	164.656 (23.9) (0.620)	174.318 (27.1) (0.618)

Table: The results of four experiments for the example, each using 100 trial runs with $p_1 = 191.184$, and $\sigma = 20.0$. For each pair (ϵ, N_p), we display the triple $\mu(p_1)$, $\mu(\sigma)$, and $\mu(\epsilon)$ – the average estimates of the distribution parameters for p_1, and the data error.

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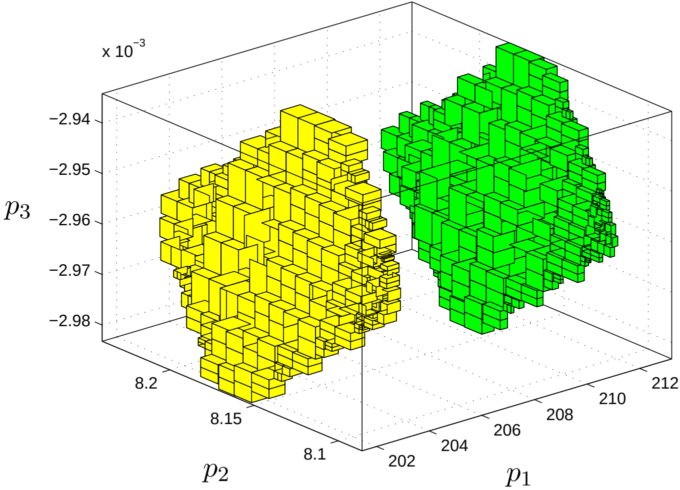

Figure: The set of consistent parameters for two subjects from the example.

Conclusions

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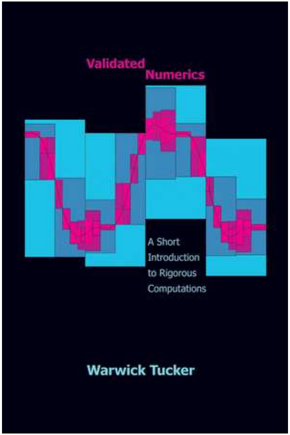

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Warwick Tucker

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