Parameter estimation via constraint propagation

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Introduction

Problem formulation

A classic inverse problem/parameter estimation setting: given a finitely parametrized model function

$$y = f(x; p_1, p_2, \ldots, p_m) = f(x; p),$$

together with some (noisy) data

$$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$$

and a search region $\mathcal{P}$ in parameter space, try to find parameters that give a *good agreement* between the data and the model.

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and a search region $\mathcal{P}$ in parameter space, try to find parameters that give a *good agreement* between the data and the model.

- Here, f can be almost anything (a function, an ODE, a PDE, some process...). This means that no single method is best.

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- **Instability:** many inverse problems are extremely unstable (ill-conditioned): a small perturbation in data produces a large change in the fitted parameter.

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- If the parameters enter f linearly, this is "straight-forward".
- Otherwise, we have moved the problem to *global optimization*.
- The selection of weights is almost always a delicate issue.

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A set-valued approach

Assume that the model is uncertain, and that the data is perturbed via some unknown mechanism.

Rather than seaching for the least-squares best fit, we attempt to locate nearby models that are *consistent* with nearby data:

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Of course, $\mathcal{S}$ is very hard to find, but by discretizing the search space $\mathcal{P} \to \mathcal{P}_K$, we can form an inner/outer enclosure of $\mathcal{S}$:

$$\underline{\mathcal{S}} = \{\boldsymbol{p} \subset \mathcal{P}_K\colon f(x_i;\boldsymbol{p}) \subset \boldsymbol{y}_i \text{ for all } i = 1,\dots,N\}$$
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The coarser the discretization of $\mathcal{P}$, the less we trust the model.

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Set-valued computations

Interval analysis

All our computations are set-valued, and are based on the *inclusion principle*:

$$\mathrm{range}(g;\boldsymbol{x}) = \{g(x)\colon x \in \boldsymbol{x}\} \subseteq g(\boldsymbol{x})$$

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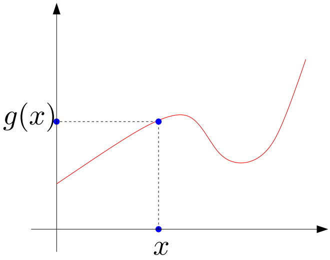

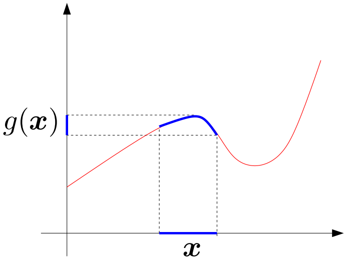

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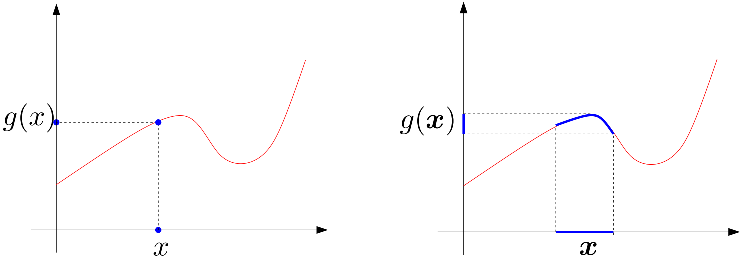

Interval Computations Web Page

`http://www.cs.utep.edu/interval-comp`

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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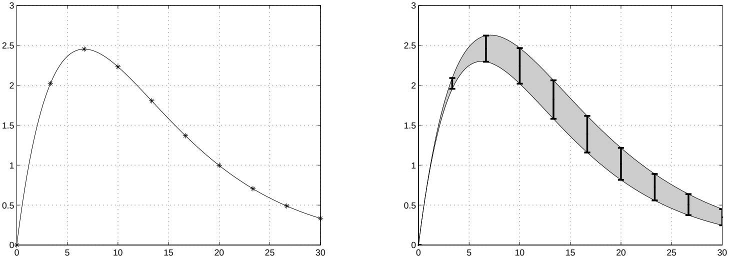

Figure: (a) $p = 0.15$, a point in $\mathcal{P}$. (b) $\boldsymbol{p} = [0.14, 0.16]$, a subset of $\mathcal{P}$. The model function is $f(x;p) = xe^{-px}$, and 10 samples are shown.

Parameter reconstruction

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.

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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 reconstruction

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 $p^\star = (0.11, -0.32)$. With a relative noise level of 90%, we get the following set of consistent parameters:

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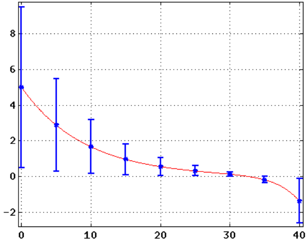

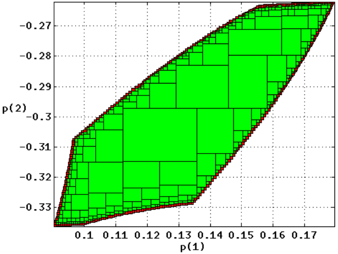

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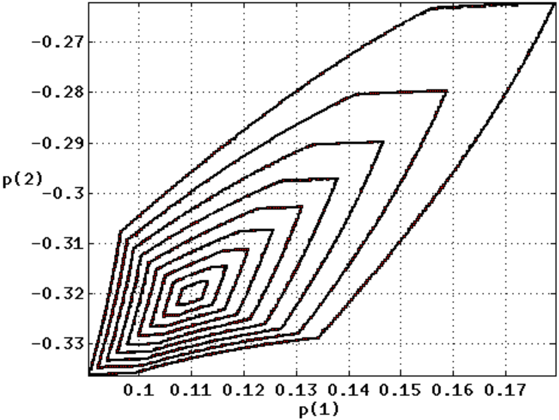
Parameter reconstruction

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



Constraint propagation

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Let $f(x;p) = xe^{-px}$, and consider the situation $\boldsymbol{p} = [0, 1]$ and $(x, \boldsymbol{y}) = (2, [1, 3])$.

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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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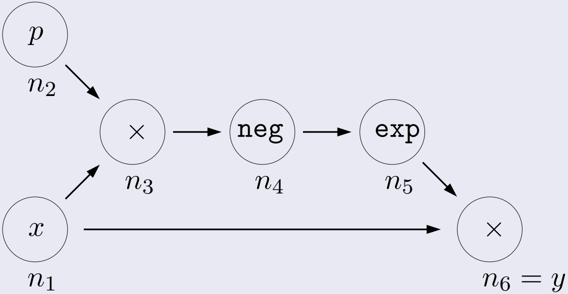

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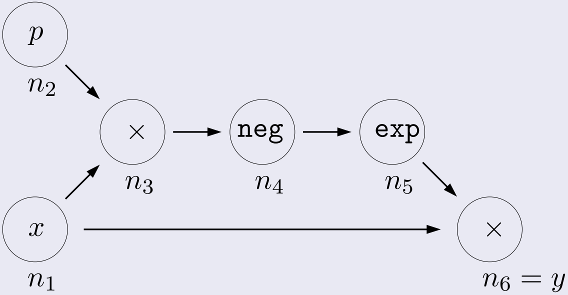

$$
\begin{aligned}
n_1 &= x \\
n_2 &= p \\
n_3 &= n_1 \times n_2 \\
n_4 &= -n_3 \\
n_5 &= e^{n_4} \\
n_6 &= n_1 \times n_5.
\end{aligned}
$$

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

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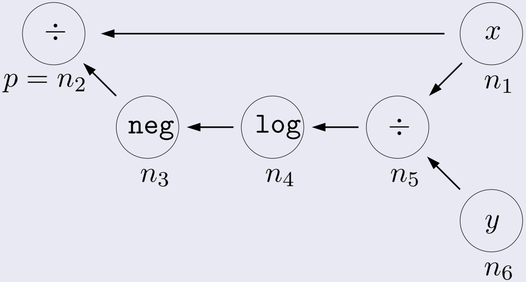

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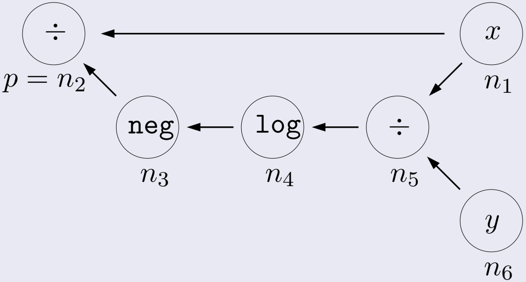

$$n_5 = n_6 \div n_1$$
$$n_4 = \log n_5$$
$$n_3 = -n_4$$
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Example

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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$$\begin{array}{lllllll} n_5 & = & n_6 \div n_1 & = & [1, 2] \div 2 & = & [\frac{1}{2}, 1] \\ n_4 & = & \log n_5 & = & \log [\frac{1}{2}, 1] & = & [-\log 2, 0] \\ n_3 & = & -n_4 & = & [0, \log 2] & & \\ n_2 & = & n_3 \div n_1 & = & \frac{1}{2}[0, \log 2] & \approx & [0, 0.34657359]. \end{array}$$

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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

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

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

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

$$\text{Data perturbation:} \qquad y_{ij} = y_{ij}^\sharp (1 + \theta_{ij}), \quad \theta_{ij} \sim U(-\epsilon, +\epsilon)$$

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 $[100, 1600]$.

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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A mixed-effects model for orange tree truncs

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Search region:

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

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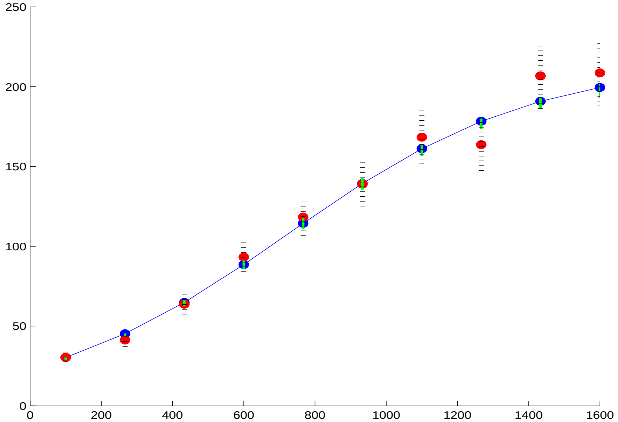

Figure: Data inflation and contraction for the example. The graph of the model function for one subject (blue line). The data points are marked with red dots. The inflated data sets are shown as striped bars, and the re-contracted data as green bars.

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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.

A mixed-effects model for orange tree truncs

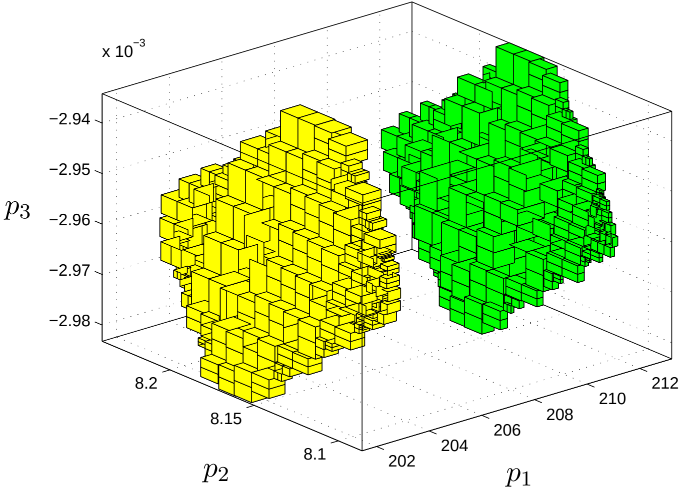

Figure: The set of consistent parameters for two subjects from the example.

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Summary

Main steps

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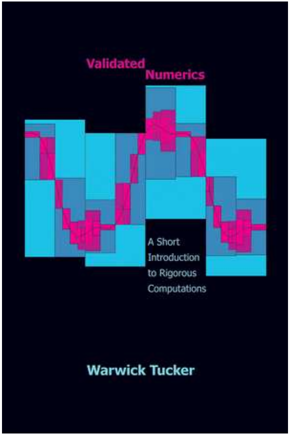

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Warwick Tucker

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