Sensitivity analysis in linear and nonlinear models: A review

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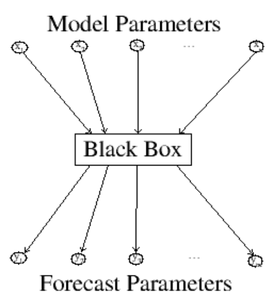
Introduction

Consider:



Question: How do the inputs affect the outputs?
General Answer: Sensitivity Analysis (SA).

However, different people mean different things by SA. E.g.
– How does input uncertainty propagate (Uncertainty A.)?
– How does the addition of a new observation affect the outcome?
– How is output uncertainty apportioned among the inputs?

And they do it for different reasons. E.g.
– Knowledge discovery.
– Ranking of the inputs.
– Dimensionality Reduction.
– Model tuning. Etc.

Introduction ...

Three components:

1) Experimental Design.
– Make or break.
– No experimental error. Computer Data. *In vitro vs. In silico.*
– How should the inputs be selected?
– To optimize accuracy and precision.
– random sampling will not give the most precise estimate.

2) Choice of SA method.
– Performance vs. inclusion/exclusion of inputs.
– One At a Time.
– High-dimensional space is mostly corners.
– Generally three types:
. – Local (derivatives, adjoint),
. – Screening (factorial designs)
. – Global (variance-decomposition)

3) Method for estimating conditional expectations.
– Monte Carlo
– Emulation (Gauss Process/Krig, Poly. Regression, NN, ...)

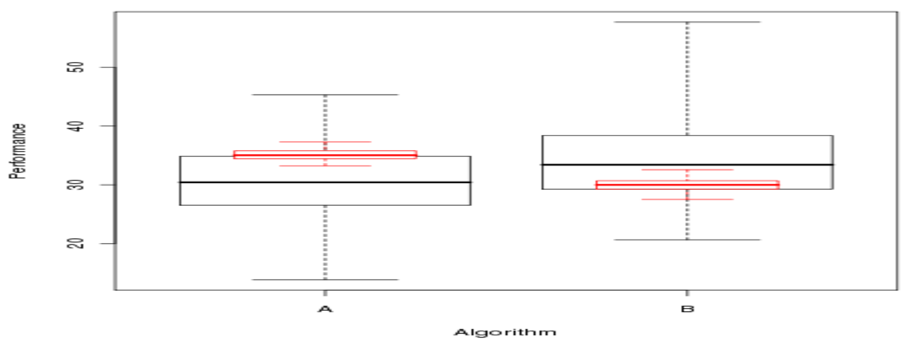
A few issues specific to computer experiments:
– No experimental error to minimize.
– Emulator must have zero error on training set.
– Error on test set must be consistent with realistic uncertainty.

Q: Why AI/CI? A: 1 and 3.

Experimental Design

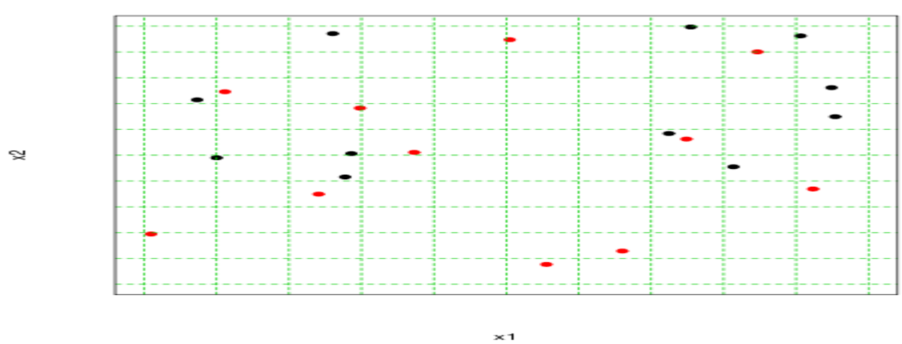
Q: What values of the inputs should be selected?

– Impossible to explore all values. So, sample!
– Simple random sample does not give most precise estimates.
.   – Who cares?



With low precision (black): Cannot pick better algorithm.
If/when forced, may take B.
But with higher precision, A wins.

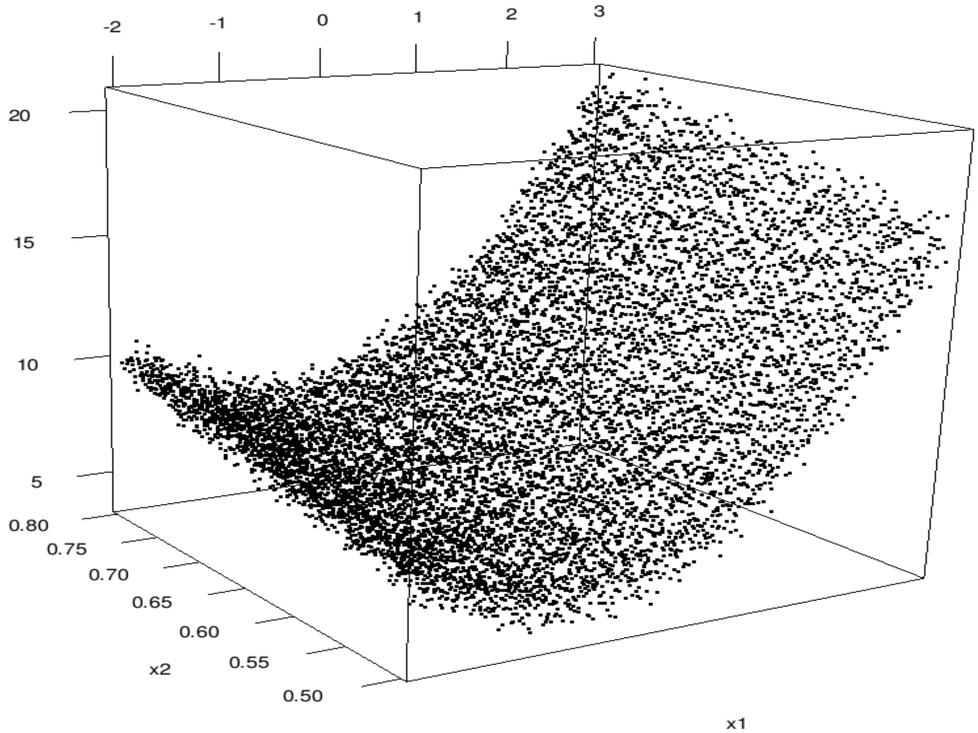
– Space-filling samples/designs give more precise estimates. E.g.,
– Latin hypercube sampling

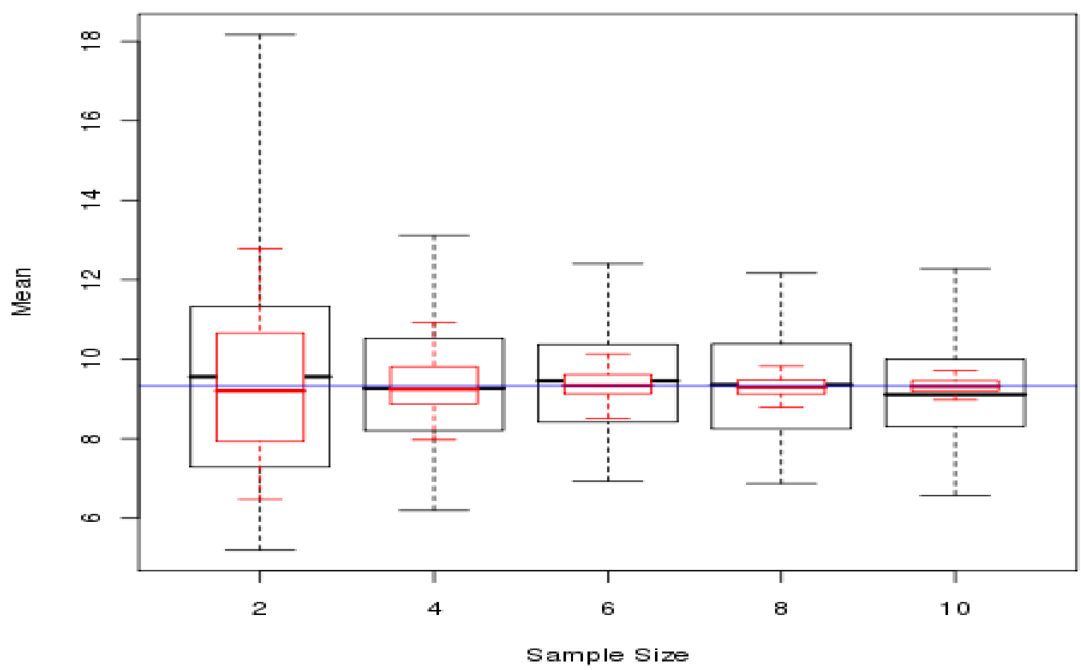


A simple random sample (black) and a latin square sample (red).
No 2 red dots have a row or col in common.

Simple random vs. Latin square sampling

Estimate mean of z-axis:





Distribution of means according to simple random (black) and latin square (red) sampling, for different sample sizes.
True mean = horizontal line.

Variance-Based SA

Two "theorems" save the day:

$$Var[Y] = E[\,Var[Y|X]\,] + Var[\,E[Y|X]\,]$$

$$Y = \eta(X_1, X_2, ...) = E[Y] + z_1(x_1) + z_2(x_2) + z_{12}(x_1, x_2) + ...$$

where

$$z_i(x_i) = E[Y|x_i] - E[Y]$$

$$z_{12}(x_1, x_2) = E[Y|x_1, x_2] - E[Y|x_1] - E[Y|x_2] + E[Y]$$

$$\ldots$$

Measures of Sensitivity

Reduction in uncertainty of Y, after X_i is learned:

$$V_i = Var[\,E[Y|X_i]\,]$$

Reduction in uncertainty of Y, after X_1 and X_2 are learned:

$$V_{12} = Var[E[Y|X_1, X_2]]$$

Uncertainty in Y remaining, after X_2 is learned:

$$V_{T1} = Var[Y] - Var[E[Y|X_2]] \quad \text{(1,2) not a typo!}$$

Main effect index of X_i::

$$S_i = V_i / Var[Y]$$

Total effect index of X_i:

$$S_{Ti} = V_{Ti} / Var[Y]$$

Example 1

$$Y = \eta(X_1, X_2) = X_1$$

	General	Indep X_1, X_2
z_1	$x_1 - E[X_1]$	$x_1 - E[X_1]$
z_2	$E[X1 \vert X_2] - E[X_1]$	0
z_{12}	$-z_2(x_2)$	0
V_1	$V[X_1]$	$V[X_1]$
V_2	$V[E[X_1 \vert X_2]]$	0
V_{12}	$V[X_1]$	0
V_{T1}	$V[X_1] - V_2$	$V[X_1]$
V_{T2}	0	0
S_1	1	1
S_2	$V_2/V[X_1]$	0
S_{T1}	$1 - S_2$	1
S_{T2}	0	0

Example 2

$$Y = \alpha + \beta_1 \, X_1 + \beta_2 \, X_2 + \beta_{12} \, X_1 \, X_2$$

Theorem: Things are messy. Proof:

$$\begin{aligned} z_1 &= \beta_1(x_1 - E[X_1]) \\ &+ \beta_2(E[X_2|X_1] - E[X_2]) \\ &+ \beta_{12}(x_1 E[X_2|X_1] - E[X_1 \, X_2]) \\ z_2 &= \text{similar} \\ z_{12} &= \beta_1(E[X_1] - E[X_1|X_2]) \\ &+ \beta_2(E[X_2] - E[X_2|X_1]) \\ &+ \beta_{12}(x_1 \, x_2 - x_1 \, E[X_2|X_1] - x_2 \, E[X_1|X_2] - E[X_1 \, X_2]) \end{aligned}$$

Even for indep. X_1, X_2, and $E[X_i] = 0$

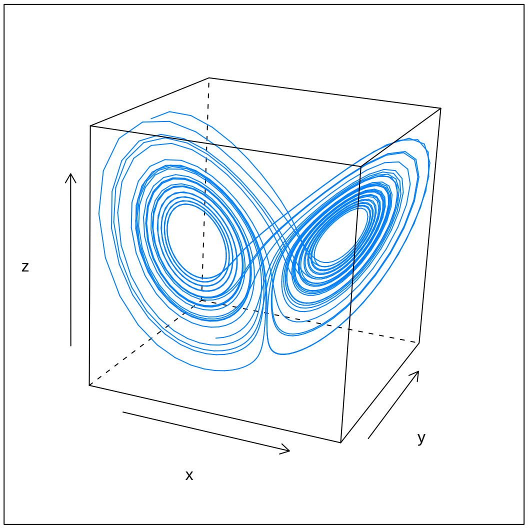
$$\begin{aligned} z_1 &= \beta_1 \, x_1 - \beta_{12} \, E[X_1 \, X_2] \\ z_2 &= \beta_2 \, x_2 - \beta_{12} \, E[X_1 \, X_2] \\ z_{12} &= \beta_{12}(x_1 \, x_2 - E[X_1 \, X_2]) \end{aligned}$$

Etc. for V_i, V_{Ti}, S_i, S_{Ti}.

Moral:
If model = linear ($\beta_{12} = 0$), the $S_i \sim$ (std regress coeff)^2.
Else, not, and complicated.

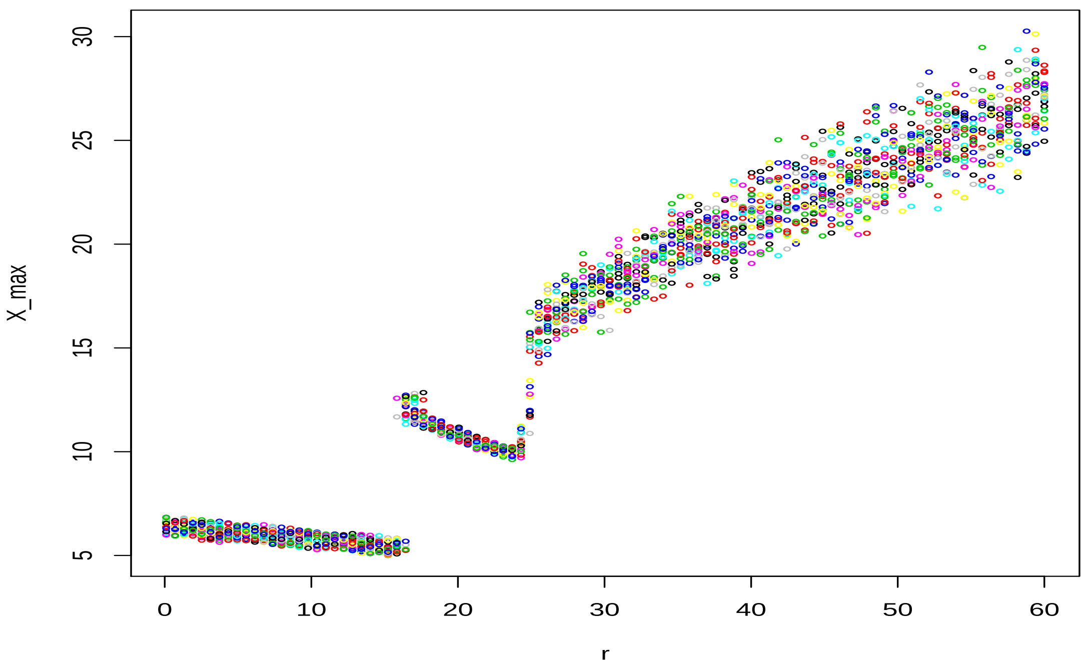
Example 3

Black Box = Lorenz, 1963



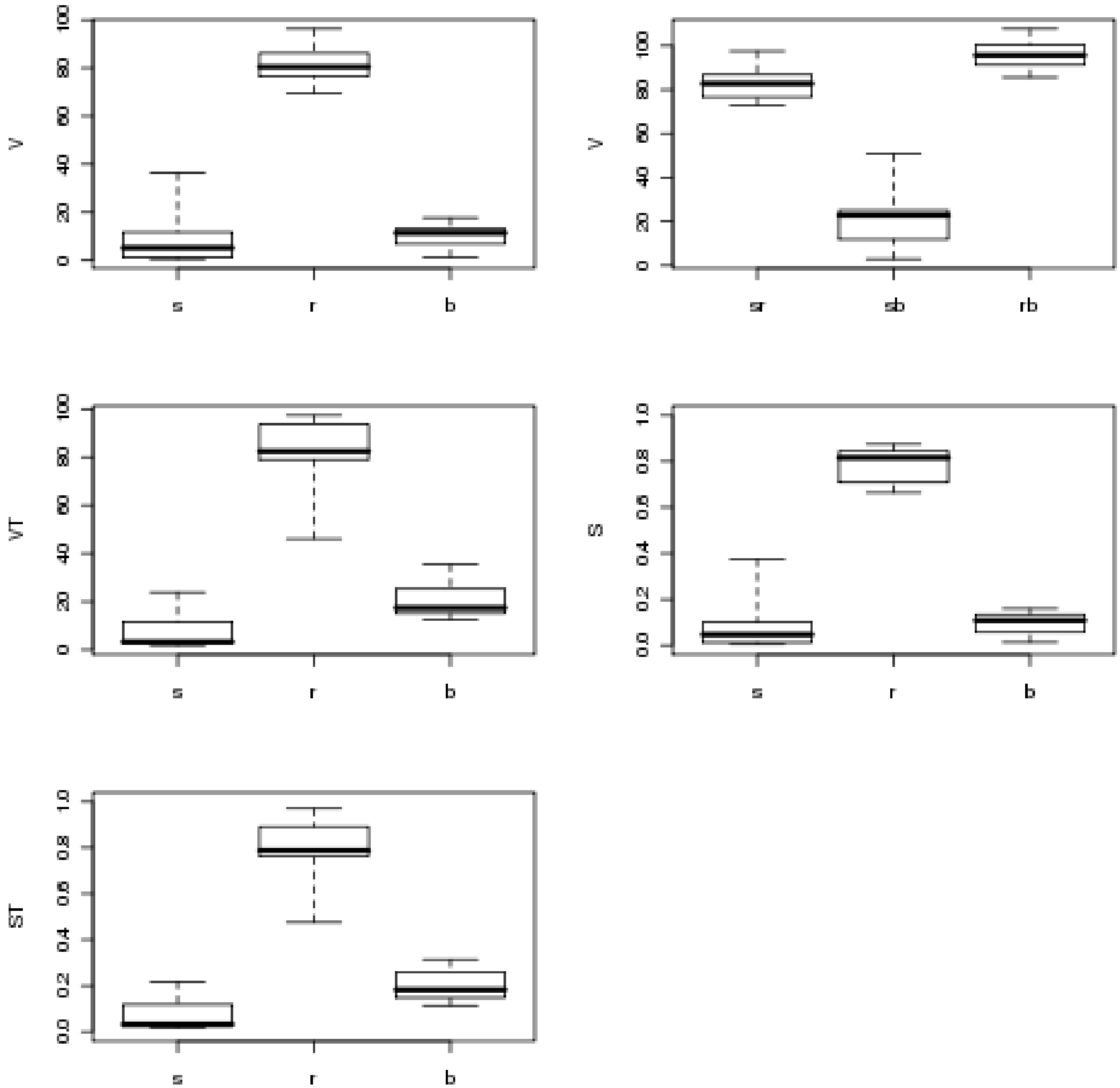
Inputs $= s, r, b.$

Outputs $= X_{max}, Y_{max}, Z_{max}.$



Main conclusion for Lorenz

All sensitivity measures:



According to most measures, X_{max} is

– most sensitive to r,

– not so sensitive to s, and b,

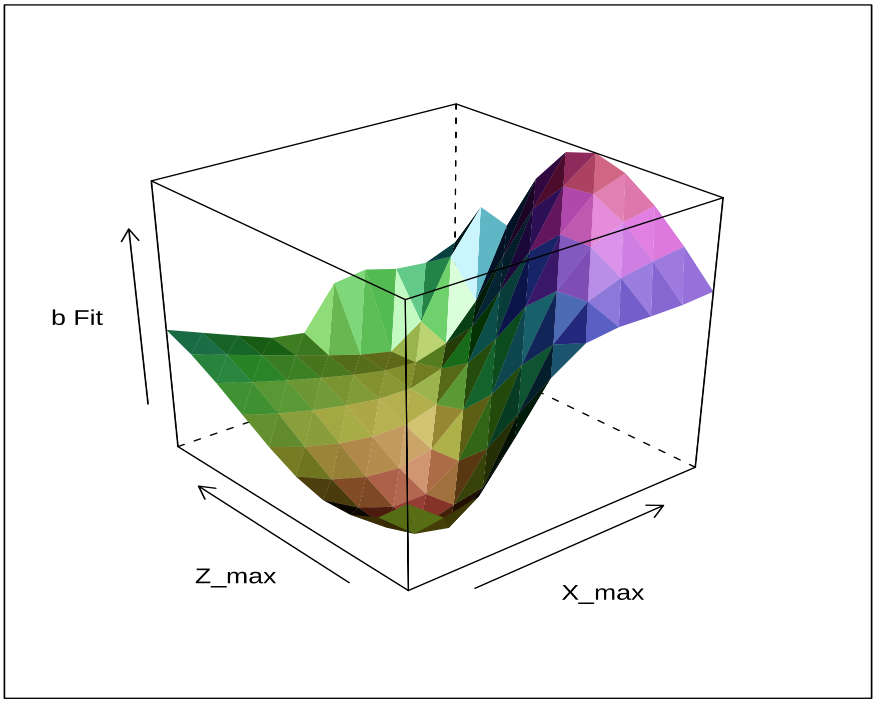
– but there exists an "interaction" between s and r,

– and between r and b,

– but not as much between s and b.

Peeking into the black box

The blackbox according to one NN emulator:



Final Remarks

– Sensitivity Analysis is intuitive, but ambiguous.
– Careful attention to experimental design is crucial.
– Variance-based methods naturally tie SA to emulators.
– Not clear (to me) if "fancy" emulators are necessary.
– Many AI techniques come with natural ranking of inputs.
– But in most, an "explanation" is lacking.
– Ranking based on variance is explanatory.
– But does not assure better performance.

Coming soon:

- Emulation with gaussian process (zero trn error) vs. NN (not).
- Extension to Multivariate (multiple output).
- Orthogonal designs to address collinearity.
- Connection with ensemble methods.

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