Computer tutorial on global sensitivity analysis

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Model problem: SIR dynamics with time varying transmission rate

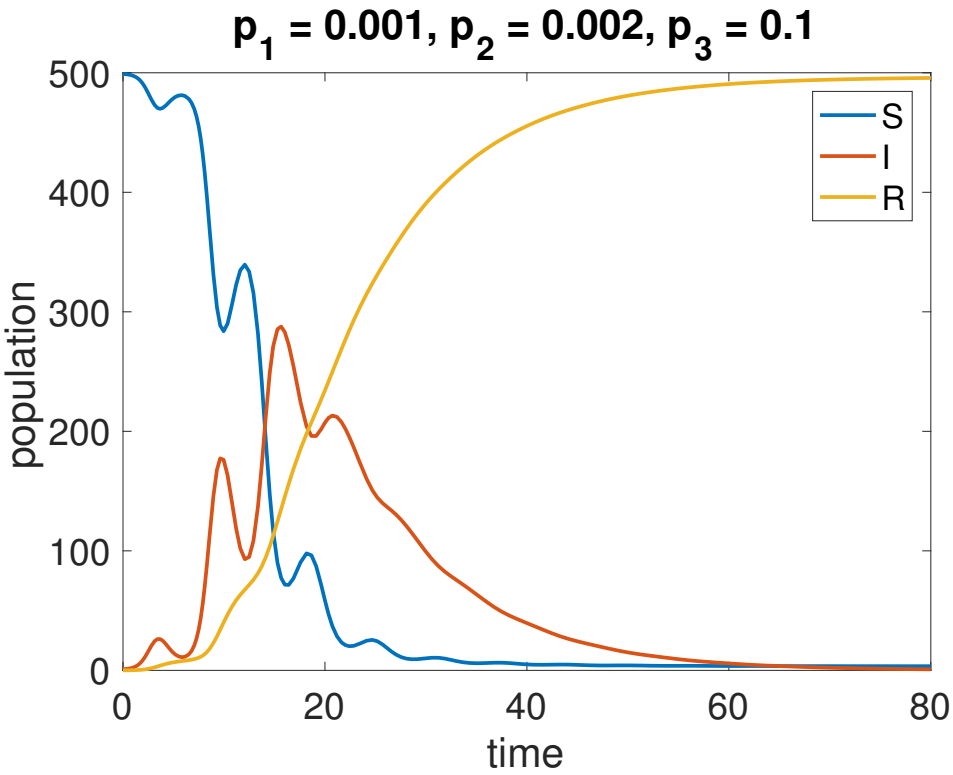
Governing equations:

$$\frac{dS}{dt} = -\beta(t)SI \qquad \text{with} \qquad \beta(t) = p_1 + p_2 \sin(t)$$
$$\frac{dI}{dt} = \beta(t)SI - p_3 I$$
$$\frac{dR}{dt} = p_3 I$$

Uncertain parameter vector:

$$\boldsymbol{p} = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

DEMO 1: Nominal system parameters



$$S(0) = 499 \quad I(0) = 1 \quad R(0) = 0$$

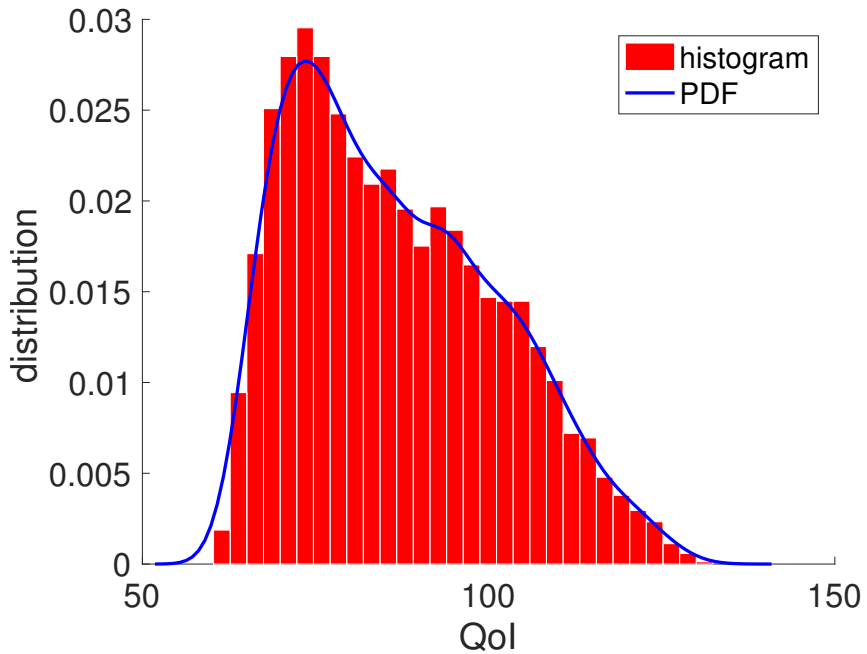
MATLAB: `demo_nominal_system.m`

DEMO 2: A scalar quantity of interest (QoI)

Parameterize uncertainty in $\boldsymbol{p}$ using $\boldsymbol{x} \in \mathbb{R}^3$ with $x_i \sim U(-1, 1)$

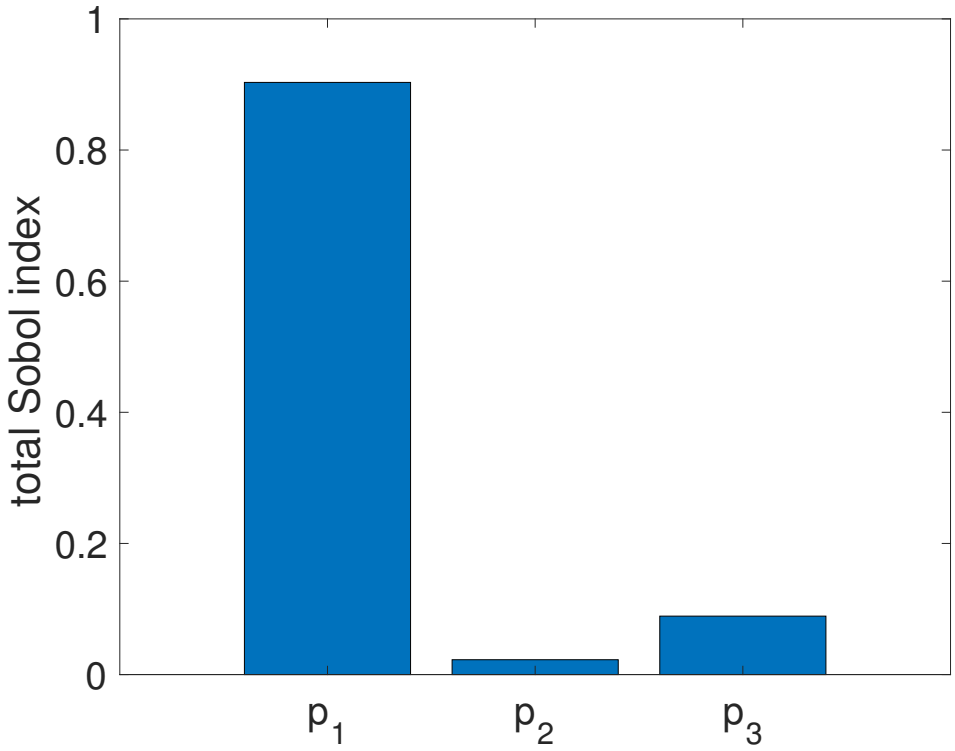
QoI: average susceptible population

$$f(\boldsymbol{x}) = \frac{1}{T} \int_0^T S(t; \boldsymbol{x})\, dt \quad \text{with } T = 80$$



MATLAB: `demo_sample.m`

DEMO 3: Sobol' indices



MATLAB: `demo_sobol_scalar.m`

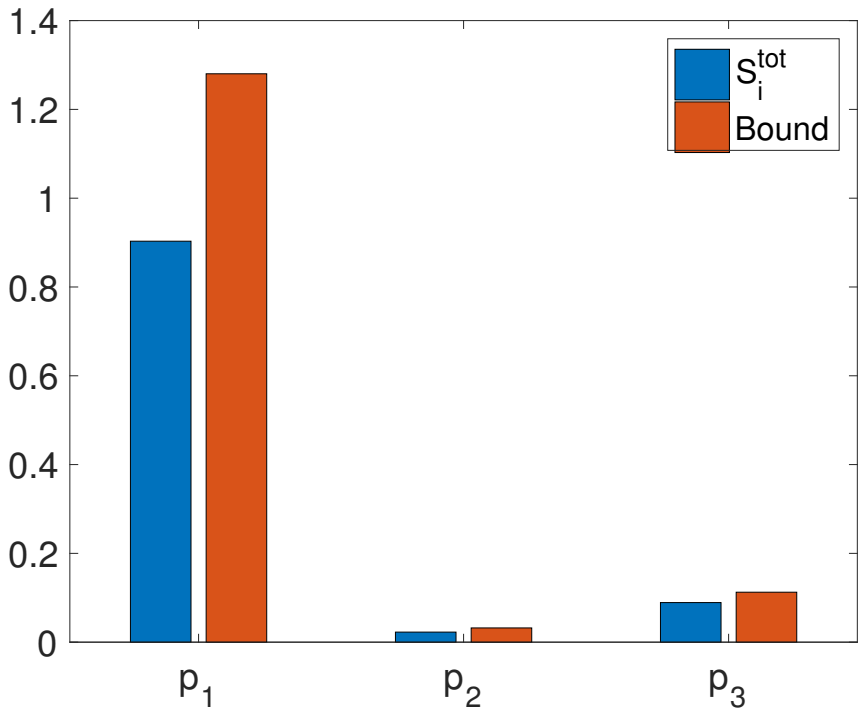
DEMO 4: Derivative based GSA

Inequality:

$$S_i^{\text{tot}}(f) \leq \frac{c}{D}\nu_i(f)$$

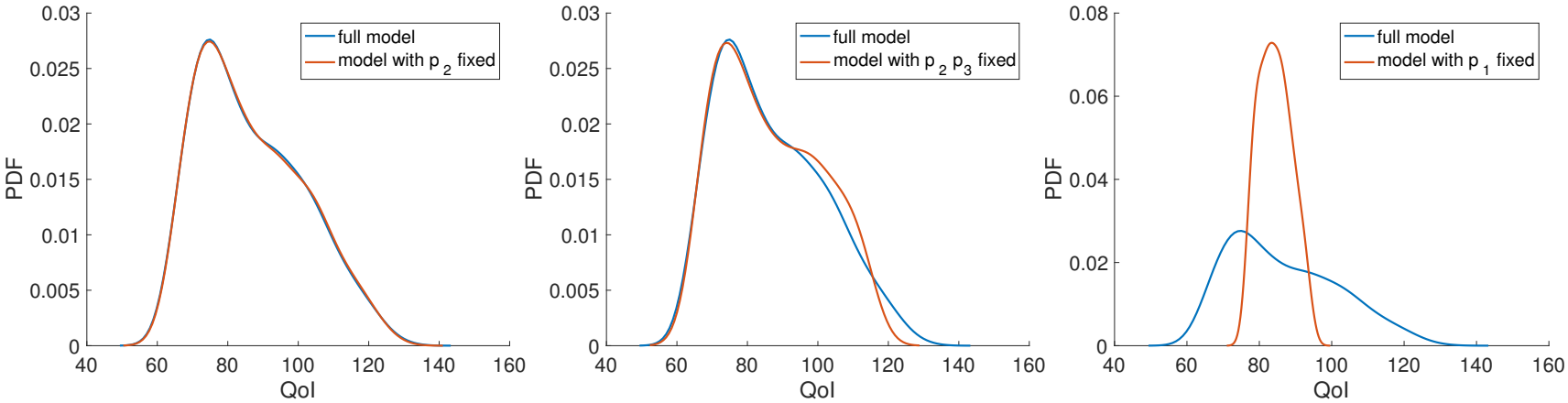
with

$$D = \text{Var}\{f\} \quad \nu_i(f) = \text{E}\left\{\left(\frac{\partial f}{\partial x_i}\right)^2\right\} \quad c = \frac{4}{\pi^2}$$



MATLAB: `demo_dgsm.m`

DEMO 5: Fixing parameters



Recall the model

$$\frac{dS}{dt} = -\beta(t)SI \qquad \text{with} \qquad \beta(t) = p_1 + p_2 \sin(t)$$

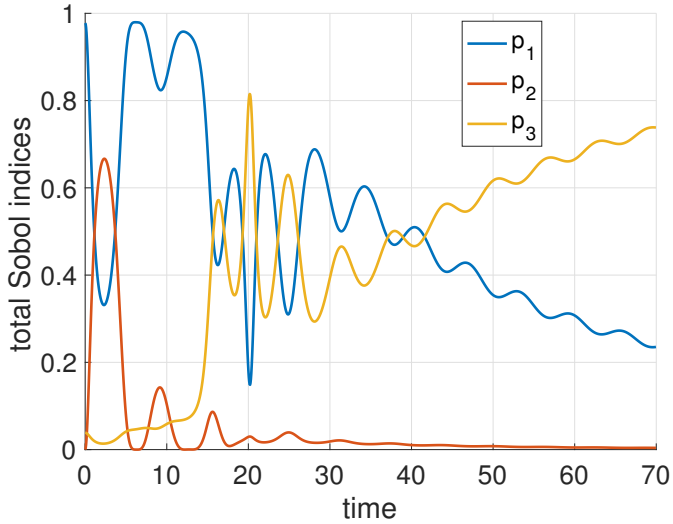
$$\frac{dI}{dt} = \beta(t)SI - p_3 I$$

$$\frac{dR}{dt} = p_3 I$$

MATLAB: `demo_fixing_var.m`

DEMO 6: Sobol' indices over time

Sobol' indices for $I(t; \boldsymbol{x})$ over time

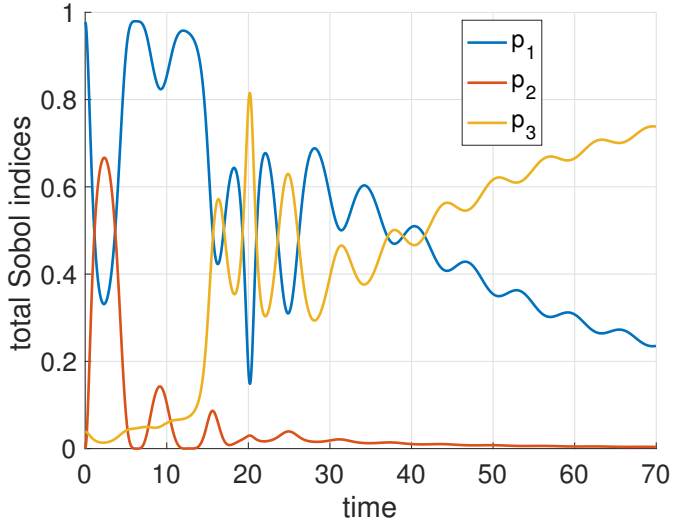


Note: $S_i^{tot}(t)$ = total contribution of ith input to variance **at time** t

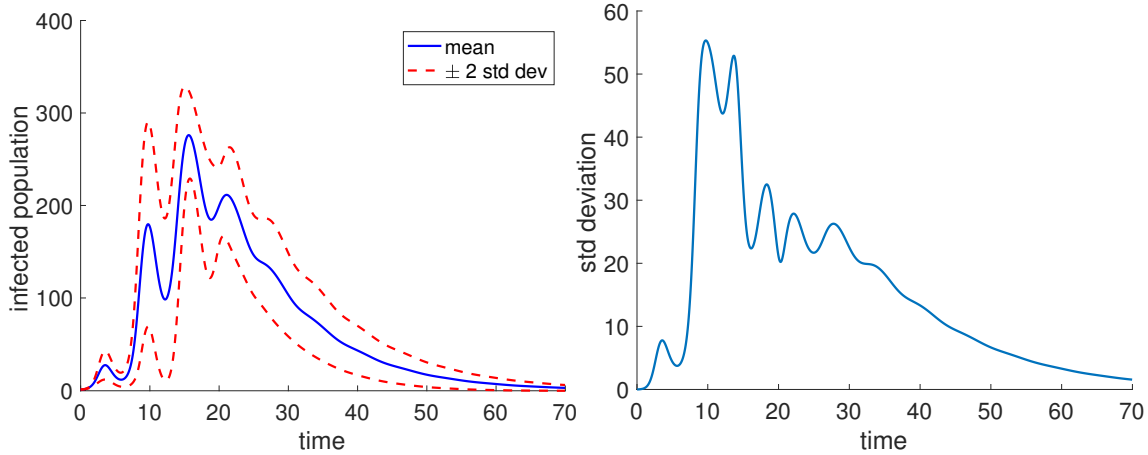
MATLAB: `demo_sobol_time.m`

DEMO 6: Sobol' indices over time

Sobol' indices for $I(t; \boldsymbol{x})$ over time



Note: $S_i^{tot}(t)$ = total contribution of ith input to variance **at time** t
variance changes over time $\Rightarrow$ pointwise-in-time Sobol' indices have limited use



MATLAB: `demo_sobol_time.m`

Getting started with the Matlab codes

- Download `rtg_codes.zip` from
  `https://aalexan3.math.ncsu.edu/rtg/rtg.html`
  (can also go to
  `http://rtg.math.ncsu.edu/workshop-2018/Schedule_2018/`)
- Expand the .zip file by clicking on it
- Start Matlab
- In Matlab command-prompt type

```
>> cd ~/Downloads/rtg_codes
```

Some suggested computational experiments

- Generate system trajectory with different sets of nominal parameters
- Compute Sobol' indices / DGSMs with different sample sizes
- Change ranges of uncertainty on parameters
- Consider different scalar QoIs (redefine `sir_scalar_qoi.m`)
- Think more about the time-dependent case (look at `demo_sobol_time_generalized.m`)
- Consider different time-dependent QoIs (redefine `sir_timedep_qoi.m`)
- ...

Further reading

Books

- Ralph Smith, Uncertainty Quantification: Theory, Implementation, and Applications, 2014.
- A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana. and S. Tarantola, Global sensitivity analysis: the primer. John Wiley & Sons. 2008.
- Le Maitre, Olivier, and Omar M. Knio. Spectral methods for uncertainty quantification: with applications to computational fluid dynamics. 2010.

Some relevant papers

- I.M. Sobol'. Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. Mathematics and computers in simulation, 55(1):271–280, 2001.
- I.M. Sobol' and S. Kucherenko. Derivative based global sensitivity measures and their link with global sensitivity indices. Mathematics and Computers in Simulation, 79(10), 2009.
- I.M. Sobol', S. Tarantola, D. Gatelli, S. Kucherenko, and W. Mauntz. Estimating the ap- proximation error when fixing unessential factors in global sensitivity analysis. Reliability Engineering & System Safety, 92(7), 2007.
- S. Kucherenko and B. Iooss, Derivative-based global sensitivity measures. Handbook of uncertainty quantification, 2017.
- J. Hart and P. Gremaud. An approximation theoretic perspective of Sobol' indices with dependent variables. Submitted. `https://arxiv.org/pdf/1801.01359.pdf`. 2018.
- J. Hart, A. Alexanderian, P. Gremaud Efficient computation of Sobol'indices for stochastic models. SIAM Journal on Scientific Computing, 39(4), 2017.
- A. Alexanderian, P.A. Gremaud, and R.C. Smith. Variance-based sensitivity analysis for time-dependent processes. In revision. `https://arxiv.org/abs/1711.08030`. 2017.