SENSITIVITY ANALYSIS OF STATIC QUANTITIES DERIVED FROM DYNAMICAL SYSTEMS

Let $x' = f(x, t; p, \sigma)$ be our dynamical system where p is our set of parameters and σ is our level of noise (any of these quantities may be vectors). For now, let's assume there is no noise in the system ($\sigma = 0$) and we'll come back to the case with nosie later.

We are often interested in static quantities derived from such systems such as the values of any equlibria, the stability of the equilibria, or more domain-specific quantities like the basic reproduction number. These quantities are called static because they are independent of time (you might also call them autonomous). Let Q be the static quantity we're interested in: $Q = g(p)$. Here $p = (p_1, \ldots, p_n)$ might include our set of initial conditions which can also be thought of like parameters.

We're interested in better understanding the effect of the variation of parameters on the quantity Q. For example, if Q changes a lot with only a small change in p_1, then we need to make sure our estimate of p_1 is really accurate because inaccuracy in p_1 will lead to more inaccuracy in Q. On the other hand, if Q barely changes as p_2 is varied, then we don't have to focus as much on p_2 and, in fact, may be able to find a way to exclude p_2 from our model. However, the function g can be quite complicated and we may have many parameters we're interested in studying. We can't simply plot $Q = g(p)$ to understand how Q depends on the values of p. We need a way to measure the relative influence of the parameters on Q.

Local Sensitivity Analysis

The *local sensitivity* of Q with respect to the parameter p_i is defined to be

$$\mathscr{S}_Q^{p_i} = \frac{\partial Q}{\partial p_i}$$

This is called local because we can only evaluate this for a particular set of parameter values; we're not exploring the entire parameter space. If we're reasonably confident in the values of all the parameters, then a local sensitivity analysis is a good way to understand which parameters have the greatest influence on Q. However, this approach is very dependent on the magnitude of p_i. If p_i is measured in kilometers and p_j in meters, we would expect a relatively small change in p_i to have a larger impact on Q than a large change in p_j. We can resolve this considering instead the *elasticity* of Q with respect to p_i

$$\varepsilon_Q^{p_i} = \left(\frac{p_i}{Q}\right)\frac{\partial Q}{\partial p_i} \approx \frac{\%\Delta Q}{\%\Delta p_i}$$

This measures the percentage change in the value of Q due to a 1% change in p_i. This is still a local measure of influence but is more appropriate for comparing influence among the full set of parameters. These both measure the *monotonicity* of Q with respect to p_i. If $\mathscr{S}$ and ε are positive (negative), then Q increases (decreases) with p_i. We can calculate the full set of elasticities,$\left\{\varepsilon_Q^{p_i}\right\}_{i=1}^{n}$, and order them to see which parameters are most influential on the value of Q.

Global Sensitivity Analysis

But what if we are really unsure about our parameter values? Or we want to explore a model that can be applied to a wide range of systems (= parameter sets)? The goal of a *global sensitivity analysis*is to understand how Q is influenced by parameters through the whole parameter space. Exploring parameter space can quickly become daunting beyond two parameter. Consider the equation $Q = x^2y + xz$. We could maybe draw some level sets of Q in three dimensions to get an idea of what's going on but we'll only get a part of the picture.

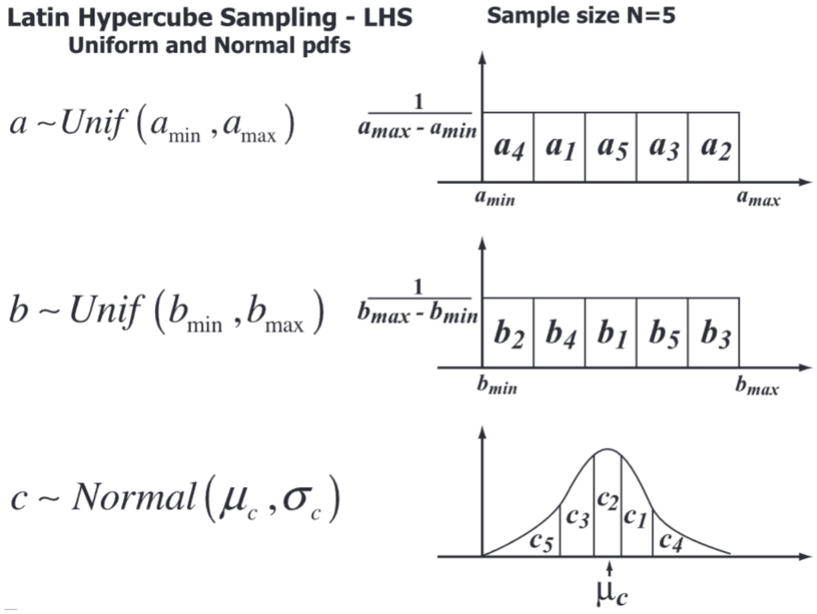
To start a global sensitivity analysis, we have to decide on the parameter space we want to explore. There are two philosophies here: 1) parameters represent real quantities with uncertainty and 2) we should explore the full feasible range of the parameters. In the first case, we specify the distributions for each parameter e.g. $p_1 \sim N(\mu, \sigma^2)$. In the second case, we specify the feasible intervals for each parameter i.e. $m_i \le p_i \le M_i$ for

$i = 1, \dots, n$. While we could try to evaluate Q for all the p_i's through their feasible ranges, this quickly gets memory and time intensive with any meaningful level of resolution beyond, say, 4 inputs. So in practice, we also treat the p_i's as random variables in this case, with $p_i \sim \text{Uniform}\,(m_i, M_i)$. So from now on, think of $P = (p_1, \dots, p_n)$ as a random variable.

Latin Hypercube Sampling. We now need to evaluate our output function across our parameter values. As I said previously, even at relatively low dimensions this becomes a very intensive process. Latin Hypercube Sampling provides a method to systematically explore the entire parameter space in an efficient manner.

Let $p_1, \dots, p_n$ be our parameters. Suppose that we want to collect K samples of each parameter. K should be large so that we get a good cross-section of our parameter values. But if we just take K samples of each parameter, we'll have to calculate the value of Q a total of K^n times. If we have $n = 3$ parameters that we want $K = 1000$ samples of and each evaluation of Q takes 0.001 seconds, this would take ~ 277 hours!

Latin Hypercube Sampling is a method to efficiently explore the "full" parameter space in only nK evaluations (with the example above, this would take only 3 seconds!). How does this work? Here's a picture



For each parameter, divide it's range into K sub-intervals so that each interval has equal probability. For a uniform distribution, this amounts to a simple dividing of the interval. For a normal distribution, notice how the sub-intervals containing higher probability densities are "thinner". Now from each sub-interval, sample one point according to the probability distribution. After this we end up with a set of nK parameter samples $\{p_{i,j}\}$ where $i = 1, \dots, n$ and $j = 1, \dots, K$

Calculating sensitivity. We now have a set $\{p_{i,j}\}$ of inputs which give us the set $\{Q_j\}$ of outputs. We can instead think of these as matrices:

$$X = \begin{bmatrix} p_{11} & \cdots & p_{n1} \\ p_{12} & \cdots & p_{n2} \\ \vdots & \ddots & \cdots \\ p_{1K} & \cdots & p_{nK} \end{bmatrix}, Y = \begin{bmatrix} Q_1 \\ Q_2 \\ \vdots \\ Q_K \end{bmatrix}$$

Now remember, we're thinking of P as a random variable. What are the rows of X? These are simply samples of the random variable P. Q is some function of these random variables and hence is itself a random variable; the rows of Y are samples of Q. Now how do we measure the strength of a relationship between two random variables?

Correlation and partial correlation. With two random variables, an input X and output Y, we measure *correlation*, the strength of the **linear** relationship between these two random variables as

$$c_{XY} = \frac{\operatorname{Cov}(X,Y)}{\sqrt{\operatorname{Var}(X)\operatorname{Var}(Y)}} = \frac{E[XY] - E[X]E[Y]}{\sqrt{E[X^2] - E[X]^2}\sqrt{E[Y^2] - E[Y]^2}}$$

which is also called the *Pearson correlation coefficient.* Using the Cauchy-Schwarz inequality, we know that $-1 \leq c_{XY} \leq 1$. In fact, if $c_{XY} = 1$, then $Y = aX + b$ (similarly if $c_{XY} = -1$, then $Y = -aX + b$). In other words, in this case there is a "perfect" linear relationship between Y and X. If $c_{XY} = 0$, then there is no linear relationship between the random variables. Note that this does **not** mean there is **no** relationship between $Y$and X.

Example. Here's a cute counter-example: let $X \sim N(0,1)$. Then $E[X] = E\left[X^3\right] = 0$. Let $Y = X^2$. Then $\operatorname{Cov}(X,Y) = E[XY] - E[X]E[Y] = E\left[X^3\right] - E[X]E[Y] = 0$. But Y is clearly dependent on X!

But we don't just want to understand the influence of X on Y, we want to know how the parts of X (the p_i's) influence Y. For this, we can calculate *partial correlation coefficients.* Partial correlation characterizes the **linear** relationship between parameter p_i and Q after the linear effects on Q of the remaining parameters are discounted. The partial correlation coefficient between p_i and Q is the correlation coefficient between the two residuals $(p_i - \hat{p_i})$ and $\left(Q - \hat{Q}\right)$ where $\hat{p_i}$ and $\hat{Q}$ are the linear regression models:

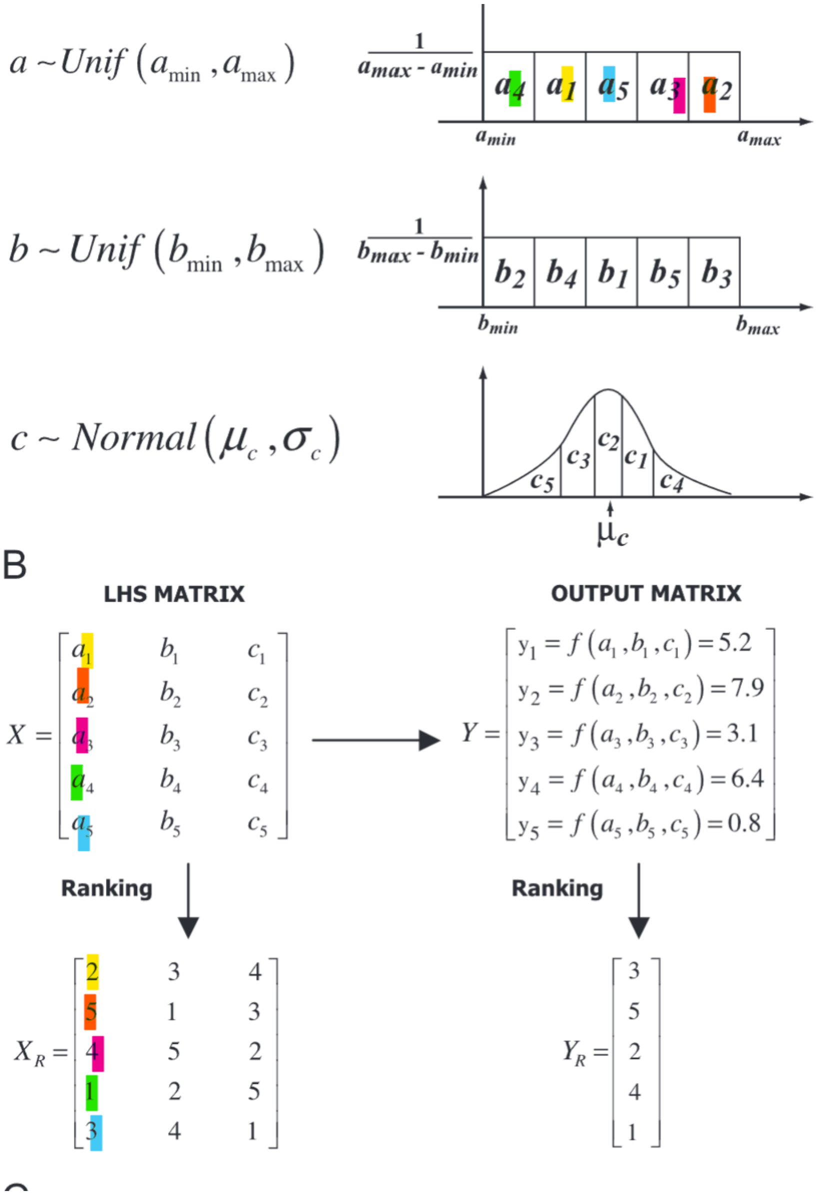
$$\hat{p_i} = c_0 + \sum_{j=1, j\neq i}^{n} c_j p_j$$
$$\hat{Q} = b_0 + \sum_{j=1, j\neq i}^{n} b_j p_j$$

So correlation tells us whether there is a strong, **linear** relationship between our input and output and we can compute it even for individual inputs. But ruling out a linear relationship, there can still be strong correlations (in the general sense) between variables. Consider our example from above: we would want to be able to detect that when X increases, so does Y(when X is positive) because we know what $Y = X^2$ looks like. This sort of relationship is called **monotonic**: when one quantity increases (decreases) when another quantity increases. If we aim more broadly and don't insist on a linear relationship, we can actually learn more.

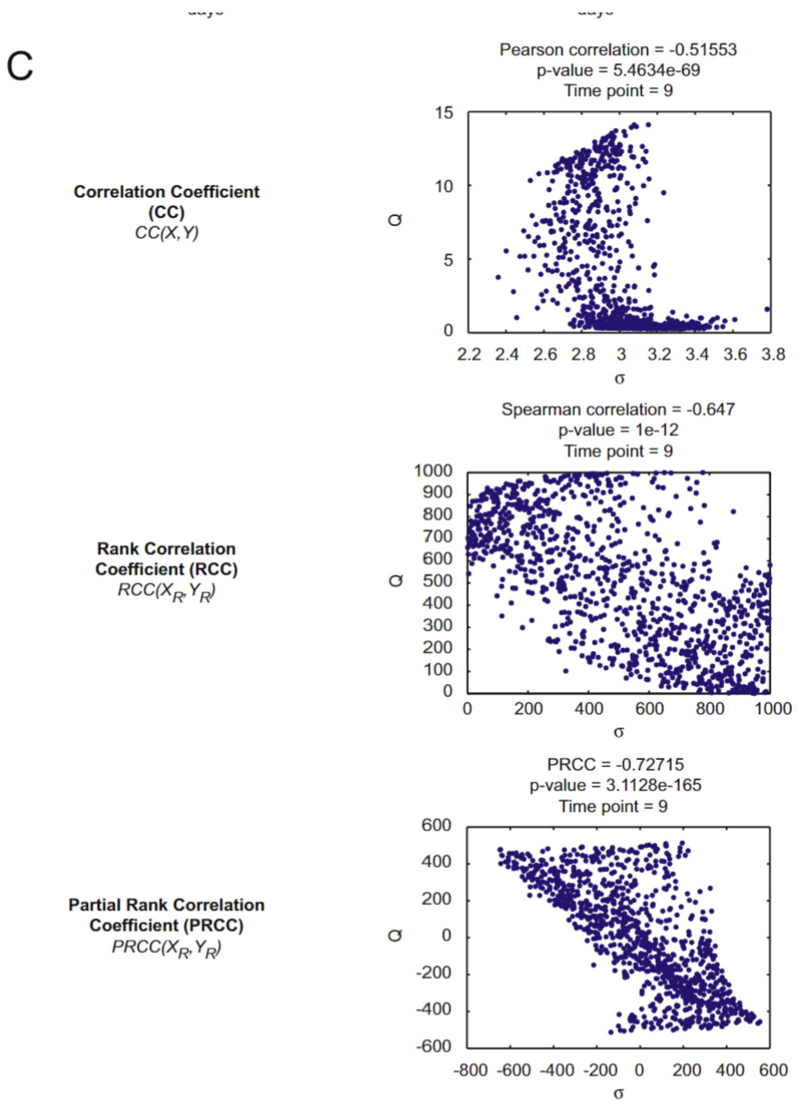
Rank correlation coefficients. Going from "regular" correlation coefficients to rank correlation is pretty simple. All we do is replace the actual values of our input and output samples with their relative "rank" if we sorted them in increasing order. So we might end up with new matrices that look like

$$X_R = \begin{bmatrix} 1 & 7 & 3 \\ 2 & 6 & 4 \\ 12 & 5 & 1 \\ 5 & 4 & 10 \\ \vdots & \ddots & \dots \\ 3 & \dots & 20 \end{bmatrix}, Y_R = \begin{bmatrix} 12 \\ 8 \\ 1 \\ 5 \\ \vdots \\ 2 \end{bmatrix}$$

Note that for X we are doing the sort in each column (remember, column i corresponds to parameter i). We've basically thrown out all the information besides the relative size of quantity. If large values of p_i are associated with large values of Q and small values of p_i with small values of Q, then that is evidence of a monotonic relationship between p_i and Q. Notice how this could detect the relationship between X and $Y = X^2$ in the example above because now we are essentially forcing step sizes between adjacent values of X and Y.


$a \sim Unif(a_{\min}, a_{\max})$
$\frac{1}{a_{max} - a_{min}}$
a_4 a_1 a_5 a_3 a_2
a_{min}
a_{max}
$b \sim Unif(b_{\min}, b_{\max})$
$\frac{1}{b_{max} - b_{min}}$
b_2 b_4 b_1 b_5 b_3
b_{min}
b_{max}
$c \sim Normal(\mu_c, \sigma_c)$
c_5 c_3 c_2 c_1 c_4
μ_c
B
LHS MATRIX
OUTPUT MATRIX
$X = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \\ a_4 & b_4 & c_4 \\ a_5 & b_5 & c_5 \end{bmatrix}$
$Y = \begin{bmatrix} y_1 = f(a_1, b_1, c_1) = 5.2 \\ y_2 = f(a_2, b_2, c_2) = 7.9 \\ y_3 = f(a_3, b_3, c_3) = 3.1 \\ y_4 = f(a_4, b_4, c_4) = 6.4 \\ y_5 = f(a_5, b_5, c_5) = 0.8 \end{bmatrix}$
Ranking
Ranking
$X_R = \begin{bmatrix} 2 & 3 & 4 \\ 5 & 1 & 3 \\ 4 & 5 & 2 \\ 1 & 2 & 5 \\ 3 & 4 & 1 \end{bmatrix}$
$Y_R = \begin{bmatrix} 3 \\ 5 \\ 2 \\ 4 \\ 1 \end{bmatrix}$

Comparing measures of sensitivity.



Only the partial rank correlation coefficients are able to detect a monotonic, decreasing relationship between σ and Q.

Variance-based Sensitivity Analysis

We'll talk more about this later. These are good for finding influential but non-monotonic relationships. For example, Q could be varying strongly with p_i but not in one direction. We'd still characterize p_i as influential but none of the previous methods would be able to detect its influence.

The general idea behind these methods is that variation in parameters results in variation in the output. We want to isolate how much of the variance in the output is due to variation in a given parameter, a process called variance decomposition. These methods return measures of fractional variacne accounted for by individual parameters or groups of parameters. The problem is that when all the parameters are varying, it's very difficult to detect the "signal" in the output from the focal parameter around the "noise" of the variation of the other parameters. One method to overcome this is the so-called extended Fourier amplitude sensitivity test. Essentially, each parameter is assigned a "frequency" at which is oscillates among its range. You can then calculate the variance in the output with respect to each parameter-frequency. If a parameter is particularly influential, we'll see a big spike at its frequency in the variance-frequency plot.

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Let's start from the most general set up. Think of a "model" simply as the description of a relationship between some inputs and some outputs. Let $\vec{y} = (y_1, \ldots, y_m)$ be the set of outputs we're interested in with $\vec{x} = (x_1, \ldots, x_n)$ our inputs. A model can be described as a function from our space of inputs (and some additional stuff) to the space of outputs, $f : X \to Y$. Now if we want to be more sophisticated, we should take into account that our model likely depends on some other parameters we did not or cannot measure, call them $\theta = (\theta_1, \ldots, \theta_k)$ as well as some randomness that we can't git rid of, σ. Then we basically have

$$\vec{y} = f\left(\vec{x}; \theta, \sigma\right)$$

The function f could be derived mechanistically: encapsulating ideas about how we think the entries of $\vec{x}$ affect $\vec{y}$. Or, like with a stastical model, we simply assume that each input has a linear or multiplicative effect on the output. We might even just describe f as the map that takes our measured inputs to our measured outputs (like from a spreadsheet).

If X or Y are low-dimensional and f is a "simple" function, we can just inspect f directly to describe how the entries of $\vec{x}$ affect any of the entries of $\vec{y}$. But generally, models are more complicated; input variables may interact with each other in complex, non-linear ways which can hide their effect on the outputs we're interested in. We to somehow account for variation in all the inputs (not to mention that our parameters θ might be wrong, or we're dealing with noise σ) when evaluating their influence on the outputs.

What is correlation?

Let's say we just have two values, an input X and output Y. Correlation measures the strength of the linear relationship between these two random variables:

$$c_{XY} = \frac{\mathrm{Cov}\left(X, Y\right)}{\sqrt{\mathrm{Var}\left(X\right)\mathrm{Var}\left(Y\right)}}$$

Using the Cauchy-Schwarz inequality, we know that $-1 \leq c_{XY} \leq 1$. In fact, if $c_{XY} = 1$, then $Y = aX + b$ (similarly if $c_{XY} = -1$, then $Y = -aX + b$). In other words, in this case there is a "perfect" linear relationship between Y and X. If $c_{XY} = 0$, then there is no linear relationship between the random variables. Note that this does **not** mean there is **no** relationship between $Y$and X.

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So correlation tells us whether there is a strong **monotonic** relationship between our input and output.