

Research Notes

June 10, 2020

Supply Chain Regression Analysis

Variable definitions:

- I : set of end nodes (pharmacy outlets); $|I| = n$
- J : set of intermediate nodes (suppliers); $|J| = m$
- π_i : Falsification probability for a product obtained from end node $i, i \in I$
- θ_j : Falsification probability for a product obtained from intermediate node $j, j \in J$
- $\mathbf{A} \in \mathbb{R}^{n \times m}$: Transition matrix between intermediate nodes and end nodes; entry (i, j) is the probability that end node i procures from intermediate node j
- \dot{s}, \ddot{s} : Sensitivity and specificity, respectively, of the diagnostic tool used during sampling
- $\hat{\mathbf{q}} \in \mathbb{R}^n$: Vector of observed positive test proportions at each end node

Given a transition matrix, end node sampling results, and diagnostic sensitivity/specificity, what can we say about the falsification probabilities $\boldsymbol{\theta}$ and $\boldsymbol{\pi}$?

We can solve a system of equations to derive an estimate of the intermediate node falsification probabilities, $\hat{\boldsymbol{\theta}}$, using the hat matrix of \mathbf{A} :

$$\hat{\boldsymbol{\theta}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \hat{\mathbf{q}} \quad (1)$$

And then use $\hat{\boldsymbol{\theta}}$ to derive an estimate for $\boldsymbol{\pi}$:

$$\hat{\boldsymbol{\pi}} = \hat{\mathbf{q}} - \mathbf{A} \hat{\boldsymbol{\theta}} \quad (2)$$

However, for any vector of observed positive test proportions, the total system, $(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\pi}})$ is non-determined: for any $\hat{\mathbf{q}}$, there always exists a solution $(\hat{\boldsymbol{\theta}} = \mathbf{0}, \hat{\boldsymbol{\pi}} = \hat{\mathbf{q}})$.

Single-source procurement

Suppose that each end node i only procures from a single intermediate node j , such that I_j denotes the set of end nodes procuring from intermediate node j . Sorting the end nodes according to their intermediate supplier, the transition matrix \mathbf{A} looks as follows:

$$\mathbf{A} = \begin{bmatrix} e_1 \\ \vdots \\ e_2 \\ \vdots \\ \vdots \\ e_m \\ \vdots \\ \vdots \end{bmatrix}$$

Where each e_j is a standard basis vector of 0's with a 1 in the j th position. $\mathbf{A}^T \mathbf{A}$ becomes:

$$\begin{aligned} \mathbf{A}^T \mathbf{A} &= \text{diag}(|I_1|, |I_2|, \dots, |I_m|) \\ (\mathbf{A}^T \mathbf{A})^{-1} &= \text{diag}\left(\frac{1}{|I_1|}, \frac{1}{|I_2|}, \dots, \frac{1}{|I_m|}\right) \end{aligned}$$

$$(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T = \begin{bmatrix} \frac{1}{|I_1|} & \frac{1}{|I_1|} & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \frac{1}{|I_2|} & \frac{1}{|I_2|} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & \frac{1}{|I_m|} & \frac{1}{|I_m|} \end{bmatrix}$$

We observe that the product of the hat matrix and the falsification proportion observations results in an estimate $\hat{\boldsymbol{\theta}}$ that simply averages the observed proportions across the "children" of each intermediate node j .

Adjusted single-source procurement

Now suppose that each end node i procures from a primary intermediate j with probability $(1 - \epsilon)$, and some secondary intermediate with probability ϵ . Let I_{ij} denote the set of end nodes with primary intermediate i and secondary intermediate j . If we retain a sorting similar to that described in the single-source case, $\mathbf{A}^T \mathbf{A}$ becomes a square matrix with $\sum_{k \in I_{ij}, \forall j \in J} (1 - \epsilon)^2 + \sum_{k \in I_{ji}, \forall j \in J} \epsilon^2$ in the i th diagonal entry, and $\sum_{k \in I_{ij}} \epsilon(1 - \epsilon) + \sum_{k \in I_{ji}} \epsilon(1 - \epsilon)$ in the non-diagonal entries at row i , column j .

Balanced supply chain

Suppose further that the supply chain is perfectly balanced and non-decomposable, such that each intermediate node has an identical distribution of children of different procurement probabilities. We consider three scenarios: 1) The $(1 - \epsilon), \epsilon$ case, where each end node procures from a primary intermediate node with probability $(1 - \epsilon)$ and a secondary node with probability ϵ , 2) The $(1 - \epsilon), \frac{\epsilon}{m-1}$ case, where each end node procures from a primary intermediate node with probability $(1 - \epsilon)$ and every other intermediate node with probability $\frac{\epsilon}{m-1}$, and 3) The ρ -decay case, where for a given ρ , each end node procures from the j th-most frequently solicited intermediate node with probability $\frac{\rho^{j-1}}{(1-\rho^m)/(1-\rho)}$.

$(1 - \epsilon), \epsilon$ case

For the $(1 - \epsilon), \epsilon$ case, each intermediate node has $\frac{n}{m} \in \mathbb{Z}$ primary children and $\frac{n}{m(m-1)} \in \mathbb{Z}$ secondary children (so n must be a multiple of $m(m-1)$). Let a denote the i th diagonal entry of $\mathbf{A}^T \mathbf{A}$, where $a = \frac{n}{m}(1 - \epsilon)^2 + \frac{n}{m}\epsilon^2 = \frac{n}{m}(1 - 2\epsilon + 2\epsilon^2)$, and let b denote the (i, j) th non-diagonal of $\mathbf{A}^T \mathbf{A}$, where $b = \frac{2n}{m(m-1)}\epsilon(1 - \epsilon) = \frac{n}{m(m-1)}(2\epsilon - 2\epsilon^2)$.

Consider $(a - b)$, the "preference gap" between an intermediate node's primary children and any group of its secondary children who all possess the same primary preference. Minimizing $(a - b)$ with respect to ϵ yields:

$$a - b = \frac{n}{m}(1 - 2\epsilon + 2\epsilon^2) - \frac{n}{m(m-1)}(2\epsilon - 2\epsilon^2) = \frac{n}{m}[1 - 2(\frac{m}{m-1})\epsilon(1 - \epsilon)] \quad (3)$$

$$\begin{aligned} \frac{d}{d\epsilon}(a - b) &= 0 = \frac{-2}{m-1} - 2 + (\frac{4}{m-1} + 4)\epsilon \\ \epsilon &= \frac{1 + \frac{1}{m-1}}{2 + \frac{2}{m-1}} = \frac{1}{2} \end{aligned}$$

which follows intuition. Importantly, note that when $\epsilon = \frac{1}{2}$:

$$a - b = \frac{n}{m}(1 - \frac{1}{2} \frac{m}{m-1})$$

which implies that $(a - b) \geq 0 \forall m \geq 2$, which again is true for any supply chain we might consider.

To generate the inverse of $\mathbf{A}^T \mathbf{A}$, consider that $\mathbf{A}^T \mathbf{A} = bP + (a - b)I$, where P is an all-ones matrix. It can be shown that the $(\mathbf{A}^T \mathbf{A})^{-1}$ is then $\frac{-b}{(a-b)(bm+a-b)}P + \frac{1}{a-b}I$. The diagonal entries of $(\mathbf{A}^T \mathbf{A})^{-1}$ are then $\frac{m-1-2\epsilon+2\epsilon^2}{n(\frac{m-1}{m}-2\epsilon+2\epsilon^2)}$, and the non-diagonal entries become $\frac{-2\epsilon+2\epsilon^2}{n(\frac{m-1}{m}-2\epsilon+2\epsilon^2)}$.

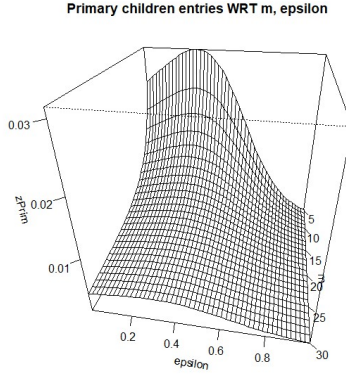


Figure 1: Relative change in entry values of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for primary children of intermediate node j with respect to m and ϵ

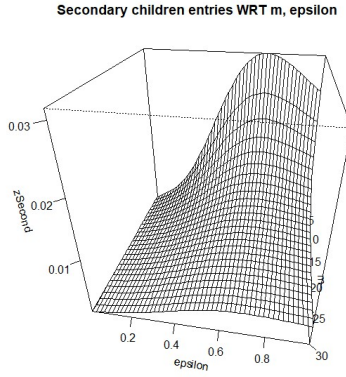


Figure 2: Relative change in entry values of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for secondary children of intermediate node j with respect to m and ϵ

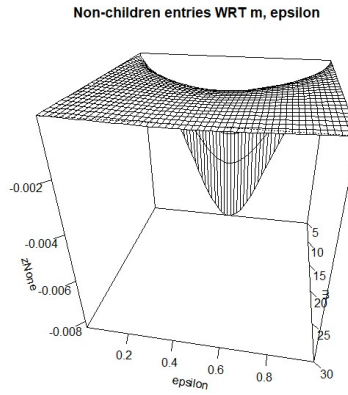


Figure 3: Relative change in entry values of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for non-children of intermediate node j with respect to m and ϵ

The $m \times n$ matrix $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$, then, has three element types, where row i signifies an intermediate node, and column j signifies an end node:

1. j is a **primary** child of i : $\frac{(1-\epsilon)(m-1)-2\epsilon(1-\epsilon)}{n(\frac{m-1}{m}-2\epsilon(1-\epsilon))}$
2. j is a **secondary** child of i : $\frac{\epsilon(m-1)-2\epsilon(1-\epsilon)}{n(\frac{m-1}{m}-2\epsilon(1-\epsilon))}$
3. j is a **no** child of i : $\frac{-2\epsilon(1-\epsilon)}{n(\frac{m-1}{m}-2\epsilon(1-\epsilon))}$

See Figures 1, 2 and 3. As anticipated, we observe that values of ϵ nearer to 0.5 increase the weight in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ given to secondary children. Interestingly, these same ϵ values result in a greater off-setting/negative effect for non-children. This effect translates to a tendency to reduce the $\hat{\theta}_i$ estimate for intermediate node i when the supply chain becomes significantly convoluted. The result is that the $\hat{\theta}$ values tend to equalize with ϵ values near 0.5.

These effects become drastically less pronounced as m , the number of intermediate nodes, increases. However, bearing in mind that we are analyzing a supply chain where each end node receives only 2 preferences, it seems intuitive that increasing the availability of preferences, in conjunction with m , should result in correspondingly more dramatic curves for the elements of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$. Importantly, we note that there exists an overall *interactive* impact of ϵ and m on $\hat{\theta}$.

$(1 - \epsilon), \frac{\epsilon}{m-1}$ case

In the $(1 - \epsilon), \frac{\epsilon}{m-1}$ case, each end node procures from a primary intermediate node with probability $(1 - \epsilon)$ and every other intermediate node with probability $\frac{\epsilon}{m-1}$, where $\epsilon \neq \frac{m-1}{m}$ (details below). Observe that for $\epsilon > \frac{m-1}{m}$, the "primary" intermediate node is then procured from less than all other suppliers. Each intermediate node has $\frac{n}{m} \in \mathbb{Z}$ primary children and $\frac{n}{m}(m-1) \in \mathbb{Z}$ secondary children (so now n need only be a multiple of m).

As with the previous case, letting a denote the i th diagonal entry of $\mathbf{A}^T \mathbf{A}$, with $a = \frac{n}{m}(1 - 2\epsilon + \frac{m}{m-1}\epsilon^2)$, and letting b denote the (i, j) th non-diagonal of $\mathbf{A}^T \mathbf{A}$, with $b = \frac{n}{m(m-1)}[2\epsilon - \frac{m}{(m-1)}\epsilon^2]$, allows the calculation of the entries of $(\mathbf{A}^T \mathbf{A})^{-1}$ as follows:

- **Diagonal:** $\frac{1 - \frac{2}{m-1}\epsilon + \frac{m}{(m-1)^2}\epsilon^2}{\frac{n}{m} \left[1 - \frac{2m}{m-1}\epsilon + \frac{m^2}{(m-1)^2}\epsilon^2 \right]}$
- **Non-Diagonal:** $\frac{\frac{-2}{m-1}\epsilon + \frac{m}{(m-1)^2}\epsilon^2}{\frac{n}{m} \left[1 - \frac{2m}{m-1}\epsilon + \frac{m^2}{(m-1)^2}\epsilon^2 \right]}$

Figures 4 and 5 illustrate these entries. Compare these expressions with those for the $(1 - \epsilon), \epsilon$ case and note they align for $m = 2$: $\frac{m-1-2\epsilon+2\epsilon^2}{n(\frac{m-1}{m}-2\epsilon+2\epsilon^2)}$ and $\frac{-2\epsilon+2\epsilon^2}{n(\frac{m-1}{m}-2\epsilon+2\epsilon^2)}$ for the diagonal and non-diagonal entries, respectively. Additionally, observe that the effect of the non-diagonal entries of $(\mathbf{A}^T \mathbf{A})^{-1}$ diminishes with increasing m , and that the weight of the diagonal entry decreases with increasing ϵ , as we should anticipate. Importantly, $(\mathbf{A}^T \mathbf{A})^{-1}$ is undefined when $1 - \frac{2m}{m-1}\epsilon + \frac{m^2}{(m-1)^2}\epsilon^2 = 0$, i.e., when $\epsilon = \frac{m-1}{m}$. Note that in the case of $\epsilon = \frac{m-1}{m}$, each end node procures from every supplier node with probability $\frac{1}{m}$, indicating a perfectly distributed likelihood across suppliers, and implying that designating the effect of falsification detection at any end node upon a supplier node would assign likelihood evenly across all suppliers. At values near $\epsilon = \frac{m-1}{m}$, we see strongly positive/negative values for diagonal/non-diagonal entries of $(\mathbf{A}^T \mathbf{A})^{-1}$, which suggests much more volatility of $\hat{\theta}$ estimates with respect to detection at end nodes.

In contrast with the $(1 - \epsilon), \epsilon$ case, because every end node procures from every supplier, the $m \times n$ matrix $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ only has two element types for row i and column j , corresponding to supplier i and end node j , as follows:

- j is a primary child of i : $\frac{(1-\epsilon) - \frac{2\epsilon}{m-1} + \frac{m\epsilon^2}{(m-1)^2}}{\frac{n}{m} \left[1 - \frac{2m\epsilon}{m-1} + \frac{m^2\epsilon^2}{(m-1)^2} \right]}$

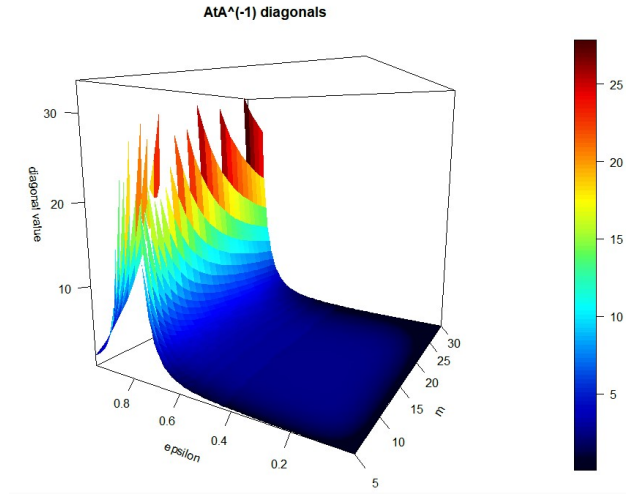


Figure 4: Relative change in diagonal values of $(\mathbf{A}^T \mathbf{A})^{-1}$ with respect to m and ϵ for the $(1 - \epsilon), \frac{\epsilon}{m-1}$ case

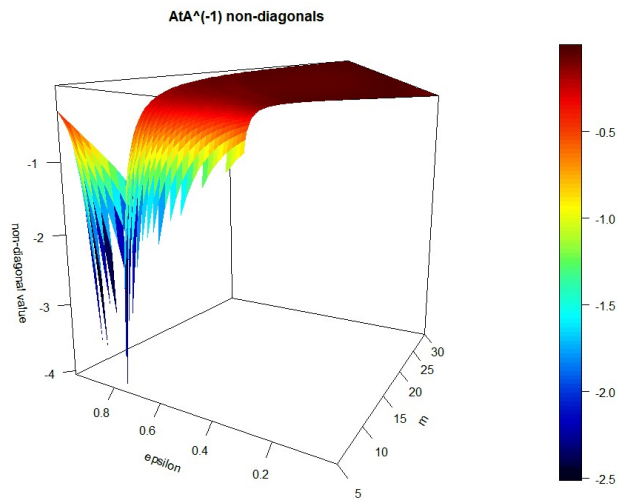


Figure 5: Relative change in non-diagonal values of $(\mathbf{A}^T \mathbf{A})^{-1}$ with respect to m and ϵ for the $(1 - \epsilon), \frac{\epsilon}{m-1}$ case

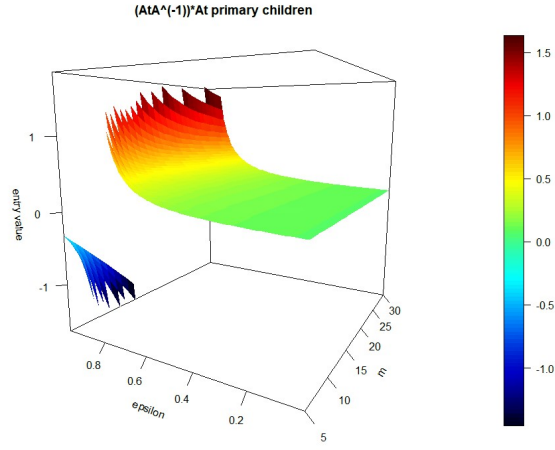


Figure 6: Relative change in primary children values of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ with respect to m and ϵ for the $(1 - \epsilon), \frac{\epsilon}{m-1}$ case

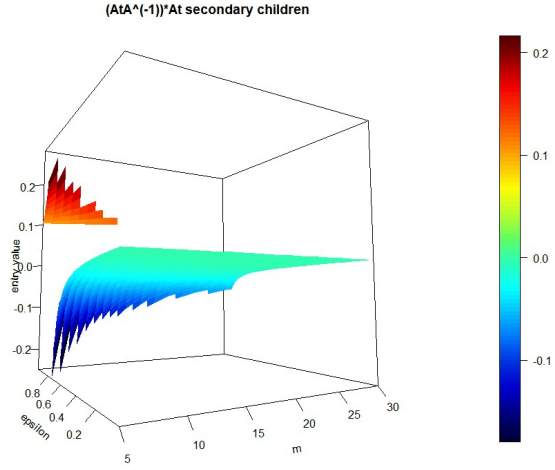


Figure 7: Relative change in secondary children values of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ with respect to m and ϵ for the $(1 - \epsilon), \frac{\epsilon}{m-1}$ case

- j is a secondary child of i :
$$\frac{-\epsilon}{m-1} + \frac{m\epsilon^2}{(m-1)^2} \frac{n_i}{m} [1 - \frac{2m\epsilon}{m-1} + \frac{m^2\epsilon^2}{(m-1)^2}]$$

Figures 6 and 7 illustrate these entries of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$. As one might anticipate, more balanced distributions of procurement likelihood across intermediate nodes translates to much more volatility in computing $\hat{\theta}$ estimates. Under these ϵ conditions, $\hat{\theta}$ is subject to significant adjustments upon the detection of falsification at any end node.

ρ -decay case

In the ρ -decay case, for a given ρ each end node procures from the j th-most frequently solicited intermediate node with probability $\rho^{j-1} \frac{1-\rho}{1-\rho^m}$. Low ρ values correspond with strong preferences for few suppliers, while high ρ values correspond with more even procurement distributions.

To construct the \mathbf{A} matrix, note that each row corresponding to an end node i is a permutation γ_i of the row $\frac{1-\rho}{1-\rho^m} [\rho^0 \ \rho^1 \ \dots \ \rho^{m-1}]$. Since we have n rows each summing to 1, each column of \mathbf{A} must sum to $\frac{n}{m}$. Combinatorially, there are many ways to construct such a matrix (on the order of $O((n!)^m)$). We consider matrices where $n = m(m-1)$, so that \mathbf{A} consists of blocks of $\frac{n}{m}$ rows, where each block consists of a column of ρ^0 entries and $(m-1)$ columns of a doubly-stochastic permutation matrix of size $(m-1) \times (m-1)$. For the entries of $\mathbf{A}^T \mathbf{A}$ to be balanced, it must be the case that there are $\frac{n}{m}$ of each $\rho^k, k \in \{0, 1, \dots, m-1\}$ in each column of \mathbf{A} . \mathbf{A} appears as follows:

$$\mathbf{A} = \frac{1-\rho}{1-\rho^m} \begin{bmatrix} \rho^0 & \rho^1 & \dots & \rho^{m-2} & \rho^{m-1} \\ \rho^0 & \rho^2 & \dots & \rho^{m-1} & \rho^1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho^0 & \rho^{m-1} & \dots & \rho^1 & \rho^{m-2} \\ \\ \rho^1 & \rho^0 & \dots & \rho^{m-2} & \rho^{m-1} \\ \rho^2 & \rho^0 & \dots & \rho^{m-1} & \rho^1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho^{m-1} & \rho^0 & \dots & \rho^1 & \rho^{m-2} \\ \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \\ \rho^{m-1} & \rho^{m-2} & \dots & \rho^1 & \rho^0 \\ \rho^1 & \rho^{m-1} & \dots & \rho^2 & \rho^0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho^{m-2} & \rho^1 & \dots & \rho^{m-1} & \rho^0 \end{bmatrix}$$

With this structure, any two columns of \mathbf{A} are aligned such that, pairwise, there exists two of each pair $\rho^i, \rho^j, \forall i \neq j$. The resulting entries of $\mathbf{A}^T \mathbf{A}$ are as follows:

- **Diagonal:** $\frac{(1-\rho)^2}{(1-\rho^m)^2} \cdot \frac{n}{m} \sum_{j=0}^{m-1} \rho^{2j}$
- **Non-Diagonal:** $\frac{(1-\rho)^2}{(1-\rho^m)^2} \cdot 2 \sum_{\substack{i < j \\ i, j \in \{0, 1, \dots, m-1\}}} \rho^i \rho^j$

Denote $S_1 = \sum_{j=0}^{m-1} \rho^{2j}$ and $S_2 = 2 \sum_{\substack{i < j \\ i, j \in \{0, 1, \dots, m-1\}}} \rho^i \rho^j$. Figures 8 and 9 depict these summations with

respect to m and ρ . Note that both S_1 and S_2 increase approximately linearly in m and exponentially in ρ . Following the ideas of the previous cases yields the following for the entries of $(\mathbf{A}^T \mathbf{A})^{-1}$, illustrated in Figures 10 and 11:

- **Diagonal:** $\frac{(m-2)S_2 + \frac{n}{m}S_1}{(\frac{n}{m})^2(S_1)^2 + \frac{n(m-2)}{m}(S_1)(S_2) - (m-1)(S_2)^2} \cdot \frac{(1-\rho^m)^2}{(1-\rho)^2}$
- **Non-Diagonal:** $\frac{-S_2}{(\frac{n}{m})^2(S_1)^2 + \frac{n(m-2)}{m}(S_1)(S_2) - (m-1)(S_2)^2} \cdot \frac{(1-\rho^m)^2}{(1-\rho)^2}$

We can take advantage of the fact that $n = m(m-1)$ to simplify these entries for $(\mathbf{A}^T \mathbf{A})^{-1}$:

- **Diagonal:** $\frac{\frac{m-2}{m-1}S_2 + S_1}{[(m-1)S_1 - S_2][S_1 + S_2]} \cdot \frac{(1-\rho^m)^2}{(1-\rho)^2}$

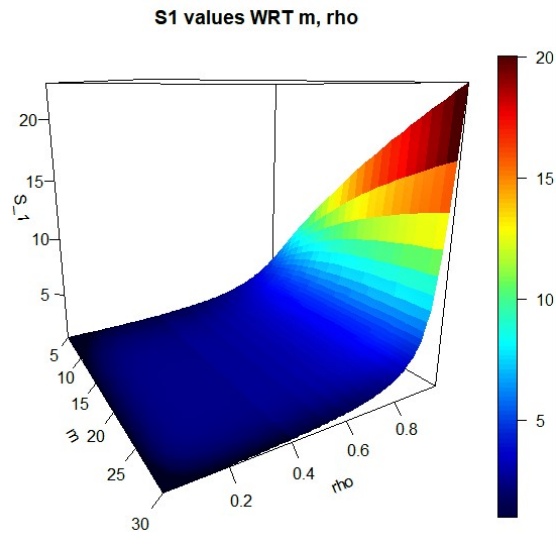


Figure 8: Relative change in S_1 values with respect to m and ρ

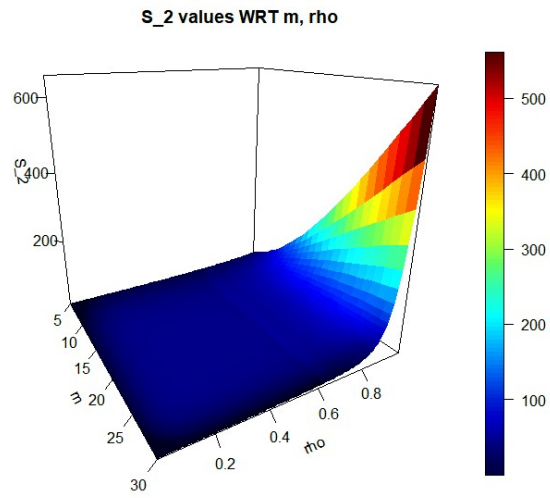


Figure 9: Relative change in S_1 values with respect to m and ρ

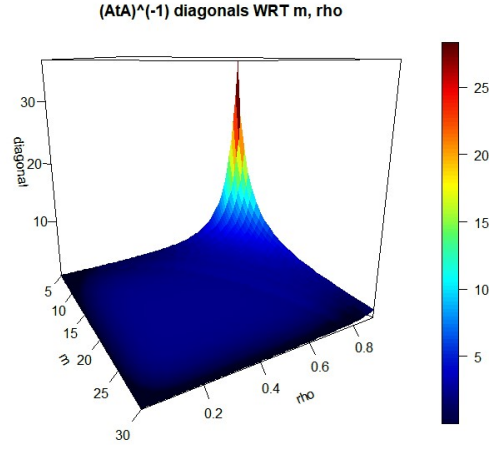


Figure 10: Relative change in diagonals of $(\mathbf{A}^T \mathbf{A})^{-1}$ with respect to m and ρ

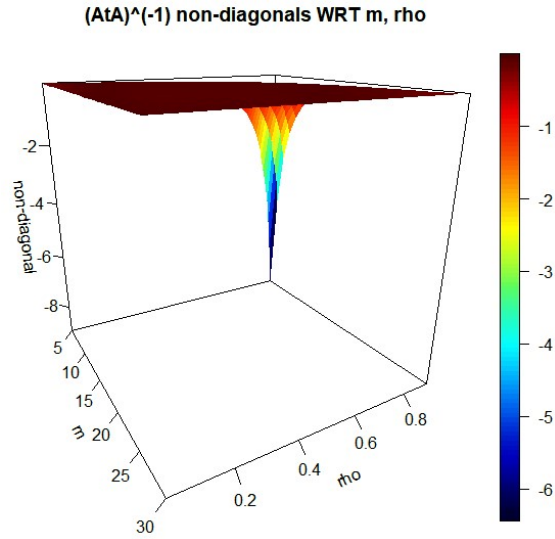


Figure 11: Relative change in non-diagonals of $(\mathbf{A}^T \mathbf{A})^{-1}$ with respect to m and ρ

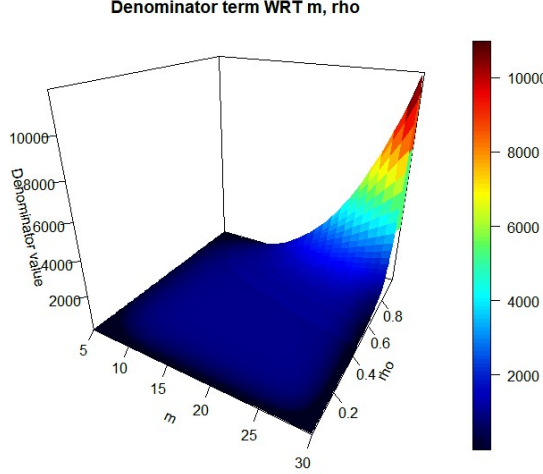


Figure 12: Relative change in denominator term of $(\mathbf{A}^T \mathbf{A})^{-1}$ with respect to m and ρ

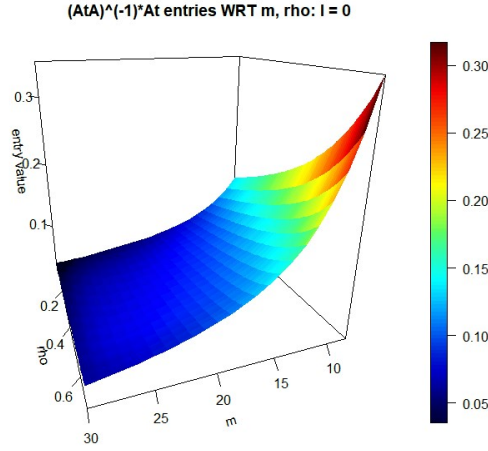


Figure 13: Relative change in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for a 1st child with respect to m and ρ

- **Non-Diagonal:** $\frac{\frac{-S_2}{m-1}}{[(m-1)S_1 - S_2][S_1 + S_2]} \cdot \frac{(1-\rho^m)^2}{(1-\rho)^2}$

Figure 12 depicts the denominator term of the $(\mathbf{A}^T \mathbf{A})^{-1}$ entries. Observe that this term is never less than 0.

We then have m types of entries for $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$, where row i corresponds to a supplier node and column j corresponds to an end node. Somewhat differently than the $1 - \epsilon$, ϵ and $1 - \epsilon$, $\frac{\epsilon}{m-1}$ cases, the $(l+1)$ th child of a supplier node refers to an end node with procurement likelihood $\rho^l \frac{1-\rho}{1-\rho^m}$, $\forall l \in \{0, 1, \dots, m-1\}$. For supplier i , an $(l+1)$ th child j has a corresponding entry in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ as follows:

$$\frac{\rho^l \frac{1-\rho}{1-\rho^m} (S_1 + S_2) - \frac{S_2}{m-1}}{[(m-1)S_1 - S_2][S_1 + S_2]} \cdot \left(\frac{1-\rho^m}{1-\rho} \right)^2 \quad (4)$$

Figures 13, 14, 15, 16 and 17 depict how these entries change with respect to m and ρ for $l \in \{0, 1, 2, 3, m\}$. Note that for many combinations of m and ρ , the projection matrix terms are negative for $l \geq 2$. From 4, the projection matrix terms are negative whenever $\rho^l < \frac{S_2 \frac{1-\rho^m}{1-\rho}}{(m-1)(S_1 + S_2)}$.

Additionally, note in the projection matrix figures that the ranges of m and ρ are restricted in order to depict the interesting regions of the space. For large values of ρ , the entries of $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ are generally

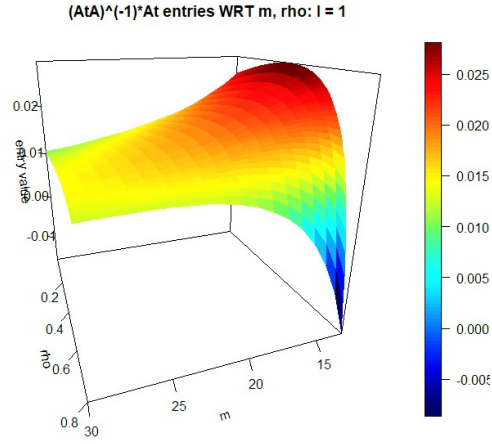


Figure 14: Relative change in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for a 2nd child with respect to m and ρ

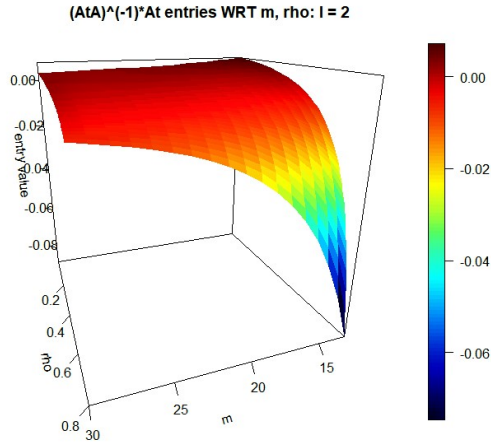


Figure 15: Relative change in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for a 3rd child with respect to m and ρ

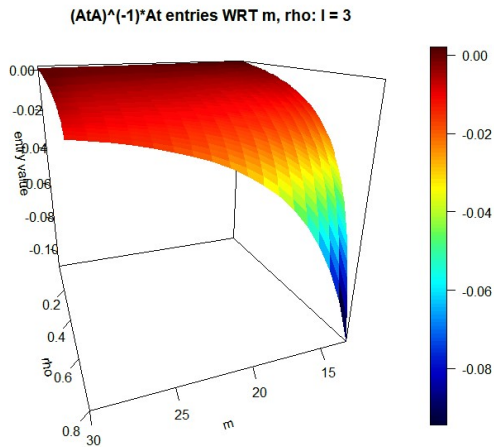


Figure 16: Relative change in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for a 4th child with respect to m and ρ

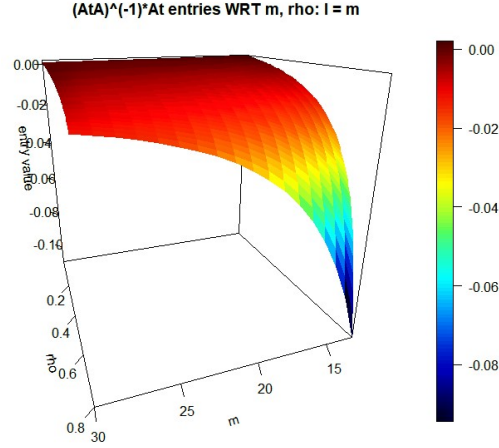


Figure 17: Relative change in $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$ for a m th child with respect to m and ρ

very negative or very positive. As with the $(1 - \epsilon)$, $\frac{\epsilon}{m-1}$ case, highly distributed procurement likelihoods can cause very high variability in $\hat{\boldsymbol{\theta}}$ estimates as falsification samples are detected.

Unbalanced supply chain

Note that $\mathbf{A}^T \mathbf{A}$ can be formed iteratively by the following process. Initialize $\alpha \leftarrow u_1 \otimes u_1$, where $u_1 = (1 - \epsilon)e_i + \epsilon e_j$, with i and j denoting the primary and secondary intermediate nodes for the first end node under consideration. A $(1 - \epsilon)^2$ term is added to the i th diagonal, a ϵ^2 term is added to the j th diagonal, and $\epsilon(1 - \epsilon)$ terms are added to the (i, j) th and (j, i) th locations of α . Form u_2 similarly, and set $\alpha \leftarrow \alpha + (u_2 \otimes u_2)$. Iterating through all $k \in I$, the resulting α is then $\mathbf{A}^T \mathbf{A}$.

DOESN'T WORK - A NEEDS TO BE INVERTIBLE AT EVERY STEP

Try initializing $\alpha = I$ ("dummy" end node children) and removing the children at the end (how to adjust at the end?). After one step, where $u_1 = (1 - \epsilon)e_{i_1} + \epsilon e_{j_1}$, we get:

$$\alpha_1 \leftarrow I + u_1 \otimes u_1 = \begin{bmatrix} 1 & 0 & \dots & 0 & \dots & 0 & \dots \\ 0 & 1 & \dots & 0 & \dots & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 + (1 - \epsilon)^2 & \dots & \epsilon(1 - \epsilon) & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \epsilon(1 - \epsilon) & \dots & 1 + \epsilon^2 & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 & 1 \end{bmatrix}$$

Using Sherman-Morrison to find the inverse gives us:

$$\alpha_1^{-1} = \begin{bmatrix} 1 & 0 & \dots & 0 & \dots & 0 & \dots \\ 0 & 1 & \dots & 0 & \dots & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 - \frac{(1 - \epsilon)^2}{2 - 2\epsilon + 2\epsilon^2} & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots & 1 - \frac{\epsilon^2}{2 - 2\epsilon + 2\epsilon^2} & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 & 1 \end{bmatrix}$$

For α_2 , we have **7 potential cases** [A lot of algebra involved for the other cases, does it make sense to follow them all?], depending on whether $i_2, j_2 \in \{i_1, j_1, J \setminus \{i_1, j_1\}\}$.

- **Case 1:** The simplest case is when $i_2, j_2 \in \{J \setminus \{i_1, j_1\}\}$, where only the $\{i_2, j_2\}$ indices change:

$$\alpha_2^{-1} = \begin{bmatrix} 1 & 0 & \dots & \overset{i_1}{0} & \dots & \overset{j_1}{0} & \dots & \overset{i_2}{0} & \dots & \overset{j_2}{0} & \dots & 0 \\ 0 & 1 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \overset{i_1}{0} & 0 & \dots & 1 - \frac{(1 - \epsilon)^2}{2 - 2\epsilon + 2\epsilon^2} & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \overset{j_1}{0} & 0 & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots & 1 - \frac{\epsilon^2}{2 - 2\epsilon + 2\epsilon^2} & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \overset{i_2}{0} & 0 & \dots & 0 & \dots & 0 & \dots & 1 - \frac{(1 - \epsilon)^2}{2 - 2\epsilon + 2\epsilon^2} & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \overset{j_2}{0} & 0 & \dots & 0 & \dots & 0 & \dots & \frac{-\epsilon(1 - \epsilon)}{2 - 2\epsilon + 2\epsilon^2} & \dots & 1 - \frac{\epsilon^2}{2 - 2\epsilon + 2\epsilon^2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix}$$

Note that the update terms have limited ranges, as $\epsilon \in (0, 1)$.

Formulas to play with:

Woodbury:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Sherman-Morrison:

$$(A + uu^T)^{-1} = A^{-1} - \frac{A^{-1}uu^T A^{-1}}{1 + u^T A^{-1}u}$$

ANOVA

First we consider the variance of the observation vector, $\hat{\mathbf{q}}$. Each element \hat{q}_i is the result of a binomial trial with t_i samples, a probability q_i of a positive test, and an underlying probability π_i of a falsified sample, where π_i is sampled from some distribution $\Pi(\cdot)$, $\forall i \in I$, with mean μ_Π and variance σ_Π^2 . Taking into account the diagnostic sensitivity and specificity, where \dot{s} denotes the sensitivity (bounded below by 0.5) and \ddot{s} denotes 1 less the specificity (bounded above by 0.5), we calculate q_i as:

$$q_i = \dot{s}\pi_i + \ddot{s}(1 - \pi_i) = \ddot{s} + \pi_i(\dot{s} - \ddot{s})$$

The variance of each observed \hat{q}_i is then:

$$\begin{aligned} \mathbb{V}[\hat{q}_i | \boldsymbol{\pi} \in \Pi] &= \frac{q_i(1 - q_i)}{t_i} = \frac{2\pi_i^2 \dot{s}\ddot{s} + \dot{s}\pi_i + 2\ddot{s}^2\pi_i - \dot{s}\pi_i^2 - \ddot{s}\pi_i^2 - 2\dot{s}\ddot{s}\pi_i - \ddot{s}\pi_i - \ddot{s}^2 + \ddot{s}}{t_i} \\ &= \frac{\ddot{s}(1 - \ddot{s}) + 2\dot{s}\ddot{s}\pi_i(\pi_i - 1) + \dot{s}\pi_i(1 - \pi_i) + 2\ddot{s}^2\pi_i - \ddot{s}\pi_i(\pi_i - 1)}{t_i} \end{aligned}$$

With perfect specificity ($\ddot{s} = 0$), we obtain:

$$\mathbb{V}[\hat{q}_i | \boldsymbol{\pi} \in \Pi] = \frac{\dot{s}\pi_i(1 - \pi_i)}{t_i}$$

With perfect sensitivity ($\dot{s} = 1$), we obtain:

$$\mathbb{V}[\hat{q}_i | \boldsymbol{\pi} \in \Pi] = \frac{\ddot{s}(1 - \ddot{s}) + \pi_i(1 - \pi_i)(1 - \ddot{s}) + 2\ddot{s}^2\pi_i}{t_i}$$

The variance of $\hat{\boldsymbol{\theta}}$ then becomes, from Equation 1:

$$\mathbb{V}[\hat{\boldsymbol{\theta}} | \hat{\mathbf{q}}] = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \Sigma(\hat{\mathbf{q}}) ((\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T)^T$$

The mean square error (MSE) term:

$$MSE_{\hat{\mathbf{q}}} = \frac{\|\hat{\boldsymbol{\pi}}\|^2}{n - (m + 1)} = \frac{\|\hat{\mathbf{q}} - \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \hat{\mathbf{q}}\|^2}{n - (m + 1)}$$

being an unbiased estimator of $\mathbb{V}[\mathbf{q}] = \mathbb{V}[\ddot{s} + \boldsymbol{\pi}(\dot{s} - \ddot{s})] = (\dot{s} - \ddot{s})^2 \sigma_\Pi^2$, and where $\frac{(n - (m + 1)) MSE_{\hat{\mathbf{q}}}}{(\dot{s} - \ddot{s})^2 \sigma_\Pi^2}$ follows a χ^2 distribution with $n - (m + 1)$ degrees of freedom.

In the case of single-source procurement, the resulting variance matrix for $\hat{\boldsymbol{\theta}}$ becomes:

$$\mathbb{V}[\hat{\boldsymbol{\theta}}] = \begin{bmatrix} \frac{1}{|I_1|^2} \sum_{i \in I_1} \mathbb{V}[\hat{q}_i] & 0 & \dots & 0 \\ 0 & \frac{1}{|I_2|^2} \sum_{i \in I_2} \mathbb{V}[\hat{q}_i] & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{|I_m|^2} \sum_{i \in I_m} \mathbb{V}[\hat{q}_i] \end{bmatrix}$$

Questions & Thoughts

- Add weights to observations by number of data points collected (Q matrix we discussed previously)?
- How closely does the simulation model verify align with these calculations?
- Is there an impact of variable market shares for different importers? $|I_1| \geq |I_2| \geq \dots \geq |I_m|$
- Correct that the process of forming $\mathbf{A}^T \mathbf{A}$ for adjusted single-source procurement above can be generalized for general distribution vector \mathbf{u} ?

Future Research Ideas

- Expanding to three-tier supply chains, so large countries and global suppliers might be included? Might be implications for value in cross-country coordination and data-sharing
- How might these models affect the choice of detection device investment?
- What are the implications for decisions of which region and/or specific outlets to sample from? (Potentially the most direct implications from this analysis)
- What types of statistics + hypothesis testing can be conducted under different supply chains and test results?