Notes

SCK team

1 Notation

- Average emission per source: $x_1, \dots, x_m$ where $m = 200$.
- Measured concentrations $y_1, \dots, y_n$ where $n = 4636$. These are consecutive measurements for several measurement stations.
- $M_{i,(j,\Delta)}$ is a block in the sensitivity matrix M that represents the contribution of x_j from $\Delta - 1$ days ago to the observed concentration y_i.
- Scaling factors $s_1, \dots, s_m$ (in `scalings.csv`). These are put in a diagonal matrix S.
- $\mathbf{1}_q = [1 \ \dots \ 1]^T \in \mathbb{R}^q$ is the constant vector consisting of only ones.
- $\otimes$ is the Kronecker product. In particular,

$$\underbrace{\begin{bmatrix} a_1 \\ \vdots \\ a_p \end{bmatrix}}_{\in \mathbb{R}^p} \otimes \underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{\in \mathbb{R}^q} = \underbrace{\begin{bmatrix} a_1 \\ \vdots \\ a_1 \\ a_2 \\ \vdots \\ a_2 \\ \vdots \\ a_p \end{bmatrix}}_{\in \mathbb{R}^{pq}}.$$

2 Model

With $n = 1, \dots, 4636$ and $m = 1, \dots, 200$, the initial model is

$$y_i \approx \hat{y}_i = \sum_{j=1}^{m} \sum_{\Delta=1}^{15} M_{i,(j,\Delta)} \frac{x_j}{s_j}.$$

That is, for each emission source j, we simulate the contribution of 15 days, and add this together for all j. A matrix formulation of this reads

$$\begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \begin{bmatrix} M_{1,(1,1)} & M_{1,(1,2)} & \cdots & M_{1,(n,15)} \\ \vdots & \vdots & & \vdots \\ M_{m,(1,1)} & M_{m,(1,2)} & \cdots & M_{m,(n,15)} \end{bmatrix} \begin{bmatrix} s_1^{-1} x_1 \\ \vdots \\ s_1^{-1} x_1 \\ s_2^{-1} x_2 \\ \vdots \\ s_n^{-1} x_n \end{bmatrix}$$

$$= \begin{bmatrix} M_{1,(1,1)} & M_{1,(1,2)} & \cdots & M_{1,(n,15)} \\ \vdots & \vdots & & \vdots \\ M_{m,(1,1)} & M_{m,(1,2)} & \cdots & M_{m,(n,15)} \end{bmatrix} \left(\begin{bmatrix} s_1 & & \\ & \ddots & \\ & & s_n \end{bmatrix}^{-1} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \otimes \mathbf{1}_{15} \right)$$

where s_i are the scalings.

Now we present a different interpretation. Instead of $S^{-1}x \otimes \mathbf{1}_{15}$, we make a vector $\tilde{x} := S^{-1}x \otimes \mathbf{1}_{365}$. This is a vector of length 365×200 that gives the emission from day 1 to day 365 for each source. This is assumed to be constant for all days. Therefore, $\tilde{x}$ consists of $m = 200$ blocks, each of which is constant.

With this formulation, the predicted concentration in station y_i is

$$\hat{y}_i = \begin{bmatrix} \cdots & M_{1,(1,1)} & \ldots & M_{1,(1,15)} & 0 & \ldots & M_{1,(2,1)} & \ldots & M_{1,(2,15)} & \ldots \end{bmatrix} (S^{-1}x \otimes \mathbf{1}_{365}).$$

Now assume that in each station, there is one observation per day, named y_{kt}, where $k = 1, \ldots, K$ where K is the number of stations and $t = 1, \ldots, 365$. The index $t = 1$ corresponds to the most recent measurement. Then

$$\begin{bmatrix} \hat{y}_{1,1} \\ \hat{y}_{1,2} \\ \vdots \\ \hat{y}_{2,1} \\ \vdots \\ \hat{y}_{K,365} \end{bmatrix} = \underbrace{\begin{bmatrix} M_{(1,1),(1,1)} & M_{(1,1),(1,2)} & \cdots & M_{(1,1),(1,15)} & 0 & \cdots & \cdots & M_{(1,1),(2,1)} & \cdots & 0 \\ 0 & M_{(1,2),(1,1)} & \cdots & M_{(1,2),(1,14)} & M_{(1,2),(1,15)} & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & & \vdots \\ M_{(2,1),(1,1)} & M_{(2,1),(1,2)} & \cdots & M_{(2,1),(1,15)} & 0 & \cdots & \cdots & M_{(2,1),(2,1)} & \cdots & 0 \\ \vdots & & & & & & & & & \\ \vdots & & & & & & & & & \end{bmatrix}}_{:= M_{shift}} \tilde{x}$$

where

$$\tilde{x} := S^{-1}x \otimes \mathbf{1}_{365} = \begin{bmatrix} s_1^{-1}x_1 \\ \vdots \\ s_1^{-1}x_1 \\ s_2^{-1}x_2 \\ \vdots \\ s_m^{-1}x_m \end{bmatrix}.$$

If we weigh each day and each emission source by some factor, we get

$$\hat{y} = M_{shift} W (S^{-1}x \otimes \mathbf{1}_{365})$$

where W is a diagonal matrix containing the weights. If W is what we should be looking for, then we can use well-known numerical techniques for solving linear matrix equations. For theoretical purposes, we describe the problem as a large linear system involving Kronecker products. Writing $W = \operatorname{diag}(w)$ for some vector w, the above can be reformulated as a liner operation applied to w as follows:

$$\hat{y} = ((S^{-1}x \otimes \mathbf{1}_{365})^T \otimes M_{shift}) \operatorname{vec}(\operatorname{diag} w)$$

where $\operatorname{vec} \circ \operatorname{diag}$ is a constant linear map that can be inferred from the dimensions of the problem.