Here's Some Math

Brynnydd Hamilton, Jake Gebbie

January 11, 2023

1 Single model "textbook" solution, no prior

This math follows Section 1.3.4. in Dynamical Insights from Data, and derives the equation behind the "solve_textbook" method in BLUEs.jl. We seek to solve the system

$$\mathbf{y} = \mathbf{E}\mathbf{x} \tag{1}$$

where \mathbf{y} is some vector of observations, \mathbf{x} is some vector of parameters and \mathbf{E} is a model matrix that relates the two. Our observations \mathbf{y} has some associated noise covariance matrix $\mathbf{C_{nn}}$ Here we solve an overdetermined problem, so length(\mathbf{y}) < length(\mathbf{x}), and \mathbf{E} has more rows than columns. We define a residual \mathbf{n}

$$\mathbf{n} = \mathbf{y} - \mathbf{E}\mathbf{x} \tag{2}$$

We seek to minimize a cost function defined by the weighted inner product of the residual

$$J = \mathbf{n}^{\mathbf{T}} \mathbf{C}_{\mathbf{n}\mathbf{n}}^{-1} \mathbf{n} = (\mathbf{y} - \mathbf{E}\mathbf{x})^{\mathbf{T}} \mathbf{C}_{\mathbf{n}\mathbf{n}}^{-1} (\mathbf{y} - \mathbf{E}\mathbf{x})$$
(3)

To minimize it, we want to minimize J with respect to \mathbf{x} . To accomplish this, we take the first partial derivative $\frac{\partial J}{\partial \mathbf{x}}$, set it equal to 0, and solve for our solution estimate $\tilde{\mathbf{x}}$

$$\frac{\partial J}{\partial \mathbf{x}} = \frac{\partial \mathbf{n}}{\partial \mathbf{x}} \frac{\partial J}{\partial \mathbf{n}} \tag{4}$$

$$\frac{\partial J}{\partial \mathbf{n}} = (\mathbf{C_{nn}}^{-1} + \mathbf{C_{nn}}^{-T})\mathbf{n} = 2\mathbf{C_{nn}}^{-1}\mathbf{n}$$
 (5)

$$\frac{\partial \mathbf{n}}{\partial \mathbf{x}} = -\mathbf{E}^T \tag{6}$$

$$\frac{\partial J}{\partial \mathbf{x}} = \frac{\partial \mathbf{n}}{\partial \mathbf{x}} \frac{\partial J}{\partial \mathbf{n}} = -2\mathbf{E}^T \mathbf{C_{nn}}^{-1} \mathbf{n} = -2\mathbf{E}^T \mathbf{C_{nn}}^{-1} (\mathbf{y} - \mathbf{E}\mathbf{x}) = -2\mathbf{E}^T \mathbf{C_{nn}}^{-1} \mathbf{y} + 2\mathbf{E}^T \mathbf{C_{nn}}^{-1} \mathbf{E}\mathbf{x}$$
(7)

We then set the above equation equal to zero, and now solve for the solution estimate $\tilde{\mathbf{x}}$

$$-2\mathbf{E}^{T}\mathbf{C_{nn}}^{-1}\mathbf{y} + 2\mathbf{E}^{T}\mathbf{C_{nn}}^{-1}\mathbf{E}\tilde{\mathbf{x}} = 0$$
(8)

$$\tilde{\mathbf{x}} = (\mathbf{E}^T \mathbf{C_{nn}}^{-1} \mathbf{E})^{-1} (\mathbf{E}^T \mathbf{C_{nn}}^{-1} \mathbf{y})$$
(9)

2 Multiple model "textbook" solution, no prior

For our eventual application, we will have multiple, disparate observational vectors $\mathbf{y_i}$, that each have their own associated noise covariance matrix $\mathbf{C_{nn}}_{(i)}$, as well as their own model matrix \mathbf{E}_i . However, they will all be associated with the same parameter vector \mathbf{x} . Therefore, we are solving the simultaneous system

$$\mathbf{y}_i = \mathbf{E}_i \mathbf{x} \tag{10}$$

For each observational vector, we can define a corresponding noise vector

$$\mathbf{n}_i = \mathbf{y_i} - \mathbf{E}_i \mathbf{x} \tag{11}$$

Each system will have its own cost function, and we want to minimize all of them simultaneously, so we will minimize the sum of the cost functions

$$J = \sum_{i}^{N} \mathbf{n}_{i}^{T} \mathbf{C}_{\mathbf{nn}(i)} \mathbf{n}_{i}$$
(12)

As this is a simple sum, the math will remain relatively similar to Equations 4 - 7, with the new version of Equation 7 as follows

$$\frac{\partial J}{\partial \mathbf{x}} = \sum_{i}^{N} -2\mathbf{E}_{i}^{T} \mathbf{C_{nn}}_{(i)}^{-1} \mathbf{y}_{i} + 2\mathbf{E}_{i}^{T} \mathbf{C_{nn}}_{(i)}^{-1} \mathbf{E}_{i} \mathbf{x}$$
(13)

If we set Equation 13 equal to 0, and solve for $\tilde{\mathbf{x}}$, we would have to calculate

$$\tilde{\mathbf{x}} = \left(\sum_{i}^{N} \mathbf{E}_{i}^{T} \mathbf{C}_{\mathbf{nn}(i)}^{-1} \mathbf{E}_{i}\right)^{-1} \left(\sum_{i}^{N} \mathbf{E}_{i}^{T} \mathbf{C}_{\mathbf{nn}(i)}^{-1} \mathbf{y}_{i}\right)$$
(14)