Model misspecification and bias in the least-squares algorithm: Connecting Omitted Variable Bias to AVO three-term projections

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Abstract

These are some additional notes to be read in conjunction with my September 2021 TLE paper [2] on model misspecification and omitted variable bias (OVB). Having finished the paper, I started looking at the Ball et al. paper in Geophysics, from 2018 [1], on three-term AVO projections. (Better late than never; but apologies to the authors for not including this reference in my paper). It is easy to see how bias is also captured in the AVO projection operators, and here I show how.

Introduction

To recap: The key result from omitted variable bias relates the included variable least-squares estimation to the variables which are omitted:

$$\begin{aligned} \mathbf{A}_i^{-g}\mathbf{d} &= \hat{\mathbf{m}}_i + \mathbf{A}_i^{-g}\mathbf{A}_o\hat{\mathbf{m}}_o && (1)\\ &= \mathsf{unbiased\ variable} + \mathsf{bias} && (2)\\ &= \mathsf{unbiased\ variable} + \mathsf{data\ independent\ weight\ term} \times \mathsf{omitted\ variable(s)}\,. && (3) \end{aligned}$$

The model parameters estimated in the reduced regression (lhs) are equal the unbiased least squares estimate of the model parameters in the full model (first term on rhs) plus a bias term. The bias term splits into a data-independent weight term, in the following also called *bias weights*, multiplied with the omitted variables. The weight term (matrix) $\mathbf{A}_i^{-g}\mathbf{A}_o$ has one entry for each combination of included and omitted variable.

As an example, I then applied this to the case of two-term AVO[1], compared to three-term AVO, assuming for now that the data follow the three-term AVO equation, so that the fit with three variables is unbiased.

This gave:

$$\begin{aligned} \mathbf{A}_{i=(2t)}^{-g}\mathbf{d} &\equiv \begin{pmatrix} \hat{R}(0)^{(2t)} \\ \hat{G}^{(2t)} \end{pmatrix} \\ &= \begin{pmatrix} \hat{R}(0)^{(3t)} \\ \hat{G}^{(3t)} \end{pmatrix} + \frac{1}{\mathsf{var}(\sin^2(\theta))} \begin{pmatrix} \langle \sin^4(\theta)\rangle\langle\sin^2(\theta)\tan^2(\theta)\rangle - \langle\sin^2(\theta)\rangle\langle\sin^4(\theta)\tan^2(\theta)\rangle \\ \mathsf{cov}\left(\sin^2(\theta), \sin^2(\theta)\tan^2(\theta)\right) \end{pmatrix} \hat{C}^{(3t)}\,. \end{aligned} \quad (4)$$

[1]Two-term AVO is often called *truncated* AVO. However, keep in mind that linearised isotropic three-term AVO is a weak refectivity approximation, and may therefore also be considered a truncated version of AVO (see [6] and [3].

Now notice how either of these equations can be written as:

$$\begin{pmatrix} \hat{R}(0)^{(2t)} \\ \hat{G}^{(2t)} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \text{data independent weight term}_{R(0)} \\ 0 & 1 & \text{data independent weight term}_{G} \end{pmatrix} \begin{pmatrix} \hat{R}(0)^{(3t)} \\ \hat{G}^{(3t)} \\ \hat{C}^{(3t)} \end{pmatrix} \tag{5}$$

$$= P_{23,\mathsf{Shuey}} \begin{pmatrix} \hat{R}(0)^{(3t)} \\ \hat{G}^{(3t)} \\ \hat{C}^{(3t)} \end{pmatrix} \tag{6}$$

Thus, the AVO projection operator that *truncates* a given AVO model (in this case, from three to two terms) also gives the bias weights I calculated using omitted variable bias. So OVB provides insight into the shape of the AVO projections operator given by [1] (which is not to say one couldn't find this result directly starting from the projection operator itself; it's all linearly connected). The 2x2 unit matrix in the projection operator is the result of multiplying the 2x2 inverse covariance matrix of the truncated variables (in my notation: the included variables) with the corresponding covariance matrix of the full system, which has the same two variables (and hence 2x2 covariance) plus the additional (in my notation: the omitted) variables.

We can further use the linear relation between the Shuey and Fatti AVO parameterisations

$$\begin{pmatrix} R(0) \\ G \\ C \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -8\gamma^2 & 4\gamma^2 - 1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} R_{I_P} \\ R_{I_S} \\ R_\rho \end{pmatrix} = P_{\mathsf{Shuey,Fatti}} \begin{pmatrix} R_{I_P} \\ R_{I_S} \\ R_\rho \end{pmatrix} . \tag{7}$$

As discussed, we must question if forward model relations also hold for least squares parameters. I show in the appendix that the forward relation does indeed also hold in inverse space, so we can combine the two projection matrices to create relations between the variables. Using

$$\begin{pmatrix} \hat{R}_{I_P} \\ \hat{R}_{I_S} \\ \hat{R}_\rho \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{-8\gamma^2} & \frac{1}{8}\frac{4\gamma^2+1}{\gamma^2} - 1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} \hat{R}(0) \\ \hat{G} \\ \hat{C} \end{pmatrix} \tag{8}$$

we find the two-term relationship between inverted model parameters, at three-term level:

$$\hat{\mathbf{m}}^{(12)3t}_{\mathsf{Fatti}} = \begin{pmatrix} \hat{R}^{(3t)}_{I_P} \\ \hat{R}^{(3t)}_{I_S} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & \frac{1}{-8\gamma^2} \end{pmatrix} \begin{pmatrix} \hat{R}(0)^{(3t)} \\ \hat{G}^{(3t)} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{8}\frac{4\gamma^2+1}{\gamma^2} - 1 \end{pmatrix} \hat{C}^{(3t)} \tag{9}$$

This confirms that if we work with unbiased least squares estimates, i.e. we fit the three-term AVO equation, we honor the known modeling relation between shear-impedance and intercept and gradient in the Shuey model for $\gamma^2 = 1/4$:

$$\hat{R}^{(3t)}_{I_S} = \frac{1}{2}\hat{R}(0)^{(3t)} - \frac{1}{2}\hat{G}^{(3t)} . \tag{10}$$

However, if we are fitting just the two terms, then the unbiassed relationship in model parameter space no longer holds due to the bias in the two-term fit results.

To propagate the bias from the Shuey fit to the Fatti parameters we use equation 3:

$$\hat{\mathbf{m}}^{(12)(3t)} = \hat{\mathbf{m}}^{(12)(2t)} - A^{(12)-g} A^{(3)} \hat{\mathbf{m}}^{(3)(3t)} \tag{11}$$

Inserting this just for the Shuey model parameters we get:

$$\begin{aligned} \hat{\mathbf{m}}^{(12)(3t)}_{\mathsf{Fatti}} &= \begin{pmatrix} \hat{R}^{(3t)}_{I_P} \\ \hat{R}^{(3t)}_{I_S} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & \frac{1}{-8\gamma^2} \end{pmatrix} \begin{pmatrix} \hat{R}(0)^{(2t)} \\ \hat{G}^{(2t)} \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & \frac{1}{-8\gamma^2} \end{pmatrix} A^{(12)-g}_{\mathsf{Shuey}} A^{(3)}_{\mathsf{Shuey}} \hat{C}^{(3t)} + \begin{pmatrix} 0 \\ \frac{1}{8}\frac{4\gamma^2+1}{\gamma^2} - 1 \end{pmatrix} \hat{C}^{(3t)} \end{aligned} \tag{12}$$

Let's use this to look at the bias for R_{I_S} in the context of the data example we used previously, where $\gamma^2 = 1/4$. I also use the Gardner relation $C = c\hat{R}(0)^{(2t)}$ to remove the curvature. We find

$$\hat{R}^{(3t)}_{I_S\,\mathsf{Fatti}} = \frac{1}{2}\hat{R}(0)^{(2t)}\left(1 + c(\mathsf{bias}_G - \mathsf{bias}_{R(0)})\right) - \frac{1}{2}\hat{G}^{(2t)}\,. \tag{13}$$

This tallies with the analysis in the paper[2], see equation 22.

Keep in mind that here we have assumed that the three-term AVO fit is unbiased, which is not generally the case, as I dicuss in my paper [2].

1 Appendix: Least squares in linearly transformed AVO spaces

If an AVO formulation in basis a

$$\mathbf{A}_a\mathbf{m}_a = \mathbf{d} \tag{14}$$

is re-parameterized in terms of new variables in basis b, using the invertible matrix $\mathbf{P}$

$$\mathbf{A}_b = \mathbf{A}_a\mathbf{P} \tag{15}$$

then the least squares solution to the problem in the new basis is

$$\hat{\mathbf{m}}_b = \mathbf{P}^{-1}\hat{\mathbf{m}}_a \tag{16}$$

which can be shown by simple insertion. The least squares models are identical. It follows that

$$\mathbf{P}^{-1} \quad = \quad \mathbf{A}_b^{-g}\mathbf{A}_a\,. \tag{17}$$

If $\mathbf{A}_b = \mathbf{A}_a\mathbf{P}$ and supposing we have obtained model parameter estimates in model a, we therefore have three possible ways of obtaining the corresponding parameter estimates $\hat{\mathbf{m}}_b$ in model b:

$$(1)\ \hat{\mathbf{m}}_b \quad = \quad \mathbf{P}^{-1}\hat{\mathbf{m}}_a \tag{18}$$
$$(2)\ \hat{\mathbf{m}}_b \quad = \quad \mathbf{A}_b^{-g}\mathbf{A}_a\hat{\mathbf{m}}_a \text{ or } \mathbf{N}_a = \mathbf{N}_b \tag{19}$$
$$(3)\ \hat{\mathbf{m}}_b \quad = \quad \mathbf{A}_b^{-g}\hat{\mathbf{d}}_a \tag{20}$$

In simple least squares, any of these three methods give us the same result for $\hat{\mathbf{m}}_b$ as from independently fitting model b to the data[2].

The *data resolution matrix* [4] $\mathbf{N}$ tells us how well the predicted data matches the observed data:

$$\hat{\mathbf{d}} = \mathbf{A}\hat{\mathbf{m}} = \mathbf{A}(\mathbf{A}^{-\mathbf{g}}\mathbf{d}) = \left(\mathbf{A}\mathbf{A}^{-\mathbf{g}}\right)\mathbf{d} = \mathbf{N}\mathbf{d}\,. \tag{21}$$

This matrix, like the design matrix $\mathbf{A}$, is not dependent on the data values. Menke [4] shows that the least squares generalized inverse $\mathbf{A}^{-g}$ is obtained either by minimizing the $L2$ norm of the prediction error, or as the inverse that minimizes the spread of the data resolution matrix $\mathbf{N}$. The data resolution matrix $\mathbf{N}$ is clearly a projection matrix (it is also symmetric and idempotent), taking the input data vector $\mathbf{d}$ and projecting it onto the least squares solution vector $\hat{\mathbf{d}}$. Tukey termed the matrix $(\mathbf{A}\mathbf{A}^{-\mathbf{g}})$ the *hat-maker*, since it puts the hat on the data $\mathbf{d}$. Another name is *influence matrix* since N_{ij} is the rate at which the ith fitted value changes as the jth observation is varied, to wit, the influence that observation has on that fitted value.

The first of the three equations 18-20 states that the transform in the inverted domain is the same *as if* the models were *identical*, i.e. as if they *forward model* identical AVO. Notice however, that this assumption was not made in the argument; only the basis vectors were linearly transformed. So this results states that the *estimated* least squares

[2] More complex schemes such as iterative reweighted least squares (IRLS) may change this slightly, but more intuitive insight can be gained by sticking to simple least squares. One way to think of IRLS is that the weights it determines and applies to the data allow us to use simple least squares again.

model parameters are such that the estimated least-squares models are made to look *identical*, even if they were not identical in model space. This happens as long as the AVO operators have the same range.

The second conversion equation expresses this concept using the data resolution matrix. By definition, two AVO parameterisations have the same least squares models $\hat{\mathbf{d}}_a = \hat{\mathbf{d}}_b$ if

$$\begin{aligned} \mathbf{N}_a &= \mathbf{N}_b \qquad (22) \\ \mathbf{A}_a\mathbf{A}_a^{-g} &= \mathbf{A}_b\mathbf{A}_b^{-g} \qquad (23) \end{aligned}$$

This can be written as:

$$\mathbf{A}_a = \mathbf{N}_b\mathbf{A}_a \qquad (24)$$

in which case the model parameters in the two basis sytems are related by conversion eq. (2) above:

$$\hat{\mathbf{m}}_b = \mathbf{A}_b^{-g}\mathbf{A}_a\hat{\mathbf{m}}_a\,. \qquad (25)$$

This last result was given (but not derived) by Thomas et al. in [5].

Finally, the last of the three conversion equations, an immediate rewrite of (2), states that we can convert to the second set of elastic parameters $\hat{\mathbf{m}}_b$ by regressing onto the model data $\hat{\mathbf{d}}_a$ obtained from fitting the data to the first set of parameters $\mathbf{m}_a$. The conversions do not require the original data [5]. Conversion (3) answers the following question: Which set of model fit parameters in model b gives us the same model fit of the data as in model a? If models a and b are *identical*, i.e. exact algebraic re-formulations, their forward models also agree, and are trivially related via the conversion matrix $\mathbf{P}^{-1}$. However, it is sufficient to have linearly transformed basis vectors for the least squares model estimates to be related in this way. In other words, AVO models with different *forward* models, but related in this way give the same least squares model *estimates*. Thomas et al. [5] already showed several examples of such behaviour for two-term AVO models (their Figures 1 and 2). The above explains how and why this happens.

So far we have identified two possibilities for AVO with the same range:

$$\mathbf{A}_b = \mathbf{A}_a\mathbf{P} \text{ and AVO models } \begin{array}{lll} (1) & \text{identical} & \mathbf{m}_b = \mathbf{P}^{-1}\mathbf{m}_a \\ (2) & \text{equivalent} & \mathbf{m}_b \neq \mathbf{P}^{-1}\mathbf{m}_a \end{array} \implies \hat{\mathbf{m}}_b = \mathbf{P}^{-1}\hat{\mathbf{m}}_a = \mathbf{A}_b^{-g}\mathbf{A}_a\hat{\mathbf{m}}_a\,. \qquad (26)$$

Remember that *identical* means that the *forward models* match, whereas for *equivalent* but not identical AVO models the forward models are different.

In both instances the AVO operators have the same range. We are simply chosing different basis vectors in the same data space to describe the AVO data vector. In case one, the forward models match and the linear relationship between the model parameters is replicated by the regression. However, if the forward models do not match, we find that due to the range of the AVO operators being equivalent, we still get the same linear relation in the model estimate space, as if they did! Case (2) in eq. 26 shows this clearly, since the relation between the inverted parameters is now explicitly not honoured by the forward model. However in both cases, the two least squares AVO models, and hence residuals, are identical. This is not necessarily good news. Firstly, it means the least squares model fits do not distinguish between such different models. Secondly, as I have shown, for the least squares models to be identical when the forward models are not, bias has to be at work.

That leaves us, lastly, with the third possibility for AVO spaces when mis-specifying the model: How do we compare AVO models which are not equivalent? Remember this means the AVO design matrices $\mathbf{A}$ are no longer linearly related. The Fatti and Shuey AVO parameterisations with just two terms are an example. In this case neither their forward models nor the least squares estimates match. As proposed by Thomas et al. [5] we can use the same transform matrix as before to relate such models. This is based, as we now see, on the third variant of the conversion equation. It means we effectively take the least squares model obtained in the first of the AVO parameterisations, and least-squares fit the second AVO model to this data. As before, this makes no statement about bias in either of the two models, and, in general, is a conversion between two biased AVO models.

All three cases in overview:

$$\begin{array}{llll} \mathbf{A}_b = \mathbf{A}_a\mathbf{P} \text{ and AVO models} & \begin{array}{lll} (1) & \text{identical} & \mathbf{m}_b = \mathbf{P}^{-1}\mathbf{m}_a \\ (2) & \text{equivalent} & \mathbf{m}_b \neq \mathbf{P}^{-1}\mathbf{m}_a \end{array} & \implies & \hat{\mathbf{m}}_b = \mathbf{P}^{-1}\hat{\mathbf{m}}_a = \mathbf{A}_b^{-g}\mathbf{A}_a\hat{\mathbf{m}}_a\,. \\ \mathbf{A}_b \neq \mathbf{A}_a\mathbf{P} \text{ and AVO models} & (3) \quad \text{not equivalent} \quad \mathbf{m}_b \neq \mathbf{P}^{-1}\mathbf{m}_a & \implies & \hat{\mathbf{m}}_b = \mathbf{A}_b^{-g}\mathbf{A}_a\hat{\mathbf{m}}_a\,. \end{array} \qquad (27)$$

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