When and when not to use optimal model averaging

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Abstract

Traditionally model averaging has been viewed as an alternative to model selection with the ultimate goal to incorporate the uncertainty associated with the model selection process in standard errors and confidence intervals by using a weighted combination of candidate models. In recent years, a new class of model averaging estimators has emerged in the literature, suggesting to combine models such that the squared risk, or other risk functions, are minimized. We argue that, contrary to popular belief, these estimators do not necessarily address the challenges induced by model selection uncertainty, but should be regarded as attractive complements for the machine learning and forecasting literature, as well as tools to identify causal parameters. We illustrate our point by means of several targeted simulation studies.

1 Background

Regression models are the cornerstone of statistical analyses. The motivation for their use is diverse: they might (a) be purely descriptive, (b) target prediction and forecasting problems, (c) help identifying associations or (d) even causal parameters. The motivation for variable selection in regression models is based on the rationale that associational relationships between variables are best understood by reducing the model's dimension. An example would be regression growth models for which a multitude of variables are potentially relevant to describe the relationships in the data (Sala-I-Martin et al, 2004). The problem with this approach is that in finite samples (i) the regression parameters after model selection are often biased and (ii) the respective standard errors are too small because they do not reflect the uncertainty related to the model selection process (Leeb and Pötscher, 2005; Burnham and Anderson, 2002; Hjort and Claeskens, 2003).

   A wave of publications in the 1990's (Chatfield, 1995; Draper, 1995; Hoeting et al, 1999) proposed that the drawback of model selection can be overcome by model averaging. With model averaging one calculates a weighted average of the parameter estimates of a set of candidate models, for example using regression models with a different set of included variables. The weights are determined in such a way that 'better' models receive a higher weight. For example, models with a lower AIC may receive a higher weight (Buckland et al, 1997). The variance of these type of estimators is typically calculated such that both the variance related to the parameters of each model and the variance between the different model estimates is taken into account. Note that this approach tackles problem (ii), the incorporation of model selection uncertainty into the standard errors of the regression parameters; but it may not necessarily tackle problem (i) as the regression parameters may still be biased. In fact, model averaging estimators behave similarly to shrinkage estimators because regression coefficients

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which belong to variables which are not supported among many candidate models are shrunk and are therefore possibly biased. The obvious conclusion is that model averaging is useful to identify associations in regression models and yields more realistic confidence intervals than model selection does. It can therefore serve as a descriptive and exploratory tool in data analysis and be applied in the context of (a) and (c).

However, the pitfalls of this classical model averaging scheme are clear: the estimators produced by a classical weight choice are not optimal from a statistical point of view. The weights are chosen such that one gets improved standard errors. But ideally the weights of an estimator would also result in an averaged estimator which minimizes a risk function, for example the squared risk with respect to some function of μ (at least asymptotically). This may yield an estimator with good properties, potentially even with good predictive abilities. These type of estimators are known as 'Optimal Model Averaging' (OMA) estimators and were mostly inspired by the seminal paper of Hansen (2007). He considered a set of nested regression models and proposed to choose weights such that the weighted estimator minimizes a criterion similar to Mallow's C_p. With this, the weights are constructed such that the mean squared prediction error is small, therefore one obtains a good bias-variance tradeoff as well as other properties, for example an (asymptotically) optimal estimator based on definitions common in the model averaging literature. The construction of Hansen's estimator corresponds to motivation (b) outlined above. It is no surprise that other authors then also developed optimal model averaging estimators – based on the same idea, but in the context of different model classes, different loss/risk functions, different model sets, and so on – see Cheng et al, 2015; Gao et al, 2016; Hansen, 2008; Hansen and Racine, 2012; Liang et al, 2011; Liu and Kuo, 2016; Liu et al, 2016; Zhang et al, 2014; Zhang et al, 2015; Zhang et al, 2016b and the references therein. The interesting part is that the authors of these papers, with few exceptions (e.g. Zhang et al, 2015; Zhang et al, 2016b), often motivate their estimators by saying that the purpose for their construction is to overcome the problems of model selection and to include the uncertainty associated with the model selection process. This is surprising as the methodology developed by Hansen and others does not tackle (ii) as needed for (a) and (c), but is rather geared towards (b). Moreover, the construction of confidence intervals is typically not discussed in these papers (but see Zhang and Liu (2017) on interval estimation). Our paper is motivated by this misunderstanding.

We argue that there are at least two different schools of model averaging, each with their own justification and benefit. However, the recent developments in the literature in finding an optimal model averaging estimator should not be confused with the original motivation of 'correcting' model selection estimates to include the uncertainty of the model selection process. The motivation of model selection and model averaging originates from the attempts to understand associational structures in models of moderate-to-high dimension (see items (a) and (c)). Optimal model average estimators should rather be seen as additional tools for statistical forecasting and learning problems (see item (b)).

In this paper we are going to demonstrate several points concerning the relationship and differences between different model averaging schemes:

- we investigate the coverage probability of selected popular model averaging estimators. While recently there has been a moderate interest in understanding the construction of confidence intervals when applying model averaging (Kabaila et al, 2016, Wang and Zhou, 2012, Schomaker and Heumann, 2014, Turek and Fletcher, 2012, Fletcher and Dillingham, 2011), this topic has been rather under-researched; in particular, it remains unclear how standard model-averaged confidence intervals perform in terms of coverage, and how this compares to naive intervals after model selection.

- we undertake simulation studies to compare different model averaging approaches under different motivating questions; i.e explanatory, predictive and causal questions of interest.

- we demonstrate that optimal model averaging can be successfully incorporated into 'super

learning', a recently proposed data adaptive approach which combines several learners to improve predictive performance.

- motivated by the above point, we show that OMA can complement procedures which identify causal effects, such as the sequential g-formula. We therefore show that OMA may be of interest even in the context of (d).

- moreover, we have implemented optimal model averaging estimators in such a way that they can be used easily for super learning and in causal inference.

All above points are meant to understand and illustrate under which circumstances the use of optimal model averaging has benefits, and when this is not the case.

2 Methodological Framework

Below we review the methods discussed and evaluated in the remainder of this paper. Section 2.1 introduces criterion based model averaging whereas Sections 2.2, 2.3, and 2.4 introduce optimal model averaging estimators. Section 2.5 describes the concept of super learning. The description of the below methods is brief on purpose, as the contribution of this paper relates to comparison of optimal and traditional model averaging schemes by discussion and simulation.

Consider n observations for which both a response vector $y = (y_1, \ldots, y_n)'$ and a covariate matrix $X = (x_1', \ldots, x_n')'$, $x_i = (x_{i1}, \ldots, x_{ip})$, are available. Each variable of X is denoted as $X_j = (x_{1j}, \ldots, x_{nj})'$. To relate the response with a set of explanatory variables one could use a (regression) model $M_\kappa = f(y|X; \beta)$ for which the parameter vector β has to be estimated. If we consider a *set* of candidate models, $\mathcal{M} = \{M_1, \ldots, M_k\}$, for describing y based on varying combinations of X_j's, then a model selection procedure chooses one single 'best' model out of the set $\mathcal{M}$; typically based on some criterion, for example Akaikes Information Criterion (AIC, Akaike, 1973; Rao et al, 2001).

2.1 Criterion Based Model Averaging

With criterion based model averaging, one calculates a weighted average $\hat{\bar{\beta}} = \sum_\kappa w_\kappa \hat{\beta}_\kappa$ from the k estimators $\hat{\beta}_\kappa$ ($\kappa = 1, \ldots, k$) of the set of candidate (regression) models $\mathcal{M}$ where the weights are calculated in a way such that 'better' models receive a higher weight. A popular weight choice would be based on the exponential AIC,

$$w_\kappa^{\text{AIC}} = \frac{\exp(-\frac{1}{2}\text{AIC}_\kappa)}{\sum_{\kappa=1}^k \exp(-\frac{1}{2}\text{AIC}_\kappa)}, \tag{1}$$

where AIC_κ is the AIC value related to model $M_\kappa \in \mathcal{M}$ (Buckland et al, 1997). It has been suggested to estimate the variance of the scalar $\hat{\bar{\beta}}_j \in \hat{\bar{\beta}}$ via

$$\widehat{\text{Var}}(\hat{\bar{\beta}}_j) = \left\{ \sum_{\kappa=1}^k w_\kappa \sqrt{\widehat{\text{Var}}(\hat{\beta}_{j,\kappa}|M_\kappa) + (\hat{\beta}_{j,\kappa} - \hat{\bar{\beta}}_j)^2} \right\}^2, \tag{2}$$

where $\hat{\beta}_{j,\kappa}$ is the jth regression coefficient of the κth candidate model. While formula (2) from Buckland et al (1997) is the most popular choice to calculate standard errors in model averaging, it has also been criticized that the coverage probability of interval estimates based on (2) may not always reflect the nominal level (Hjort and Claeskens, 2003).

From the Bayesian perspective the quality of a regression model $M_\kappa \in \mathcal{M}$ may be judged upon the estimated posterior probability that this model is correct, that is

$$\Pr(M_\kappa|y) \propto \Pr(M_\kappa) \int \Pr(y|M_\kappa, \beta_\kappa) \cdot \Pr(\beta_\kappa|M_\kappa) \, d\beta_\kappa, \tag{3}$$

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where $\Pr(M_\kappa)$ is the prior probability for the model M_κ to be correct, $\Pr(y|M_\kappa, \beta_\kappa) = \mathcal{L}(\beta)$ represents the likelihood, and $\Pr(\beta_\kappa|M_\kappa)$ reflects the prior density of β_κ when M_κ is the model under consideration. Since, for a large sample size, $\Pr(M_\kappa|y)$ can be approximated via the Bayes-Criterion of Schwarz (BCS, BIC), it is often suggested that the weight

$$w_\kappa^{\text{BIC}} \quad = \quad \frac{\exp(-\frac{1}{2}\text{BIC}_\kappa)}{\sum_{\kappa=1}^{k} \exp(-\frac{1}{2}\text{BIC}_\kappa)}, \tag{4}$$

should be used for the construction of the Bayesian Model Averaging estimator. The BIC corresponds to $-2\mathcal{L}(\hat{\beta}) + p\ln n$, where p corresponds to the number of parameters. The variance of $\hat{\bar{\beta}}_j$ can be estimated in various (similar) ways, depending on the assumptions about the priors and the practical approach of solving the integral in (3). Broadly, variance estimation is based on variance decomposition such as the law of total variance, i.e. using

$$\widehat{\text{Var}}(\hat{\bar{\beta}}_j) \quad = \quad \widehat{\text{E}}_\mathcal{M}(\widehat{\text{Var}}(\hat{\beta}_{j,\kappa}|y, M_\kappa)) + \widehat{\text{Var}}_\mathcal{M}(\widehat{\text{E}}(\hat{\beta}_{j,\kappa}|y, M_\kappa)), \tag{5}$$

see also Draper (1995). Practically, this yields similar, but not identical results as (2). Based on the above variance estimates, Bayesian credibility intervals can be constructed.

There are many variations and subtleties when it comes to the implementation of the above estimators. For example, for computational feasibility, one may restrict the number of candidate models. Reviews on Frequentist and Bayesian Model Averaging can be found in Wang et al (2009) and Hoeting et al (1999).

2.2 Mallow's Model Averaging

Hansen considers a situation of k nested linear regression models for k variables. Let $\hat{\beta}_\kappa$ be the estimated regression parameter of model M_κ, and $\hat{\bar{\beta}} = \sum_{\kappa=1}^{k} w_\kappa \hat{\beta}_\kappa$ be a model averaging estimator with $\hat{\mu}_w = X_k \hat{\bar{\beta}}$. Based on similar thoughts as in the construction of Mallow's C_p (Mallows, 1973), Hansen suggests to minimize the mean squared (prediction) error [MSPE] by minimizing the following criterion:

$$\tilde{C}_p \quad = \quad (y - X_k\hat{\bar{\beta}})'(y - X_k\hat{\bar{\beta}}) + 2\sigma^2 K_w, \tag{6}$$

where $K_w = \text{tr}(P_w)$, $P_w = \sum_{\kappa=1}^{k} w_\kappa X_\kappa (X_\kappa' X_\kappa)^{-1} X_\kappa'$ and σ^2 is the variance which needs to be estimated from the full model. Consequently, the weight vector w is chosen such that $\tilde{C}_p$ is minimized

$$w^{\text{MMA}} \quad = \quad \arg\min_{w \in \mathcal{H}} \tilde{C}_p, \tag{7}$$

with $\mathcal{H} = \{w = (w_1, \ldots, w_k) \in [0,1]^k : \sum_{\kappa=1}^{k} w_\kappa = 1\}$. Model averaging based on the weight choice (7) is often called Mallow's Model Averaging (MMA). MMA has beneficial properties, i.e. it minimizes the MSPE and is asymptotically optimal, see Hansen (2007, Theorem 1, Lemma 3) for more details. Moreover, it has been shown that the MMA estimator has a smaller MSE than the OLS estimator (Zhang et al, 2016a).

Since the first part of (6) is quadratic in w_κ and the second one linear, one can obtain the model averaging estimator by means of quadratic programming.

The assumptions of a discrete weight set and nested regression models sound restrictive, but it has been shown that both assumptions are not necessarily required and MMA can be applied to non-nested regression models as well; given that this is computationally feasible (Wan et al, 2010).

2.3 Jackknife Model Averaging

Jacknife Model Averaging (JMA) as proposed by Hansen and Racine (2012) for linear models, builds on leave-one-out (LOO) cross validation. For Model M_κ the LOO residual vector is $\tilde{\epsilon}^\kappa = y - \hat{y}^\kappa$, with $\hat{y}^\kappa = x_i^\kappa (X_{(-i)}^{\kappa'} X_{(-i)}^\kappa)^{-1} X_{(-i)}^{\kappa'} y_{(-i)}$ where the index $_{(-i)}$ describes that the respective matrix excludes observation i, $i = 1, \ldots, n$. It can be shown that there is a simple algebraic relationship which allows the computation of the LOO residuals in one rather than n operations:

$$\tilde{\epsilon}^\kappa = D_\kappa \hat{\epsilon}^\kappa \tag{8}$$

where $\hat{\epsilon}^\kappa$ is the standard least squares residual vector $y - P_\kappa y$ with the hat matrix $P = X(X'X)^{-1}X'$; and D_κ is a $n \times n$ diagonal matrix with $D_{ii,\kappa} = (1 - P_{ii,\kappa})^{-1}$, $i = 1, \ldots, n$.

For k candidate models the linear weighted LOO residuals are $\tilde{\epsilon}_w = \sum_\kappa w_\kappa \tilde{\epsilon}^\kappa$, $\kappa = 1, \ldots, k$. An estimate of the true expected squared error is $CV_w = n^{-1} \tilde{\epsilon}'_w \tilde{\epsilon}_w$ and an appropriate weight choice would thus be

$$w^{\text{JMA}} = \arg \min_{w \in \mathcal{H}} CV_w, \tag{9}$$

As with MMA, the weights can be obtained with quadratic programming. The estimator has similar properties as the MMA estimator (Hansen and Racine, 2012). Model averaging with the weight choice (9) is called Jackknife Model Averaging.

2.4 Lasso Averaging

Shrinkage estimation, for example via the LASSO (Tibsharani, 1996), can be used for model selection. This requires the choice of a tuning parameter which comes with tuning parameter selection uncertainty. LASSO averaging estimation (LAE), or more general shrinkage averaging estimation (Schomaker, 2012), is a way to combine shrinkage estimators with different tuning parameters.

Consider the LASSO estimator for a simple linear model:

$$\hat{\beta}_{\text{LE}}(\lambda) = \arg \min \left\{ \sum_{i=1}^n (y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\}. \tag{10}$$

The complexity parameter $\lambda \geq 0$ tunes the amount of shrinkage and is typically estimated via the generalized cross validation criterion or any other cross validation criterion. The larger the value of λ, the greater the amount of shrinkage since the estimated coefficients are shrunk towards zero.

Consider a sequence of candidate tuning parameters $\lambda = \{\lambda_1, \ldots, \lambda_L\}$. If each estimator $\hat{\beta}_{\text{LE}}(\lambda_i)$ obtains a specific weight w_{λ_i}, then a *LASSO averaging estimator* takes the form

$$\hat{\bar{\beta}}_{\text{LAE}} = \sum_{i=1}^L w_{\lambda_i} \hat{\beta}_{\text{LE}}(\lambda_i) = w_\lambda \hat{B}_{\text{LE}}, \tag{11}$$

where $\lambda_i \in [0, c]$, $c > 0$ is a suitable constant, $\hat{B}_{\text{LE}} = (\hat{\beta}_{\text{LE}}(\lambda_1), \ldots, \hat{\beta}_{\text{LE}}(\lambda_L))'$ is the $L \times p$ matrix of the LASSO estimators, $w_\lambda = (w_{\lambda_1}, \ldots, w_{\lambda_L})$ is an $1 \times L$ weight vector, $w_\lambda \in \mathcal{W}$ and $\mathcal{W} = \{w_\lambda \in [0, 1]^L : 1'w_\lambda = 1\}$.

A general measure for the cross validation error with squared loss function would be

$$OCV_k = n^{-1} \tilde{\epsilon}_\kappa(w)' \tilde{\epsilon}_\kappa(w) \propto w_\lambda E_k' E_k w_\lambda', \tag{12}$$

where $E_k = (\tilde{\epsilon}_k(\lambda_1), \ldots, \tilde{\epsilon}_k(\lambda_L))$ is the $n \times L$ matrix of the k-fold cross-validation residuals for the L competing tuning parameters. An optimal weight vector for this criterion is then

$$w^{\text{LAE}} = \arg \min_{w \in \mathcal{W}} OCV_k. \tag{13}$$

These weights can also be calculated with quadratic programming. More details can be found in Schomaker (2012).

2.5 Super Learning

Depending on the specific problem, optimal model averaging as described in the above sections may be a good prediction algorithm or not. To choose and combine the best prediction methods, *super learning* can be used. Super learning means considering a set of prediction algorithms, for example regression models, shrinkage estimators or model averaging. Instead of choosing the algorithm with the smallest cross validation error, super learning chooses a weighted combination of different algorithms, that is the weighted combination which minimizes the cross validation error. It can be shown that this weighted combination will perform (asymptotically) at least as good as the best algorithm, if not better (Van der Laan et al, 2008) and is known as the oracle property of super learning.

For example: consider Learner 1 (L1) to be a linear model including all available covariates and learner 2 (L2) to be Mallow's Model Averaging. Both of them have a specific k-fold cross-validation error, for a given loss function, that is CV_k^{L1} and CV_k^{L2}. Now, find the linear combination of the two predictions from L1 and L2 that best predicts the outcome. This can be achieved by non-negative least squares estimation, as (for the above mentioned oracle property to hold) the weights need to be positive and sum up to one. The final prediction algorithm is then the weighted linear combination of the two learners. The cross validation error of this combination is then asymptotically at least as low (and therefore good) as the errors CV_k^{L1} and CV_k^{L2}.

The interested reader is referred to Van der Laan and Petersen (2007) and Van der Laan and Rose (2011), and the references therein, for more details.

3 Simulation Studies

The purpose of this section is to contrast simple traditional model averaging, both frequentist and bayesian as described in Section 2.1 with optimal model averaging as described in Sections 2.2, 2.3, and 2.4 for different situations. The first setting described in Section 3.1 targets linear regression settings motivated by (a) and (c), i.e. those where regression is meant to describe associational relationships. The next Section 3.2 targets (b), that is the use of regression for prediction. Finally, in Section 3.3, we look at longitudinal data for which (d), i.e. the identification of a causal effect, is of interest.

3.1 Associations in a Linear Regression Model

In this setup, we compare different estimators of a linear regression model: the ordinary least squares estimate of the full model [OLS], the model selection estimates of the model selected by AIC [MS], traditional model averaging estimates based on the weight choices (1) [FMA] and (4) [BMA], and Mallow's model averaging estimates based on the weight choice (7) [MMA]. We selected the above estimators because they reflect the most popular approaches in the literature. Additionally, for BMA, we follow the implementation from the R-package BMA (Raftery et al, 2017), which uses a subset of candidate models based on a leaps and bounds algorithm in conjunction with "Occam's razor", see Hoeting et al (1999) for more details. Frequentist model averaging is based on all possible candidate models, model selection is based on those models selected by stepwise selection with AIC, and optimal model averaging on the set of nested models. Variance estimates for FMA and MMA are based on (2), and those of BMA are based on (5). Confidence intervals were constructed using critical values from a standard normal distribution, as often done in naive regression analyses.

The setup of our simulation is as follows: We generate 10 variables (sample size: $n = 500$) using normal, log-normal and exponential distributions: $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4 \sim \mathrm{N}(0,1)$, $\mathbf{X}_5, \mathbf{X}_6, \mathbf{X}_7 \sim \mathrm{logN}(0, 0.5)$, $\mathbf{X}_8, \mathbf{X}_9, \mathbf{X}_{10} \sim \mathrm{Exp}(1)$. To model the dependency between the covariates we use a Clayton Copula (Yan, 2007) with a copula parameter of 1 which indicates moderate correlation among the covariates. We then define $\mu_y = 1X_3 + 2X_4 + 3X_5 + 3X_6 + 2X_7 + 1X_8 + 0.5X_9$ and

generate the outcome from $N(\mu_y, \exp(2))$. Therefore, 7 out of 10 variables have an effect of different size on y.

We compare the point estimates of the five approaches in terms of unbiasedness. Secondly, we compare estimated standard errors for model averaging estimators) with those obtained from the simulation study (i.e. based on the variance of $\hat{\bar{\beta}}$ over the $R = 5000$ simulation runs). Thirdly, we evaluate the coverage probability of the respective 95% interval estimates.

3.2 Forecasting

This setup targets prediction accuracy. We generate 10 variables (sample size: $n = 500$) using again normal, log-normal and exponential distributions: $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4 \sim \mathrm{N}(0, 1)$, $\mathbf{X}_5, \mathbf{X}_6, \mathbf{X}_7 \sim \mathrm{logN}(0, 0.5)$, $\mathbf{X}_8, \mathbf{X}_9, \mathbf{X}_{10} \sim \mathrm{Exp}(1)$. To model the dependency between the covariates we again use a Clayton Copula with a copula parameter of 1. We then define $\mu_y = -5 + 0.5X_2 + 1.5X_6 + 1.5X_9 + X_6 \times X_9 + X_2^2$ and generate the outcome from $N(\mu_y, \exp(1.5))$. Therefore, 3 out of 10 variables predict y and both interactions and non-linear associations are present.

We evaluate the mean squared prediction error for the same methods evaluated in Section 3.1, i.e. OLS, MS, FMA, BMA, and MMA. In addition we evaluate the predictive performance of super learning with two different types of learner sets: the first one (SL) consists of the OLS of the full linear model, random forests (Breiman, 2001), stepwise regression based on AIC, the LASSO, the arithmetic mean, GLM's based on EM-algorithm-Bayesian model fitting (Gelman and Su, 2016), additive models (Wood, 2006), and the full linear model with interactions, with and without model selection with AIC. The second learner set (SL+) consists of all learners from the first set, but adds Jacknife Model Averaging, Lasso Averaging and Mallows Model Averaging to the learner set. All of these estimators are fitted i) with the full set of variables, ii) with the full set plus all two-way interactions and iii) with the full set plus squared transformations of all variables. For Lasso Averaging we used a λ-sequence of length 100, where the maximum λ-value is the smallest value for which all coefficients are zero, the minimum λ value is 0.0001, and all other λ-values are equally spaced between these two (on a log-scale). While this is a common approach (Friedman et al, 2010), alternative sequences can be easily specified in common software packages, such as the R-package `glmnet`.

In this simulation, both the mean squared prediction error as well as the choice of learners from the super learner algorithm are of interest. The simulation is based on 5000 runs.

3.3 Causal Inference

This simulation is inspired by the HIV treatment analyses of Schomaker and Heumann (2018) and Schomaker et al (2016). We generate longitudinal data ($t = 0, 1, \ldots, 6$) for 3 time-dependent confounders ($\mathbf{L_t} = \{L_t^1, L_t^2, L_t^3\}$), an outcome ($Y_t$), an intervention ($A_t$), as well as baseline data at $t = 0$ for 7 variables, using structural equation models (Sofrygin et al, 2017). The data generating mechanism is described in detail in Appendix C. In this simulation we are interested in the expected counterfactual outcome at the end of follow-up (i.e. $t = 6$) which would have been observed under 2 different intervention rules $\bar{d}^j$, $j = 1, 2$, which assign treatment (A_t) either always (at each time point) or depending on the confounders, i.e. $A_t = 1$ if $L_t^1 < 350$ or $L_t^2 < 15\%$ or $L_t^3 < -2$; that is we want to estimate $E(Y_6^{\bar{d}_j})$ [see Appendix C for more details regarding notation]. We denote these target quantities as ψ_1 and ψ_2 and their true values are -1.80 and -2.02 respectively. They can be estimated using appropriate methodology, for example using the sequential g-formula; see Appendix B for more details. Briefly, for each point in time, i.e. $t = 6, \ldots, 1, 0$, the conditional outcome given the covariate history needs to be estimated. To avoid model mis-specification, it is common to use super learning for this. We use super learning with two different sets of learners. The first one consists of the OLS of the full linear model, the arithmetic mean, stepwise regression based on AIC, GLM's based on EM-algorithm-Bayesian model fitting, additive models, and

linear models with interactions. The second learner set consists of all learners from the first set, but adds Jacknife Model Averaging, Lasso Averaging (as specified in Section 3.2) and Mallows Model Averaging to the learner set. All of these estimators are fitted i) with the full set of variables, ii) with the full set plus all two-way interactions and iii) with the full set plus squared transformations of all variables. The simulation is based on 1000 runs.

This simulation compares bias and coverage with respect to the two different learners and interventions respectively; moreover, we are particularly interested whether super learning, applied in a complex longitudinal setup, picks optimal model averaging estimators for the fitting process or not. This point is not immediately clear as simple learners, such as additive models and GLM's with interaction, are already complex enough to model the data-generating process described in Appendix C. Whether a weighted combination including OMA is of benefit is the motivation of this simulation.

3.4 Results

The results of the first simulation study are summarized in Table 1.

Table 1: Results of the first simulation study. 'est' refers to the estimated standard error of the respective method, averaged over the simulation runs; 'sim' refers to the simulated standard error based on the variation of the point estimates over the simulation runs.

(a)	Point Estimates									
Method	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
OLS	0.00	0.00	1.00	2.01	3.00	3.00	1.98	1.00	0.49	0.00
MS	0.02	0.02	0.95	2.04	3.04	3.03	1.98	0.97	0.38	0.02
FMA	0.04	0.04	0.90	2.06	3.06	3.06	1.93	0.93	0.37	0.02
BMA	0.04	0.03	0.77	2.18	3.18	3.17	1.85	0.82	0.22	0.02
MMA	0.10	0.06	1.03	2.01	2.97	2.93	1.85	0.86	0.31	0.00

(b)	Standard Errors									
Method	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
OLS – est	0.44	0.44	0.44	0.44	0.66	0.66	0.66	0.39	0.39	0.39
OLS – sim	(0.44)	(0.43)	(0.44)	(0.44)	(0.66)	(0.65)	(0.67)	(0.39)	(0.38)	(0.39)
MS – est	0.07	0.07	0.35	0.42	0.64	0.64	0.61	0.34	0.18	0.05
MS – sim	(0.34)	(0.33)	(0.53)	(0.44)	(0.66)	(0.66)	(0.75)	(0.46)	(0.44)	(0.30)
FMA – est	0.32	0.32	0.47	0.44	0.67	0.67	0.71	0.42	0.35	0.28
FMA – sim	(0.28)	(0.26)	(0.52)	(0.45)	(0.68)	(0.68)	(0.79)	(0.47)	(0.37)	(0.25)
BMA – est	0.13	0.12	0.45	0.44	0.67	0.67	0.73	0.41	0.25	0.11
BMA – sim	(0.17)	(0.15)	(0.63)	(0.48)	(0.74)	(0.74)	(1.00)	(0.58)	(0.36)	(0.13)
MMA – est	0.50	0.45	0.46	0.48	0.73	0.75	0.76	0.44	0.26	0.09
MMA – sim	(0.44)	(0.43)	(0.43)	(0.44)	(0.66)	(0.67)	(0.69)	(0.42)	(0.34)	(0.20)

(c)	Coverage Probability (in %)									
Method	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
OLS	94	96	95	95	95	95	95	95	95	95
MS	94	94	80	94	94	95	92	86	44	94
FMA	99	99	85	95	95	95	90	87	79	99
BMA	99	100	67	92	93	93	81	73	44	100
MMA	97	97	96	96	97	97	95	90	60	100

(d)	MSE with respect to μ_y				
Method	OLS	MS	FMA	BMA	MMA
MSE	1.214	1.261	1.197	1.526	1.213

As expected the OLS is approximately unbiased, whereas the other estimators are not necessarily unbiased, particularly around the small effects of β_3, β_8 and β_9 (Table 1a). This simple but important property is often neglected in the model averaging literature. One reason might be that optimality in the model selection literature is typically defined to be either consistency (choosing, asymptotically, the correct model out of a set of candidate models – given that the candidate model is contained in the set) or efficiency (the selected model minimizes, asymptotically, a risk function – based on the assumption of a true model of infinite dimension). See Leeb and Pötscher (2008) for more details.

Table 1b contrasts the average estimated standard errors with those obtained from the simulations, i.e. the variance of the point estimates over the 5000 simulation runs. Ideally they should be as close as possible. It can be seen that the estimated standard errors are appropriate for the OLS estimator, and too small for the model selection estimator. This highlights the problems of model selection uncertainty. Model averaging by means of using AIC weights performs much better, addressing the issues related to model selection, but there is a tendency towards over-conservativeness, rather than over-confidence. Bayesian Model Averaging, with a restricted set of candidate models based on the approach explained earlier, produces less variability and doesn't seem to produce very accurate standard errors, though they are still somewhat superior to model selection. MMA obviously doesn't perform very well when it comes to estimating the standard errors of β_9 and β_{10}; this is because of its nested model setup, but also because the approach of using (2) for variance estimation is rather pragmatic. As highlighted before, MMA has been developed for point estimation. However, where computationally feasible, the performance of MMA can potentially be improved by using the set of all (i.e. non-nested) models, and possibly by also using bootstrapping for confidence interval estimation. In our setting, this improved coverage for those variables which were specified to be in a rear position, i.e. coverage for β_9 improved from 60% to 88% and coverage of β_8 improved from 90% to 91%; but often the quadratic programming problem required minor modifications of the first part of (6) to be solvable.

A look at the coverage probabilities reveals the problems of both model selection and model averaging: particularly for the small effects the actual coverage is way below the nominal coverage. This is not necessarily surprising because the distribution of model averaging estimators can be non-normal (Hjort and Claeskens, 2003). To solve this problem re-sampling may be a viable option (Schomaker and Heumann, 2014), though there are valid theoretical concerns around this as well (Pötscher, 2006). Alternatively, one may simply use the OLS interval estimates of the full model as they are asymptotically equivalent to the estimator from Hjort and Claeskens (2003), see Wang and Zhou (2012) for more details.

The results of the second simulation study are summarized in Table 2.

It can be clearly seen that model averaging and model selection can't improve the mean squared prediction error in this setting. However, super learning provides much better predictive accuracy. In particular, super learning using optimal model averaging (SL+) has the best overall performance.

In the second simulation the most heavily utilized learners are Lasso averaging including squared variables, as well as JMA and MMA with transformations. As expected, optimal model averaging can help to improve predictive accuracy, in particular when used in conjunction with super learning.

The results of the third simulation study are summarized in Table 3 and Figure 1. It can be seen that in a complex longitudinal setup, with 6 follow-up times, and a data-generating process which includes non-linearities and interactions, a couple of learners contribute most to the estimation process; that is, additive models, MMA with squared transformations and JMA with squared transformations, as well as simple GLM's. This implies that even when learners are available which already describe the data-generating process well (here: GAM's and GLM's with interactions), optimal model averaging can still be utilized by super learning and thus be of benefit.

Model mis-specification is a crucial concern when identifying causal parameters (Van der

Table 2: Results of the second simulation study. (a) estimated mean squared prediction error, with standard error, for different model selection and model averaging techniques. Prediction with super learning contains both a set of learners with optimal model averaging techniques (SL+) and without (SL). (b) the weight for each learner, averaged over the simulaton runs, is listed as well.

(a)	Predictive Performance						
	OLS	MS	FMA	BMA	MMA	SL	SL+
MSPE	22.38	22.34	31.72	22.36	22.39	21.47	21.12
s.e.	1.45	1.45	3.09	1.46	1.45	1.41	1.39

(b)	Choice of Learners					
	learner	weight	learner	weight	learner	weight
	MMA	0.0002	LAE	0.0022	JMA	0.0002
	MMA (+Int.)	0.0038	LAE (+Int.)	0.1032	JMA (+Int.)	0.0044
	MMA (+squ.)	0.1588	LAE (+squ.)	0.3405	JMA (+squ.)	0.1588
	GLM (Bayes)	0.0000	GLM (+AIC)	0.0366	GLM (+Int.)	0.0174
	random forest	0.0357	LASSO	0.0024	GLM (+AIC/Int.)	0.0870
	mean	0.0001	GLM	0.0001	GAM	0.0138

Table 3: Results of the third simulation study: bias and coverage for different sets of learners and different interventions.

Intervention	Learner Set	Bias	Coverage
always	without OMA	0.036	90%
always	with OMA	0.036	91%
350/15%/-2	without OMA	0.12	97%
350/15%/-2	with OMA	0.10	97%

Laan and Rose (2011)) and this is the motivation for using super learning in this context. In our example, bias after estimation still exists, for both interventions of interest (Table 3). Using optimal model averaging has only a small benefit in terms of reducing bias in this particular setting.

4 Conclusion

Model averaging in its traditional sense addresses the problem of model selection uncertainty. Because model averaging can still yield biased estimates and imperfect coverage, its main benefit is in identifying associations in a moderate-to-large data set. Such a procedure can also be helpful in an explorative data analysis. However, these estimators wouldn't necessarily be the first choice for quantifying associations as exactly as possible, for complex prediction problems, or for estimation procedures which seek to identify causal parameters.

In contrast, optimal model averaging as proposed in the recent years may not be ideal to take into account model selection uncertainty as their construction principle is not based on interval estimation. However, the idea of optimal model averaging is attractive in analyses which deal with prediction and forecasting problems. Some of these estimators, such like Mallow's Model Averaging, are computationally efficient, robust, and tackle predictions from a different angle. This may benefit existing approaches, such as super learning, where a broad spectrum of learners are required. Super learning techniques are a popular tool in the process of identifying a causal quantity of interested by means of targeted maximum likelihood estimation
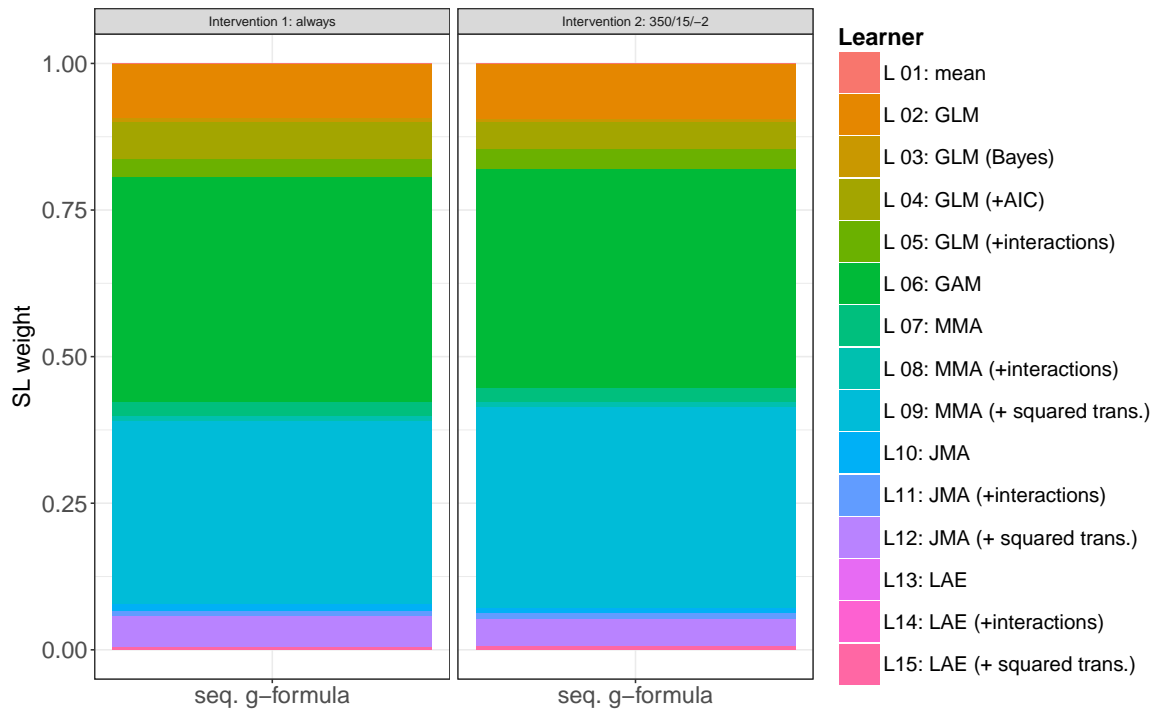
Figure 1: Results of the third simulation study: the weight for each learner, averaged over the simulation runs.

([Gruber and van der Laan](), 2012, [Petersen et al](), 2014). Therefore, the benefit of optimal model averaging techniques may reach far beyond pure prediction problems and play its role in causal analyses.

Our recommendation is that future manuscripts that propose optimal model averaging techniques focus their motivation and data examples around prediction (or the use of prediction in estimating causal quantities) rather than model selection uncertainty questions.

A Software

We have implemented Mallow's Model Averaging, Jackknife Model Averaging, and Lasso Averaging in the *R*-package MAMI ([Schomaker](), 2017a), available at `http://mami.r-forge.r-project.org/`. In addition to this, we have implemented several wrappers that make optimal model averaging easily useable for super learning ([Polley et al](), 2017), and in conjunction with causal inference packages such as `tmle` ([Gruber and van der Laan](), 2012) and `ltmle` ([Lendle et al](), 2017). Available wrappers are explained by calling `listSLWrappers()`, and examples are given in the documentation ([Schomaker](), 2017b).

B Notation and Background on the Sequential g-formula

Consider a sample of size n of which measurements are available both at baseline ($t = 0$) and during a series of follow-up times $t = 1, \ldots, T$. At each point in time we measure the outcome Y_t, the intervention A_t, time-dependent covariates $\mathbf{L}_t = \{L_t^1, \ldots, L_t^q\}$, and a censoring indicator C_t. $\mathbf{L}_t$ may include baseline variables $\mathbf{V} = \{L_0^1, \ldots, L_0^{q_V}\}$ and can potentially contain variables which refer to the outcome variable before time t, for instance Y_{t-1}. The treatment and covariate history of an individual i up to and including time t is represented as $\bar{A}_{t,i} = (A_{0,i}, \ldots, A_{t,i})$ and $\bar{L}_{t,i}^s = (L_{0,i}^s, \ldots, L_{t,i}^s)$ respectively. C_t equals 1 if a subject gets censored in the interval $(t-1, t]$, and 0 otherwise. Therefore, $\bar{C}_t = 0$ is the event that an individual remains uncensored until time t.

The counterfactual outcome $Y_{t,i}^{\bar{a}_t}$ refers to the hypothetical outcome that would have been observed at time t if subject i had received, possibly contrary to the fact, the treatment history $\bar{A}_{t,i} = \bar{a}_t$.

Similarly, $\mathbf{L}_{t,i}^{\bar{a}_t}$ are the counterfactual covariates related to the intervention $\bar{A}_{t,i} = \bar{a}_t$. The above notation refers to *static* treatment rules; a treatment rule may, however, depend on covariates, and in this case it is called *dynamic*. A dynamic rule $d_t(\bar{\mathbf{L}}_t)$ assigns treatment $A_{t,i} \in \{0, 1\}$ as a function of the covariate history $\bar{\mathbf{L}}_{t,i}$. The vector of decisions d_t, $t = 0, ..., T$, is denoted as $\bar{d}_T = \bar{d}$. The notation $\bar{A}_t = \bar{d}$ refers to the treatment history according to the rule $\bar{d}$. The counterfactual outcome related to a dynamic rule $\bar{d}$ is $Y_{t,i}^{\bar{d}}$, and the counterfactual covariates are $\mathbf{L}_{t,i}^{\bar{d}}$.

In Section 3.3 we consider the expected value of Y at time 6, under no censoring, for a given treatment rule $\bar{d}$ to be the main quantity of interest, that is $\psi = \mathbb{E}(Y_6^{\bar{d}})$.

The sequential g-formula can estimate this target quantity by sequentially marginalizing the distribution with respect to $\mathbf{L}$ given the intervention rule of interest. It holds that

$$\mathbb{E}(Y_T^{\bar{d}}) = \mathbb{E}(\mathbb{E}(\ldots \mathbb{E}(\mathbb{E}(Y_T | \bar{A}_T = \bar{d}_T, \bar{\mathbf{L}}_T) | \bar{A}_{T-1} = \bar{d}_{T-1}, \bar{\mathbf{L}}_{T-1}) \ldots | \bar{A}_0 = d_0, \mathbf{L}_0) | \mathbf{L}_0),$$

see for example Bang and Robins (2005). Equation (14) is valid under several assumptions: sequential conditional exchangeability, consistency, positivity and the time ordering $\mathbf{L}_t \rightarrow A_t \rightarrow C_t \rightarrow Y_t$. These assumptions essentially mean that all confounders need to be measured, that the intervention is well-defined and that individuals have a positive probability of continuing to receive treatment according to the assigned treatment rule, given that they have done so thus far and irrespective of the covariate history; see Daniel et al (2013) and Robins and Hernan (2009) for more details and interpretations. Note that the two interventions defined in Section 3 also assign $C_t = 0$ meaning that we are interested in the effect estimate under no censoring.

To estimate ψ one needs to the the following for $t = T, ..., 0$: (i) use an appropriate model to estimate $\mathbb{E}(Y_T | \bar{A}_{T-1} = \bar{d}_{T-1}, \bar{\mathbf{L}}_T)$. The model is fit on all subjects that are uncensored (until $T - 1$). Note that the outcome refers to the measured outcome for $t = T$ and to the prediction (of the conditional outcome) from step (ii) if $t < T$. Then, (ii) plug in $\bar{A}_t = \bar{d}_t$ to predict Y_t at time t; (iii) For $t = 0$ the estimate $\hat{\psi}$ is obtained by calculating the arithmetic mean of the predicted outcome from the second step.

C Data Generating Process in the Simulation Study

Both baseline data ($t = 0$) and follow-up data ($t = 1, \ldots, 12$) were created using structural equations using the R-package `simcausal` (Sofrygin et al, 2017). The below listed distributions, listed in temporal order, describe the data-generating process motivated by the analysis from Schomaker et al (2016). Baseline data refers to region, sex, age, CD4 count, CD4%, WAZ and HAZ respectively (V^1, V^2, V^3, L_0^1, L_0^2, L_0^3, Y_0), see Schomaker et al (2016) for a full explanation of variables and motivational question. Follow-up data refers to CD4 count, CD4%, WAZ and HAZ (L_t^1, L_t^2, L_t^3, Y_t), as well as a treatment (A_t) and censoring (C_t) indicator. In addition to Bernoulli (B), uniform (U) and normal (N) distributions, we also use truncated normal distributions which are denoted by $N_{[a,b]}$ where a and b are the truncation levels. Values which are smaller a are replaced by a random draw from a $U(a_1, a_2)$ distribution and values greater than b are drawn from a $U(b_1, b_2)$ distribution. Values for (a_1, a_2, b_1, b_2) are $(0, 50, 5000, 10000)$ for L^1, $(0.03, 0.09, 0.7, 0.8)$ for L^2, and $(-10, 3, 3, 10)$ for both L^3 and Y. The notation $\bar{\mathcal{D}}$ means "conditional on the data that has already been measured (generated) according the the time ordering".

For $t = 0$:

$$
\begin{aligned}
V^1 &\sim B(p = 4392/5826) \\
V^2|\bar{\mathcal{D}} &\sim \begin{cases} B(p = 2222/4392) & \text{if} \quad V^1 = 1 \\ B(p = 758/1434) & \text{if} \quad V^1 = 0 \end{cases} \\
V^3|\bar{\mathcal{D}} &\sim U(1,5) \\
L_0^1|\bar{\mathcal{D}} &\sim \begin{cases} N_{[0,10000]}(650, 350) & \text{if} \quad V^1 = 1 \\ N_{[0,10000]}(720, 400)) & \text{if} \quad V^1 = 0 \end{cases} \\
\tilde{L}_0^1|\bar{\mathcal{D}} &\sim N((L_0^1 - 671.7468)/(10 \cdot 352.2788) + 1, 0) \\
L_0^2|\bar{\mathcal{D}} &\sim N_{[0.06,0.8]}(0.16 + 0.05 \cdot (L_0^1 - 650)/650, 0.07) \\
\tilde{L}_0^2|\bar{\mathcal{D}} &\sim N((L_0^2 - 0.1648594)/(10 \cdot 0.06980332) + 1, 0) \\
L_0^3|\bar{\mathcal{D}} &\sim \begin{cases} N_{[-5,5]}(-1.65 + 0.1 \cdot V^3 + 0.05 \cdot (L_0^1 - 650)/650 \\ \qquad + 0.05 \cdot (L_0^2 - 16)/16, 1) & \text{if} \quad V^1 = 1 \\ N_{[-5,5]}(-2.05 + 0.1 \cdot V^3 + 0.05 \cdot (L_0^1 - 650)/650 \\ \qquad + 0.05 \cdot (L_0^2 - 16)/16, 1)) & \text{if} \quad V^1 = 0 \end{cases} \\
A_0|\bar{\mathcal{D}} &\sim B(p = 0) \\
C_0|\bar{\mathcal{D}} &\sim B(p = 0) \\
Y_0|\bar{\mathcal{D}} &\sim N_{[-5,5]}(-2.6 + 0.1 \cdot I(V^3 > 2) + 0.3 \cdot I(V^1 = 0) + (L_0^3 + 1.45), 1.1)
\end{aligned}
$$

For $t > 0$:

$$
\begin{aligned}
L_t^1|\bar{\mathcal{D}} &\sim \begin{cases} N_{[0,10000]}(13 \cdot \log(t \cdot (1034 - 662)/8) + L_{t-1}^1 + 2 \cdot L_{t-1}^2 \\ \qquad + 2 \cdot L_{t-1}^3 + 2.5 \cdot A_{t-1}, 50) & \text{if} \quad t \in \{1,2,3,4\} \\ N_{[0,10000]}(4 \cdot \log(t \cdot (1034 - 662)/8) + L_{t-1}^1 + 2 \cdot L_{t-1}^2 \\ \qquad + 2 \cdot L_{t-1}^3 + 2.5 \cdot A_{t-1}, 50) & \text{if} \quad t \in \{5,6\} \end{cases} \\
L_t^2|\bar{\mathcal{D}} &\sim N_{[0.06,0.8]}(L_{t-1}^2 + 0.0003 \cdot (L_t^1 - L_{t-1}^1) + 0.0005 \cdot (L_{t-1}^3) + 0.0005 \cdot A_{t-1} \cdot \tilde{L}_0^1, 0.02) \\
L_t^3|\bar{\mathcal{D}} &\sim N_{-5,5}(L_{t-1}^3 + 0.0017 \cdot (L_t^1 - L_{t-1}^1) + 0.2 \cdot (L_t^2 - L_{t-1}^2) + 0.005 \cdot A_{t-1} \cdot \tilde{L}_0^2, 0.5) \\
A_t|\bar{\mathcal{D}} &\sim \begin{cases} B(p = 1) & \text{if} \quad A_{t-1} = 1 \\ B(p = 1/(1 + \exp(-[-2.4 + 0.015 \cdot (750 - L_t^1) + 5 \cdot (0.2 - L_t^2) \\ \qquad - 0.8 \cdot L_t^3 + 0.8 \cdot t]))) & \text{if} \quad A_{t-1} = 0 \end{cases} \\
C_t|\bar{\mathcal{D}} &\sim B(p = 1/(1 + \exp(-[-6 + 0.01 \cdot (750 - L_t^1) + 1 \cdot (0.2 - L_t^2) - 0.65 \cdot L_t^3 - A_t]))) \\
Y_t|\bar{\mathcal{D}} &\sim N_{[-5,5]}(Y_{t-1} + 0.00005 \cdot (L_t^1 - L_{t-1}^1) - 0.000001 \cdot \left((L_t^1 - L_{t-1}^1) \cdot \sqrt{\tilde{L}_0^1}\right)^2 \\
&\quad + 0.01 \cdot (L_t^2 - L_{t-1}^2) - 0.0001 \cdot \left((L_t^2 - L_{t-1}^2) \cdot \sqrt{\tilde{L}_0^2}\right)^2 \\
&\quad + 0.07 \cdot ((L_t^3 - L_{t-1}^3) \cdot (L_0^3 + 1.5135)) - 0.001 \cdot ((L_t^3 - L_{t-1}^3) \cdot (L_0^3 + 1.5135))^2 \\
&\quad + 0.005 \cdot A_t + 0.075 \cdot A_{t-1} + 0.05 \cdot A[t] \cdot A[t-1], 0.01)
\end{aligned}
$$

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