Multilevel Models Allow Modular Specification of What and Where to Regularize, Especially in Small Area Estimation

Michael Tzen*

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1 Intro

Through the lens of multilevel model (MLM) specification and regularization, this is a connect-the-dots introductory summary of Small Area Estimation, i.e. small group prediction informed by a complex sampling design. While a comprehensive book is (Rao and Molina 2015), the goal of this paper is to get interested researchers up to speed with some current developments. We first provide historical context of two kinds of regularization: 1) the regularization ‘within’ the components of a predictor and 2) the regularization ‘between’ outcome and predictor. We focus on the MLM framework as it allows the analyst to flexibly control the targets of the regularization. The flexible control is useful when analysts want to overcome shortcomings in design-based estimates. We’ll describe the precision deficiencies (high variance) typical of design-based estimates of small groups. We then highlight an interesting MLM example from (Chaudhuri and Ghosh 2011) that integrates both kinds of regularization (between and within). The key idea is to use the design-based variance to control the amount of ‘between’ regularization and prior information to regularize the components ‘within’ a predictor. The goal is to let the design-based estimate have authority (when precise) but defer to a model-based prediction when imprecise. We conclude by discussing optional criteria to incorporate into a MLM prediction and possible entry points for extensions.

2 Rebrand Shrinkage as Regularization

As of 2018, there are roughly 91,100 Google Scholar results when searching with “shrinkage AND statistic”. There are about 49,900 search results for “shrinkage AND machine learning”. The boom can be historically traced to (James and Stein 1961) decomposing a predictor’s Mean Squared Error, (Efron and Morris 1971) evaluating the James-Stein performance of hierarchical priors (multilevel structure), and (Tibshirani 1996) using convex sparsity constraints to shrink mean components via the lasso. Shrinkage has become a general tool in statistics and machine learning. Generally speaking, there are two reasons to use shrinkage:

1. numerical reasons: add suitable constraints in an under-determined system to produce a working estimate.
2. statistical reasons: shedding off variance by taking on bias (incorporating extra information)

The word ‘shrinkage’ gives off the imagery of ‘shrinking towards zero’. There are many scenarios where zero is a good value to adjust your estimates towards (shrink). However, shrinkage does not have to be towards zero. In other scenarios, shrinkage towards a non-zero quantity makes sense. For this reason, the rest of this article will primarily use the term regularize / regularization instead of shrink / shrinkage.

Going forward, we’ll use verbiage in an applied regression context (1). For observation $i$ we have a left hand side ‘outcome’ $y_i$ and a right hand side ‘predictor’ $f()$ consisting of ‘components’ $\beta, X_i, V_i$ and $A_i$. Specifically, we have a $p$-vector of mean components $\beta$, for covariates $X_i$, and variance components $V_i$ and $A_i$. The predicted outcome is $\hat{y}_i$.

*California Center for Population Research, University of California, Los Angeles
\[ \hat{y}_i = f(\beta, X, V_i, A_i) \] (1)

We point out that depending on the scenario, some users care more about the regularized mean-components while others care more about the regularized outcome. Regularized components may further be combined to form regularized outcome predictions. Table 1 categorizes a few scenarios that we will discuss in later sections.

Table 1: Some Possible Regularization Scenarios

| Method         | Estimand          | Default Value | Regularized Towards | Main Tuner |
|----------------|-------------------|---------------|---------------------|------------|
| MLM            | outcome mean      | \( \mu(y_i)^{\text{mle}} \) | \( f(x_i, \beta, \epsilon_i) \) | \( V_i \) |
| Horseshoe      | mean component    | \( \beta^{\text{mle}} \) | 0                   | \( \lambda \) |
| Zellner’s g    | mean component    | \( \beta^{\text{mle}} \) | \( \beta^{\text{prior}} \) | \( g \) |

2.1 Regularize Mean Components

We first focus on the underlying mean components of a predictor. The original lasso (Tibshirani 1996), regularizes the parameters for the mean components \( \beta \) towards zero by optimizing a penalized loss function (2).

\[ \hat{\beta}^{\text{lasso}} = \operatorname{argmin}\{\text{Loss}(y_i, \beta, x_i) + \lambda \| \beta \|\} \] (2)

The original lasso method has a related bayesian version, based on specifying the ‘horseshoe prior’ for the mean component parameters (Carvalho, Polson, and Scott 2009). The horseshoe prior is below in (3)

\[ \beta_p \sim N(0, \lambda^2 \tau^2) \]
\[ \lambda_p \sim \text{Half-Cauchy}(0, 1) \] (3)

An alternative to the lasso, is Zellner’s g-prior introduced in the 1980s. The g-prior regularizes the MLE \( \beta^{\text{mle}} \) towards an arbitrary (possibly non-zero) value \( \beta^{\text{prior}} \). (George and Foster 2000) evaluates Zellner’s g-prior, where we abridge the specification below in (4).

\[ \beta|\psi \sim MVN(\beta^{\text{prior}}, g\psi^{-1}(X'X)^{-1}) \] (4)

2.2 Regularize Outcomes

As formulated in (C. N. Morris 1983), we briefly summarize the normally distributed MLM in equation (5). The MLM-regularized outcomes are \( \theta_i^* \). The observed outcome is \( y_i \) and \( X_i \) are covariates with unknown mean components \( \beta \). Unknown variance components \( A_i \) (possibly parameterized) modify the known variances \( V_i \). Lastly, \( V_i \) and \( A_i \) form \( R_i \), the regularization factor. The regularization factor controls how much regularization occurs between the observed outcome \( y_i \) and the linear predictor \( X_i\beta \). The within group sample size \( n_i \) plays a role in \( V_i \), which ultimately controls the regularization factor \( R_i \).

\[ y_i|\beta_i, A_i \sim N(X_i\beta, V_i + A_i) \]
\[ \theta_i|y_i, \beta, A_i \sim (\theta_i^*, V_i(1 - R_i)) \]
\[ \theta_i^* = (1 - R_i)y_i + R_iX_i\beta \]
\[ R_i = V_i/(V_i + A_i) \] (5)
This MLM-type of regularization for outcomes is sometimes referred to as ‘borrowing strength’ or ‘partial pooling’ across the set of observations \( \{y_i\} \). This verbiage makes sense if, as often done, an exchangeability structure is placed on the variance components of the MLM.

As we’ll get to in the following sections. There is a survey statistics application, called Small Area Estimation, that allows for both regularization types: regularization “between” the outcome and predictor (‘borrowing strength’ through the MLM structure) and “within” the predictor by regularizing its mean components (‘shrinkage’ through prior distributions).

We point out that Small Area Estimation is an overloaded term where some analysts do not consider incorporating the design variance. In a context without complex survey weights, a MLM can be applied but will not allow the design-based variance to control regularization. We are interested in this design-based variance controlled regularization of a MLM’s prediction. Thus, we next introduce design-based statistics which we want to improve through a model.

### 3 Additional Modeling of Design-Based Statistics

There are two frameworks to evaluate the statistical properties of a computed statistic, the design-based or model-based frameworks. When computing a statistic \( T \), the frameworks try to pinpoint where the source of randomness is coming from when taking expectations of a sample statistic, \( E_{\text{design}}\{T\} \) or \( E_{\text{model}}\{T\} \). This facilitates concrete statements of mean squared error, bias, variance, and consistency. (Sterba 2009) provides an overview of the different considerations the evaluating critic must make when choosing a framework scenario. (Skinner and Wakefield 2017) encourages the analyst to consider hybrid evaluation scenarios where the analyst must express whether they are interested in: 1) the super population or a finite population and 2) descriptive estimands or estimands characterizing relations of a system. For our discussion about regularization in MLMs, we’ll initially start with a design-based estimate, then show how certain models use the design information to control regularization. That is, we will look at examples of model-based predictions of finite population characteristics that are informed by the sample design (Pfeffermann and others 2013).

In a data set collected using a probability design, say a probability survey sample \( S \) of individuals \( j \), the analyst typically has access to the design weights \( w_j^{\text{design}} \). Here we point out the design weight could solely represent the sample weight \( w_j^{\text{sample}} \) or it could represent the survey weight \( w_j^{\text{survey}} \) (where additional adjustments have been made to the initial sample weight). See equation (6) where \( \pi_j \) is the sample selection probability for individual \( j \in S \).

\[
\begin{align*}
  w_j^{\text{design}} = \begin{cases} 
    w_j^{\text{sample}} = \frac{1}{\pi_j} & \text{known } \pi_j \\
    w_j^{\text{survey}} = h(w_j^{\text{sample}}) & \text{survey adjustments through } h
  \end{cases}
\end{align*}
\]

Going forward, we use \( w_j^{\text{design}} \) the generic terminology for the design weight. Not only does the analyst need to determine which scenario is represented by their design weights, but they also immediately face the question of “how should I use the design weights?” When the analyst’s goal is descriptive, say to compute sample estimates of finite population quantities (totals or proportions), the design-based framework is usually the de facto option. With that in mind, we first focus on estimates from the design-based framework but show how models can improve them. That is, when right hand side components, possibly from a model, are used to adjust left hand side outcomes, we only care about the adjusted left hand side outcome and how the regularization is controlled.\(^1\)

A primary option for design-based point estimates of a population quantity \( T \) is to apply the design weights to a weighted estimator, say the Horvitz-Thompson estimator, \( \hat{T}_{\text{HT}} = \sum_{j \in S} T_j \frac{1}{\pi_j} \). If the analyst is

\(^1\)This article does not assign field-specific relational interpretations of parameters, i.e. causal interpretations of right hand side parameters. See (Sterba 2009) and (Skinner and Wakefield 2017) for distinctions.
interested in estimates for a subgroup $c$ of individuals $j$, they can include the dirac indicator function $1_{j \in c}$ in their computations, resulting in the subgroup estimates $\hat{T}_{c}^{HT} = \sum_{j \in S} 1_{j \in c} T_j \frac{1}{\pi_j^{design}}$.

An important quantity is the variance of the subgroup estimate. Note that in equation (7), the dirac indicator’s role will zero out certain terms of the variance for units that are not in the subgroup $c$.

$$V(\hat{T}_c^{HT}) = (1 - \frac{n}{N}) \frac{n}{n-1} \sum_{j \in S} \left( 1_{j \in c} T_j \frac{1}{\pi_j^{design}} - \frac{1}{n} \hat{T}_c^{HT} \right)^2$$

Whether the analyst is r-inclined or stata-inclined, there are software examples for calculating subgroup estimates. Analysts can compute the respective variances using taylor-linearization (the delta-method) $\hat{V}_c^{taylor}(\hat{T}_c^{HT})$, or using alternatives like the bootstrap or the jackknife. Going forward, we simplify notation for these design-based estimates of subgroups $c$ as $\hat{T}_c := \hat{T}_c^{HT}$ and $\hat{V}_c := \hat{V}_c^{taylor}(\hat{T}_c^{HT})$.

### 3.1 Performance of Design-Based Statistics

As the name suggests, a design-based estimate has its uncertainty primarily attributed to the randomization distribution used in the sample selection design, see equation (6). These design-based estimates have been called direct estimates.\(^2\) One limitation is that these estimates usually perform fine at group-level units $c$ that have ‘large’ within unit sample size $n_c$, say states, but the performance degrades if the analyst looks at more granular group-level units $c'$ with ‘small’ within unit sample size $n_{c'}$, say census tracts.

The cost-quality assessments at various resolution scales are initially determined by the data provider. For secondary analysis, the analyst may be highly motivated to produce statistics at more granular groupings (sub-populations / sub-domains / sub-areas) than what was initially intended by the designers. An analyst, using modern statistical software packages,\(^3\) can still use their desired resolution in defining cell groups $c$ and compute design-based estimates $\hat{T}_c$ and $\hat{V}_c$. However, the analyst is likely to be underwhelmed at the estimate’s high variance (low precision). In the sub-field of Small Area Estimation, the goal is to improve the performance of these high resolution group unit estimates. Many of the Small Area Estimation methods lean on an underlying model and result in predictions, not estimates, of the groups.

### 3.2 Models with Design Information to Predict Small Group Quantities

To overcome the precision-shortcomings of direct estimates, (Fay and Herriot 1979) used a MLM to improve the direct estimates. The resulting byproduct of the MLM are design-informed model-based predictions for small areas, which we refer to as Small Area Predictions (SAP) going forward.\(^4\) The “small area” $c$ are the observational units for the MLM where the SAP predictions are regularized versions $\hat{T}_c$ of their direct estimate $\hat{T}_c$ counterparts.

The MLM of (Fay and Herriot 1979) is a special case of the MLM-class described in (C. N. Morris 1983), that we generically described in (5). The key application of (Fay and Herriot 1979) is that the direct estimates for unit $c$ are substituted as inputs $i \leftarrow c$ into the data likelihood portion of the MLM, $y_i \leftarrow \hat{T}_c$ and $V_i \leftarrow \hat{V}_c$. As discussed in the Regularize Outcomes section, this results in the MLM regularized prediction $\hat{\theta}_i \leftarrow \hat{T}_c$.

Further, (Fay and Herriot 1979) used a non-informative prior for $\beta$ but no prior for $A_i$. An Empirical Bayes procedure produced the resulting predictions. When viewing this SAP scenario through the language of mixed models, even though $V_i$ is usually an estimate, it is sometimes referred to as the ‘known’ variance of the direct estimate specified in the ‘sampling model’ while $A_i$ is a random effect term specified in the ‘linkage model’ (Rao and Molina 2015).

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\(^2\)A term commonly used to highlight their sole reliance on a unit’s measured data and its design-based probabilities of selection

\(^3\)Using the \texttt{survey} package in R (Lumley 2004).

\(^4\)They have also been called ‘indirect estimates’, to contrast against ‘direct estimates’. This article’s rebranding is to clarify that the primary MLM output of interest are predictions.
The MLM regularization trade-off tries to balance how much of the output prediction $\hat{T}_c$ is composed of the model’s linear-predictor $x_c\beta$ and how much is composed of the direct design-based estimate $\hat{T}_c$. The variance estimates $\hat{V}_c$ control the regularization-factor $R_c$. For a single small group, it’s MLM-regularized prediction $\hat{T}_c$ should rely more on the direct estimate when the direct estimate’s variance is small, (say if the sample size within the small group $c$ is large) but rely more on the linear-predictor when the variance is large.

After (Fay and Herriot 1979), many models to produce SAPs have been proposed, say incorporating spatial terms for variance components in (Mercer et al. 2014). Researchers have also looked at alternative likelihoods where (Rabe-Hesketh and Skrondal 2006) uses pseudo likelihoods and (Chaudhuri and Ghosh 2011) considering empirical likelihoods. For a bayesian treatment, (Chaudhuri and Ghosh 2011) also assessed different priors. Generally, a MLM structure will produce predictions $\hat{T}_c$ that are regularized between the direct-estimate $\hat{T}_c$ and the linear-predictor. However, the key property in SAP models with specific ‘Fay-Herriot type’ regularization is that the direct-estimate’s ‘known’ variance $\hat{V}_c$ should play a role in controlling the amount of regularization.

4 Mix and Match: A MLM with Both Kinds of Regularization

In section 3.2 we saw (Fay and Herriot 1979) apply regularization ‘between’ the direct estimate outcome and a linear predictor, first described in section 2.2, to produce design-informed predictions for small groups. Here we additionally introduce regularization ‘within’ the linear predictor as described in section 2.1. The examples in (Chaudhuri and Ghosh 2011) provide a detailed look at different MLM modeling strategies for SAP. For this discussion on regularization, we focus attention to how (Chaudhuri and Ghosh 2011) studied the behavior of different priors to regularize the mean components $\beta$.

If we first start with a MLM structure with a normal likelihood (8), we can set the stage for the desirable Fay-Herriot type of regularization ‘between’ the direct estimate and a predictor, controlled by the design-based variance.

$$\hat{T}_c|\beta, A_c \sim N(X_c\beta, \hat{V}_c + A_c)$$

$$R_c = \hat{V}_c/(\hat{V}_c + A_c)$$

$$\hat{T}_c = (1 - R_c)\hat{T}_c + R_cX_c\beta$$

(8)

To incorporate the second type of ‘within’ predictor regularization of the mean components $\beta$, (Chaudhuri and Ghosh 2011) applied the g-prior. As discussed earlier in the Regularize Mean Components section, this regularizes $\beta_{mle}$ towards $\beta_{p\text{prior}}$. Therefore, a MLM specified with (8) along with (4) will incorporate both types of regularization. The Fay-Herriot type of regularization between the direct estimate and the predictor is controlled by $R_c$ while the ‘within’ predictor regularization of mean components is controlled by the hyper parameters $g$ and $\beta_{p\text{prior}}$.

Alternatively, we can revisit the horseshoe prior previously described in (3). If the analyst has many covariates (say many higher order interactions), regularizing the mean component parameters towards 0 might be beneficial. Specifying a MLM with (8), to regularize between $\hat{T}_c$ and $X_c\beta$, with the additional horseshoe prior (3) would result in regularized small group predictions $\hat{T}_c$ whose underlying mean components $\beta$ (possibly high dimensional) are regularized towards 0 by the tuning parameter $\lambda$.

With all the flexibility a MLM provides, the analyst should first deliberate how the sample design information is incorporated into the MLM. Usually, the design weights are used one way or another to estimate the direct-estimate’s variance (as in (7)), which are then used in the MLM as the ‘known variance’ (this is how we presented our abridged summary in the proceeding discussion). (Fay and Herriot 1979) supplied the ‘known

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5 Fay uses the parametric normal distribution for the data likelihood. For binary outcomes, (Mercer et al. 2014) uses the asymptotic normal approximation (of the binomial data) for the data likelihood. The data likelihood in (Chaudhuri and Ghosh 2011) is an empirical likelihood where exponential family bartlet identities form the moment constraints.

6 In a single article, (Chaudhuri and Ghosh 2011) ambitiously evaluated a semi-parametric data likelihood along with parametric and non-parametric priors for mean components.
variance’ by backsolving from the coefficient of variation (where design weights were applied to the quantities of the coefficient of variation). Since (Mercer et al. 2014) modeled the MLM likelihood with the normal approximation of binomial outcomes, they backsolved for a binomial effective sample size (starting with scaled design weights to be used as the normal likelihood’s ‘known variance’). Alternatively, (Rabe-Hesketh and Skrondal 2006) first scaled the design weights and then incorporated them into a pseudo-likelihood of their MLM. After that, the analyst should then deliberate if regularizing the components within a predictor is desirable for their application (say towards 0 or $\beta_{\text{prior}}$).

5 Discussion

We have showcased how specifying a MLM is a way to think generally about what and where to regularize to. In Small Area Estimation, the goal is to improve design-based estimates through a model’s prediction. Inspired by an example in (Chaudhuri and Ghosh 2011), we have showcased how a MLM is a flexible model that can incorporate two kinds of regularization: ‘within’ the model’s predictor mean components and, more importantly, the Fay-Herriot type of regularization ‘between’ the predictor and the direct design-based estimates where the regularization is controlled by the variance of the design-based estimates.

To figure out if a MLM based method is a good approach for the analyst, we provide a list of questions a consumer of survey data should ask themselves. Do you have a direct mean and variance estimate that already incorporates design weights (6)? Do you want to improve group level direct estimates via design-informed model-based predictions? Do you want your predictions to be regularized between the design-based estimate and the predictor (5)? Further, do you want this regularization between the design-based estimate and the predictor controlled by the design-based variance (8)? Do you want to optionally regularize the components within the predictor (3) or (4)?

If the reader thinks model-based predictions of small groups is the right method for them, (Rao and Molina 2015) is an overarching book exposing the technical details and various extensions for Small Area Estimation. When considering the extensions, one thing for readers to keep in mind is that these methods are all about outcome prediction and regularization. Some extensions incorporate additional variance component structures, say spatial random effects as in (Mercer et al. 2014). This additional spatial variance component would add ‘local’ regularization towards neighboring groups alongside the ‘global’ regularization towards the predictor.

Along with modeling extensions, (Rao and Molina 2015) also discusses two different topics, that we frame here as loosely related, calibration of design weights via auxiliary totals and benchmarking of small group estimates. The loose overlap is the high level motivating criteria; calibration and benchmarking imposes “coherence to target quantities”. While there is an immediate difference in deliverables, calibration outputs design weights as a byproduct whereas benchmarking still outputs a (modified) group prediction, there is also a difference in the type of data source used for the target quantities. For example, weight calibration is a method to produce a set of output calibrated weights where initially supplied weights are constrained so that totals using the calibrated weights are in close agreement with totals from an ideal external data source, $w_i^{\text{calibrate}} \leftarrow \text{calibrate}(w_i^{\text{survey}}, x_i^{\text{auxiliary}})$, see (Särndal 2010). However as described in (Steorts 2014), “benchmarking a small area estimate” is a method to constrain the group-level model-based predictions so that a larger group aggregate of small group predictions are in close agreement with the direct design-based estimate of that same larger group, $\hat{y}_c^{\text{benchmark}} \leftarrow \text{benchmark}(\sum_{c \in L} \hat{y}_c, \sum_{c \in L} \hat{y}_c)$ where $c \in L$ represents that small group $c$ is an element of the larger grouping $L$. Further, calibration uses an external data source for the targets (say an administrative registry) while benchmarking uses its own internal data source (the direct design-based estimate).

There are scenarios where researchers advocate supplying small group totals as auxiliary information into calibration procedures directly, as in the ‘GREG Domain Estimation’ section in (Rao and Molina 2015).  

7say, the $h(.)$ adjustment in equation (6)

8This is related to an alternative framework, model-assisted design-based estimates (Särndal 2010). See (Breidt, Opsomer, and others 2017) for new developments and (Skinner and Wakefield 2017) for the design-based or model-based context.
On the other end, researchers (Steorts and Ugarte 2014) have advocated that external data sources can also be used in benchmarking small group predictions. At a high-level, benchmarking a MLM prediction to an external data source is conceptually similar to the Multilevel Regression and Poststratification (MrP) approach of (Ghitza and Gelman 2013). However, a fundamental difference is that MrP simply uses external targets as weights to post-stratify MLM predictions whereas calibration and benchmarking use constrained matching machinery to impose coherence to their respective targets.

Discussing this loose overlap between calibration and benchmarking is an interesting methodological note. To not confuse the reader, we describe the usual “order of operations” an analyst may go through when carrying survey data through the process of producing model-based small group predictions.

0. Calibration (produce unit level weights)
   - commits the initial design weights as primary citizens
   - appeals to external authority of auxiliary data to modify initial weights
   - calibrated weights can immediately be used to produce ‘design-based’ estimates and their variances

1. Predict Outcomes (MLM incorporating design variance)
   - predictor based on covariate features
   - the ‘Fay-Herriot type’ of regularization is controlled by the design variance
   - optionally regularize mean components

2. Benchmark to Larger Groupings
   - the benchmark targets are usually direct estimates (appeal to internal authority of large grouping direct estimate)
   - optionally incorporate external data source into benchmarking of predictions (appeal to external authority of large grouping auxiliary data)

In special cases, the above order of operations has a nice side effect. If the design weights are first calibrated and the analyst then fits a particular MLM for small group predictions, then the outcome predictions have the nice property of being ‘self-benchmarked’ when using the method of (You and Rao 2002).

We mentioned the methodological comparison between calibration and benchmarking so that we can motivate demographers to keep up the crucial work of producing high quality demographic data. As illustrated in all the examples above, not only are the survey outcomes important, but a good measure of the underlying population is equally important, if not more. The second edition of (Rao and Molina 2015) had to remove the section on formal demographic methods.

Formal demographers can apply SAP techniques to their own demographic application. On the other end, we highlight two entrypoints for demographers who want to improve SAP methodology. Upstream, in specifying tailored demographic predictors in the ‘linking model’ (say non-linear terms motivated by demographic procedures like the Brass model or the Gompertz model). The challenge would be to incorporate ‘symptomatic’ demographic approaches into SAP methods. Downstream, in producing population forecasts to be used as calibration and/or benchmarking targets (say forecasts of demographic rates as in (Raftery et al. 2012)). Whether up or downstream, demographers have the useful ability to factor in the “balancing equation” of population change (more generally, incorporate knowledge of demographic processes).

Researchers in statistics and machine learning that are developing new predictive methods should ask if a proposed method allows for the Fay-Herriot type of regularization controlled by the variance of the direct design-based estimate. An immediate heuristic to incorporate predictive methods into a small area prediction system might be to consider a sequential approach. First, produce a model based prediction via trees, kernel methods, boosting, ensembling, etc. Then, incorporate the prediction as a right hand side term in a MLM structure. The second stage (via the MLM structure) would allow the Fay-Herriot type of regularization of the direct estimate towards the first-stage prediction. It would be interesting to develop methods that incorporate prediction error metrics (from the first stage) as a regularization controller in the second stage MLM. This heuristic would be a modern take on ‘composite estimation’ using current predictive techniques for the ‘indirect’ estimators as described in (Ghosh and Rao 1994).
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