Estimation of Over-parameterized Models via Fitting to Future Observations

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Yiran Jiang
Department of Statistics
Purdue University
West Lafayette, IN 47907
jiang693@purdue.edu

Chuanhai Liu
Department of Statistics
Purdue University
West Lafayette, IN 47907
chuanhai@purdue.edu

Abstract

From a model-building perspective, in this paper we propose a paradigm shift for fitting over-parameterized models. Philosophically, the mindset is to fit models to future observations rather than to the observed sample. Technically, choosing an imputation model for generating future observations, we fit over-parameterized models to future observations via optimizing an approximation to the desired expected loss-function based on its sample counterpart and an adaptive simplicity-preference function. This technique is discussed in detail to both creating bootstrap imputation and final estimation with bootstrap imputation. The method is illustrated with the many-normal-means problem, $n < p$ linear regression, and deep convolutional neural networks for image classification of MNIST digits. The numerical results demonstrate superior performance across these three different types of applications. For example, for the many-normal-means problem, our method uniformly dominates James-Stein and Efron's $g$-modeling, and for the MNIST image classification, it performs better than all existing methods and reaches arguably the best possible result. While this paper is largely expository because of the ambitious task of taking a look at over-parameterized models from the new perspective, fundamental theoretical properties are also investigated. We conclude the paper with a few remarks.

Keywords: Auto-Modeling, Bootstrap, Image Classification, Multiple Imputation, Resampling

1 Introduction

Over-parameterized models are useful in statistical analysis. The factor analysis model provides as such a well-known but simple example. These models are handled traditionally by postulating parameter restrictions for identifiability. Such parameter restrictions may not be necessary in practice, for example, when the estimated models are used for prediction or, more generally, estimation of the data sampling distribution. As a matter of fact, the idea of creating efficient expectation-maximization algorithms, as shown in the parameter-expanded expectation-maximization algorithm (Liu et al., 1998), is to make use of over-parameterized models by activating restricted parameters. Nevertheless, over-parameterized models have become more popular nowadays and more broadly, due to the use of machine learning models such as deep learning for big data.

With over-parameterization, deep learning appears to have achieved remarkable successes in quite a few application areas with massive data, including image classification. One explanation is that over-parameterized deepnets offer a flexible and yet efficient approximation to non-linear functions with varied structures, which allow for automated modeling of massive data in terms of response surface. Fitting over-parameterized models has however appeared to be a challenging or even problematic task in applications. What is practically important is that fitted deepnets with "overestimated" depth can also potentially suffer from losing good statistical properties such as efficiency and robustness (c.f., Nalisnick et al., 2019). Another type of somewhat disturbing phenomena scientists are concerned with is the replicability and reproducibility of model fitting when it is largely dependent on parameter tuning.

*Corresponding author.
A fundamental implicit assumption on over-parameterized deepnets is that there exist some parameter values, not necessarily unique, such that the corresponding models can fit the model adequately. In other words, deepnets should be sufficiently over-parameterized so that methods can be developed in the hope to automate the critical process of statistical modeling indispensable for the high quality of scientific inference. For small datasets, modeling is often done with a deep understanding of potential data generation mechanisms and careful exploratory data analysis (Tukey and Graves-Morris 1983; Tukey 1962, 1977) to discover data structures in terms of factorization of joint distributions of unobserved quantities.

With big data, one can still make use of a practitioner’s armamentarium for small data, for example, through the method of divide-and-combine in a parallel computing environment. However, among new challenges that are unique to big data analysis is that more mathematically sophisticated functions are utilizable to provide more accurate inference than simple functions that are typically used for small data. In other words, in the modeling stage of statistical inference, models to be built are not necessarily representing data generation mechanism but an mathematical representation of the simplified view of the data analyst’s understanding of uncertainty structure in the population through the observed data (see Bernardo and Smith (2009) and Le and Clarke (2017) for a different view from a Bayesian theory perspective). Thus, for efficient and valid inference with big data, it demands methods for automated exploratory data analysis that are formulated to capture essence of subjective uncertainty assessments and decision with the preference to simpler models. Our understanding is that the essence is to build a model that leads to valid and efficient prediction of observations from the underlying target population.

Methods of prediction have proved to be powerful in model checking, including Bayesian predictive checking of Box (1980) and postictive checking of Rubin (1984), and in model selection. In model selection, a model is often chosen to have a lowest prediction error among a set of candidates. Implementation of methods of prediction is typically based on the old idea of cross-validation with the key references Stone (1974, 1977), Geisser (1975), and (Efron and Tibshirani 1994, p. 255; and references therein).

Here from a model-building perspective, we propose a paradigm shift for fitting over-parameterized models. The mindset is to fit models to future observations rather than to the observed sample. Technically, choosing a model, called the imputation model, for generating future observations, we fit over-parameterized models to future observations via optimizing an approximation to a desired expected loss-function. For a simple imputation method, bootstrapping-based imputation models are focused here for explanation. The loss-function is based on its sample counterpart and an adaptive simplicity-preference or penalty function, which, unlike the commonly used approach, does component-wise penalization on model parameters. This technique is applied to both creating bootstrap imputation and final estimation with bootstrap imputation. For convenience, according to Remark 2.2, we call the proposed method Auto-Modeling (AM).

The rest of the paper is arranged as follows. Section 2 presents the general framework of the proposed method, with numerical methods presented in Section 3. Section 4 contains relevant fundamental theoretical results. Applications of the method are given in Section 5 for estimation of many-normal-means, $n < p$ linear regression, and deep convolutional neural networks (CNNs) for image classification of MNIST digits. Section 6 concludes with a few remarks.

## 2 The General Framework

### 2.1 The setting

Suppose that a sample $S = \{(x_i, y_i) : i = 1, \ldots, n\}$ of measurements $(x, y)$ on each of $n$ items from a population $\mathbb{P}$ is available and that the sample is modeled by

$$Y \mid x \sim \mathbb{P}^{(n)}_{x, \theta} \quad (Y \in \mathbb{Y}, x \in \mathbb{R}^p) \quad (2.1)$$

with unknown parameter $\theta \in \mathbb{R}^p$. The dimension of the parameter $\theta$ depends on $n$ in general. When it is appropriate, we also write $(X, Y) \sim \mathbb{P}^{(n)}_{\theta}$, $(Y \in \mathbb{Y}, X \in \mathbb{R}^q, \theta \in \mathbb{R}^p)$. In such a case, we assume that the distribution of $X$ is independent of $\theta$ and the problem of interest remains to be on $\mathbb{P}^{(n)}_{x, \theta}$ in (2.1).

Let $\ell(\theta \mid x, y)$ be the log-likelihood function of $\theta$, based on the model $\mathbb{P}^{(n)}_{\theta}$, given the observation $(x, y)$. Take

$$L(\theta \mid x, y) = -\ell(\theta \mid x, y) \quad (2.2)$$

to be the loss function. From the modeling perspective elaborated in Section 1, we define the best model as a $\mathbb{P}^{(n)}_{x, \theta}$ that minimizes the expected loss with respect to the population, that is, $\mathbb{F}_{x, \theta}$ with some $\theta$ in

$$\Theta_x = \left\{ \theta : E_{(X,Y) \sim \mathbb{P}} [L(\theta \mid X, Y)] = \min_{\tilde{\theta}} E_{(X,Y) \sim \mathbb{P}} [L(\tilde{\theta} \mid X, Y)] \right\} \quad (2.3)$$
This is elaborated further by the following simple remarks. More discussion is provided in Section 2.2 in terms of validity and efficiency from a modeling perspective.

**Remark 2.1.** The family of models is based on the sample. The best model is defined as the one in the family of models \( \mathbb{P}_\theta (\theta \in \Theta_*) \), that fits the true population with minimal average loss.

**Remark 2.2.** The notion of statistical models potentially dependent on sample size has been recognized in statistical literature, for example, in non-parametric statistics underlying the sieve method; see Grenander (1981), Geman and Hwang (1982), Shen et al. (1999), Wasserman (2006), and references therein. Our discussion is more on its generality from modeling with small data, where this notion is implicit, to modeling with big data, where simple models appear to be limited in capturing model information that data can provide. It is the latter that has motivated our use of the term auto-modeling in this paper.

### 2.2 Validity and Efficiency

The notion of the best model introduced above from the modeling perspective leads not only to the new approach to model fitting in Section 2.3 but also to an alternative conceptual understanding of model evaluation. For our discussion of model evaluation, we introduce the concepts of validity and efficiency. Our notion of validity assumes that models ought to depend on the observed data in general and sample size in particular. This explains the notation \( \mathbb{P}_{\pi, \theta} \) in (2.1). This concept of asymptotic validity or, simply, validity concerns the behavior of \( \mathbb{P}_{\pi, \theta} \) as \( n \) goes to infinity, while the concept of efficiency concerns comparisons of different models in terms of finite-sample performance. More precisely, we define

**Definition 2.1 (Validity).** A modelling strategy is said to be valid iff

\[
\lim_{n \to \infty} \mathbb{P}_{\pi, \theta} = \mathbb{P}
\]

weakly for any \( \theta \in \Theta_* \) and some distance measure for probability distributions \( \delta(\cdot, \cdot) \).

**Definition 2.2 (Efficiency).** Consider two models \( \mathbb{P}_{1, \theta}^{(n)}, \theta \in \Theta \subseteq \mathbb{R}^p_1 \) and \( \mathbb{P}_{2, \xi}^{(n)}, \xi \in \Xi \subseteq \mathbb{R}^p_2 \), with bounded likelihood functions for a fixed sample size \( n \) and some distance measure \( \delta(\cdot, \cdot) \). Model 1 \( \mathbb{P}_{1, \theta}^{(n)} \) is said to be more efficient than Model 2 \( \mathbb{P}_{2, \xi}^{(n)} \) iff \( E_{(X,Y) \sim \mathbb{P}}[L_1(\theta|X,Y)] = \min_{\theta \in \Theta_*} E_{(X,Y) \sim \mathbb{P}}[L_1(\theta|X,Y)] \) and \( \xi \in \Xi_* = \{ \xi : E_{(X,Y) \sim \mathbb{P}}[L_2(\xi|X,Y)] = \min_{\xi \in \Xi} E_{(X,Y) \sim \mathbb{P}}[L_2(\xi|X,Y)] \} \), where \( L_1 \) and \( L_2 \) are the loss functions of models \( \mathbb{P}_{1, \theta}^{(n)} \) and \( \mathbb{P}_{2, \xi}^{(n)} \), respectively.

The purpose of defining validity and efficiency is to organize data analyst’s creative thoughts in modeling, in the hope to provide a type of deep understanding of modeling at a high level. Models are mathematically simple representations of data analyst’s understanding of \( \mathbb{P} \) from the observed data and subject-matter information (with uncertainty). Accordingly, models, as simple-but-not-simpler approximations to \( \mathbb{P} \), depend on the observed data and often change as more data are available. This understanding is somewhat different from the Box school of view marked by the famous Box’s aphorism “All models are wrong but some are useful” (Box (1976)). Although applied statisticians have much to say about Box’s aphorism, different existing views can be found in many places, including the comments “it does not seem helpful just to say that all models are wrong” by Cox (1995) and “guiding principle of modern statistics” by Bickel and Doksum (2016). Perhaps, the statement of John von Neumann (1947), “Truth is much too complicated to allow anything but approximation” is more relevant in big data modeling. For more discussion from an applied statistician’s perspective, see Rubin (2019).

The definition of validity is both an importance of the scientific attitude in modeling and a guidance in the sense of choosing a model that, when generalized for data of increasing sample size, reduces modeling error. Modern deepnets provide a good example along this direction (Section 5).

While not verifiable in practice, the definition of efficiency provides the essential guiding principles of building models for the population \( \mathbb{P} \), i.e., future observations. More specifically, it emphasizes on the importance of modeling for future observations and, thereby, suggests that in the context of auto-modeling with over-parameterized models, an imputation method be used to approximate the population.
2.3 An Imputation and Estimation algorithm

The above discussion motivates our new method of finding an approximate solution to the desired optimization problem

\[ \hat{\theta} = \arg \min_\theta E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] \]  

by optimizing its sample counterpart, with a preference for simple models to control the deviation of the estimate of \( \theta \) from (2.4). Such a simplicity-preference function generates the usual penalty function and can be defined as \( \pi^{(n)}(\theta, \lambda) \), \( \theta \in \Theta \), where \( \lambda \in \Lambda \) is a set of hyper-parameters. Thus, the sample counterpart allowing for simplicity preference given by

\[ G_\hat{\theta}(\theta, \lambda) = E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] + \pi^{(n)}(\theta, \lambda) = \frac{1}{n} \sum_{i=1}^{n} L(\theta | x_i, y_i) + \pi^{(n)}(\theta, \lambda) \]  

(2.5)

where \( \hat{P} \) denotes the empirical distribution defined by the sample \( \{(x_i, y_i) : i = 1, \ldots, n\} \).

The use of \( \pi^{(n)}(\cdot, \cdot) \) here is two-fold: (i) It serves as an approximation to \( E_{(X,Y) \sim \hat{P}}[L(\theta | x, Y)] - E_{(X,Y) \sim \hat{P}}[L(\theta | x, Y)] \) in a small neighborhood of the estimate \( \hat{\theta} \); and (ii) When there is an observed discrepancy between \( E_{(X,Y) \sim \hat{P}}[L(\theta | x, Y)] \) and \( E_{(X,Y) \sim \hat{P}}[L(\theta | x, Y)] \), it provides a way of shrinking toward simpler models by restricting some \( \hat{\theta}_i \)‘s to near zero, for appropriate parameterization of \( \theta \). For this purpose, here in this paper we take \( \pi^{(n)}(\theta, \lambda) \) to be

\[ \pi^{(n)}_\lambda(\theta) = \sum_{i=1}^n \lambda_i |\hat{\theta}_i| \quad (\lambda_i \geq 0; i = 1, \ldots, n) \]  

(2.6)

which is a type of generalized \( L_1 \)-penalty for regularization and variable selection in the literature. Alternative forms of \( \pi^{(n)}_\lambda(\theta) \) can be used. For example, a type of generalized \( L_2 \)-penalty is used for image classification in Section 5.

Note that the target objective function can be written as

\[ E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] = G_\hat{\theta}(\theta, \lambda) + V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda) \]  

(2.7)

where

\[ V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda) = E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] - E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] - \pi^{(n)}(\theta, \lambda) \]  

(2.8)

When \( G_\hat{\theta}(\theta, \lambda) \) is minimized over \( \theta \) at \( \theta = \hat{\theta} \) for given \( \lambda \), the remaining term \( V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda) \) serves as a measure of validation. It is desirable to have \( \lambda \) chosen in such a way that the ultimate objective function \( E_{(X,Y) \sim \hat{P}}[L(\theta | X, Y)] \) is minimized and, thereby, one looks for a solution to have

\[ \frac{\partial V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda)}{\partial \theta_i} = 0 \]  

(2.9)

for all \( i = 1, \ldots, p \).

An alternative condition weaker than (2.9) is considered here in this paper. As a criterion for model checking in model building, the validation function \( V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda) \) defined in (2.8) is required to be approximately a constant in a neighborhood of \( \hat{\theta} \). This leads to the adaptive choice of \( \lambda \) to be obtained by optimizing over coefficients of the Taylor expansion of the validation function \( V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda) \) at \( \theta = \hat{\theta} \). For the choice of \( \pi^{(n)}(\cdot, \cdot) \) given in (2.6), the components of the adaptive parameter \( \lambda \) are given by

\[ \hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{\theta}, \hat{\theta}}(\theta, \lambda)}{\partial \theta_i} \right| \]  

(10.10)

for all \( i = 1, \ldots, p \).

Thus, the corresponding algorithmic scheme is readily available, provided that we have a satisfactory approximation to \( \hat{P} \) or an imputation of \( \hat{P} \), especially when, it is defined as the empirical distribution on imputed future observations. Here, we use a natural bootstrap-type method of multiple imputation. More precisely, a way of creating one future observation is summarized into the following three-step imputation algorithm.

Algorithm 2.1 (Bootstrap Imputation). One future observation \((x, y)\) is created in the following three steps:

Step 1. Take a bootstrap resampled data \( \{(\tilde{x}_i, \tilde{y}_i) : i = 1, \ldots, n\} \), drawn from the original sample data \( \{(x_i, y_i) : i = 1, \ldots, n\} \) with replacement. Denote by \( \tilde{P} \) the corresponding empirical distribution.
Step 2. Find the bootstrap estimate $\hat{\theta}$, that is, $\hat{\theta}$ is obtained by minimizing $G_{\hat{\theta}}(\theta, \lambda)$ over $\theta$ subject to

$$\hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda)}{\partial \theta_i} \right| \quad (i = 1, \ldots, p) \quad (2.11)$$

Step 3. Draw $x$ from $\{x_i : i = 1, \ldots, n\}$ at random and simulate $y$ from the fitted predictive model obtained in Step 2.

Give an imputation model such as the Bootstrap imputation, the final estimation of $\theta$ and $\lambda$ is straightforward. This is summarized into the following algorithm.

Algorithm 2.2 (Estimation). Let $Q$ denote an imputation distribution. Then the estimation of $\theta$ based on the sample $S = \{(x_i, y_i) : i = 1, \ldots, n\}$ is obtained by minimizing $G_{\hat{\theta}}(\theta, \lambda)$ over $\theta$ subject to

$$\hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda)}{\partial \theta_i} \right| \quad (2.12)$$

3 Numerical Optimization Methods

Numerical optimization methods for the proposed estimation method appear to be important, except for simple artificial examples that allow for analytic solutions. An intriguing problem here is to find a pair of solutions $\theta$ and $\lambda$ that minimize both $G_{\hat{\theta}}(\theta, \lambda)$ and $V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda)$, as functions of $\theta$, at $\theta = \hat{\theta}$ for some $\lambda = \hat{\lambda}$. Here we consider two simple numerical methods. For simplicity, we focus on the case $\partial V_{\hat{\theta}}(\theta, \lambda)/\partial \theta = 0$ at the numerical solution.

3.1 The method of Lagrange multipliers

A conceptual straightforward numerical method is to apply the method of Lagrange multiplier to the constrained minimization

$$\min_{\theta, \lambda} V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda) \quad (3.1)$$

subject to the system of constraints $\partial G_{\hat{\theta}}(\theta, \lambda)/\partial \theta = 0$. In this case, the Lagrange function of $(\theta, \lambda, \phi)$ to be minimized becomes

$$g(\theta, \lambda, \phi) = V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda) + \phi \frac{\partial G_{\hat{\theta}}(\theta, \lambda)}{\partial \theta} \quad (\theta \in \Theta, \lambda \in \Lambda, \phi \in \mathbb{R}^p). \quad (3.2)$$

This Lagrange function can be minimized numerically using, for example, coordinate descent methods (Wright 2015).

3.2 A coordinate descent algorithm

Note that even with simple gradient based methods, it requires evaluation of the second-order derivatives of $G_{\hat{\theta}}(\theta, \lambda)$ in (3.2). For problems with large $p$, this approach can be computationally difficult. In this case, the following simple coordinate descent algorithm can be used. Recall that solutions $(\hat{\theta}, \hat{\lambda})$ satisfy the following two conditions

$$0 = \frac{\partial G_{\hat{\theta}}(\theta, \lambda)}{\partial \theta} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(\theta|x_i, y_i)}{\partial \theta} + \frac{\partial \pi^{(n)}(\theta, \lambda)}{\partial \theta} \quad (3.3)$$

$$0 = \frac{\partial V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda)}{\partial \theta} = E_{(X, Y) \sim P} \left[ \frac{\partial L(\theta|X, Y)}{\partial \theta} \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(\theta|x_i, y_i)}{\partial \theta} - \frac{\partial \pi^{(n)}(\theta, \lambda)}{\partial \theta} \quad (3.4)$$

This motivates a coordinate algorithm that takes (3.4) as the partial derivatives with respect to $\lambda$. More specifically, set $k \leftarrow 0$, choose starting values $\theta^{(0)}$ and $\lambda^{(0)}$, and

repeat

1. Compute $\frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(\theta|x_i, y_i)}{\partial \theta}$ and $E_{(X, Y) \sim P} \left[ \frac{\partial L(\theta|X, Y)}{\partial \theta} \right]$ at the current estimate $\theta^{(k)}$;
2. Obtain $\lambda^{(k+1)}$ toward the target (3.4);
3. Obtain $\theta^{(k+1)}$ toward the target (3.3);
4. $k \leftarrow k + 1$;

repeat
until termination test satisfied.

The problem of updating \( \lambda^{(k+1)} \) in Step 2 can be implemented to minimize

\[
\left\| \frac{\partial V_{n,P}(\theta, \lambda)}{\partial \theta} \right\|_2 = \left\| E_{(X,Y) \sim P} \left[ \frac{\partial L(\theta | X, Y)}{\partial \theta} \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(\theta | x_i, y_i)}{\partial \theta} - \frac{\partial \pi^{(n)}(\theta, \lambda)}{\partial \theta} \right\|_2
\] (3.5)

over \( \lambda \).

A stochastic coordinate descent algorithm can be easily obtained as a stochastic variant of the above algorithm by replacing Steps 2 and 3 with, for example, corresponding to the ADAM updates \( \text{[Kingma and Ba, 2014]} \). This variant is used in Section 5.3 for the deep learning example. These simple algorithms are used in this paper. For all the numerical examples in this paper, they produce satisfactory convergence results. Formal theoretical properties of these numerical methods will be reported elsewhere.

## 4 Theoretical Considerations

For clarity in organizing our thoughts on theoretical and practical issues, we start with Figure 1, a pictorial representation of the main components of the proposed framework introduced in Section 2. For simplicity purpose, consider \( \tilde{P} \) to be \( \{(x_i, y_i)\}_{i=1}^{n} \) (sample without replacement) in the theoretical investigation. While the main components involve different distributions, the main concerns are on the validity of \( P_{\theta}^{(n)} \), \( \theta \in \Theta \) and the distance between the estimated \( P_{\theta}^{(n)} \) and the true but unknown population \( \tilde{P} \).

| (Combined) Estimation | Bootstrap Imputation |
|-----------------------|----------------------|
| True \( P \)          | Data \( \{(x_i, y_i)\}_{i=1}^{n} \) |
| Imputed \( Q^{(n)} \) | \( \tilde{P} = \{(\tilde{x}_i, \tilde{y}_i)\}_{i=1}^{n} \) |
|                      | \( \sum_{j=1}^{B} \) [sample with/without replacement] |
| Optimal \( P_{\theta}^{(n)} \), \( Q_{\theta}^{(n)} \) | Optimal \( \hat{P}_{\theta}^{(n)} \) |
| Estimated \( P_{\theta}^{(n)} \) | Estimated \( \hat{P}_{\theta}^{(n)} \) |
| Model \( P_{\theta}^{(n)} \), \( \theta \in \Theta \) | Model \( \hat{P}_{\theta}^{(n)} \), \( \theta \in \Theta \) |
| Data \( \{(x_i, y_i)\}_{i=1}^{n} \) | Data \( \{(\tilde{x}_i, \tilde{y}_i)\}_{i=1}^{n} \) |

**Figure 1:** The distributions involved in the proposed procedure. The left column is the list of True \( (\tilde{P}) \), imputation \( (Q^{(n)}) \), data or empirical \( (\tilde{P}) \), and estimated \( (P_{\theta}^{(n)}) \). The right column corresponds to that of the left column, but for the bootstrap method of multiple imputation of the missing population. The symbol \( \sum_{j=1}^{B} \) between the two columns stands for a mixture of \( B \) Bootstrapped populations. The optimal distributions \( P_{\theta}^{(n)} \), \( Q_{\theta}^{(n)} \), and \( \tilde{P}_{\theta}^{(n)} \) are used in the theoretical investigations in Section 4.

The theoretical support for the proposed procedure is based on the familiar observations of the theory of using likelihood-loss functions and Kullback-Leibler divergence (e.g., \( \text{Lehmann, 1983} \), \( \text{Pardo, 2006} \)). What is new in the proposed procedure is that in addition to fitting the observed data via maximum likelihood estimation, it requires explicitly reduction of the divergence between the fitted model \( P_{\theta}^{(n)} \) and a surrogate population \( Q^{(n)} \), which we refer to as the imputed population. The additional requirement is obtained by the use of simplicity preference function. Using the Kullback-Leibler divergence measure, the optimal efficiency of the model \( \{P_{\theta}^{(n)} : \theta \in \Theta \} \) is given by the model error

\[
D_{KL}(\tilde{P}, \hat{P}_{\theta}^{(n)}) = \min_{\theta \in \Theta} D_{KL}(\tilde{P}, P_{\theta}^{(n)}) \quad (4.1)
\]
Moreover, the model is said to be strictly over-parameterized if a best model with more zero parameter estimations can
be achieved by shrinkage.

Accordingly, for a given data set \( \{(x_i, y_i)\}_{i=1}^n \), methods of estimation strive for reducing the estimation error

\[
D_{KL}(\hat{\theta}^{(n)}_\theta, \theta^*_\theta)
\]  

4.1 Automated Optimal Shrinkage

Consider the auto-modeling operator \( \mathcal{A}_\theta : \mathbb{P}_{\text{obs}} \times \mathbb{P}_{\text{fut}} \rightarrow \mathbb{R}^p \), where \( \mathbb{P}_{\text{obs}} \) denotes the currently observed distribution
and \( \mathbb{P}_{\text{fut}} \) denotes the distribution for the future observations. The projected \( p \)-dimensional vector is the estimated
parameter vector by optimizing the auto-modeling objective function given by (2.7), which, in this case is specified as

\[
E_{(X,Y)\sim P_{\text{fut}}}[L(\theta|X,Y)] = G_{\mathbb{P}_{\text{obs}}} (\theta, \lambda) + V_{\mathbb{P}_{\text{fut}}, \mathbb{P}_{\text{obs}}} (\theta, \lambda)
\]  

(4.3)

Following this notation, the auto-modeling estimator in general case can be written as

\[
\theta^{(n)}_{AM} = \mathcal{A}_\theta^{(n)} (\mathbb{P}, \mathbb{P})
\]  

(4.4)

Note that the estimation is related to \( n \), since by assumption the models ought to depend on the observed sample size,
as is stated in Section 2. Furthermore, since the true distribution \( \mathbb{P} \) is unknown in practice, this is also the optimal estimator obtained by auto-modeling, which explains the notation used on the left hand side of the equation.

The main conclusion obtained in the next theorem requires the over-parameterization assumption. Firstly, we define the
parameter space \( \Theta_\Lambda \) as follows.

**Definition 4.1 (Parameter Space for Simpler Models).** The parameter space for parameters that gives a simpler model is defined as

\[
\Theta^{(n)}_\Lambda = \{ \arg \min_{\theta} G_\theta (\theta, \lambda) | \lambda \in \Lambda \}
\]  

(4.5)

with a specific type of simplicity-preference function.

Conceptually, (4.5) defines the space for estimations that can be obtained by fitting the model on the observed data along with some type of shrinkage. An example that is well-known in statistics can be seen by considering the linear regression model with simplicity-preference function \( \pi(\theta, \lambda) = \lambda \sum_i |\theta_i| (i = 1, \ldots, p) \) and \( \Lambda := \{ \lambda \lambda \geq 0 \} \), where \( \lambda \) is a scalar. In this case, \( \Theta_\Lambda \) denotes the Lasso solution path for the fitted linear regression model, which is discussed in Efron et al. (2004).

Definition 4.1 is meaningful in the sense that when using over-parameterized models, we expect the true population can be better modeled by simpler models, which can be seen as a common assumption for all sorts of regularization techniques in the literature. This naturally leads to the following definition of over-parameterization from the parameter estimation point of view.

**Definition 4.2 (Over-parameterization).** A model with parameter \( \theta \in \mathbb{R}^p \) is said to be over-parameterized with respect to currently observed \( \mathbb{P} \) if

\[
\Theta_* \cap \Theta_\Lambda \neq \emptyset
\]  

(4.6)

with a specific type of simplicity-preference function, where \( \Theta_* \) is the parameter set for the best model defined as (2.3). Moreover, the model is said to be strictly over-parameterized if a best model with more zero parameter estimations can be achieved by shrinkage.

Conceptually, by the above definition, a model is called over-parameterized with respect to \( \mathbb{P} \) if at least one best model can be obtained by fitting the model on the observed data and applying some shrinkage. The following theorem shows that under such over-parameterization assumption and some mild conditions for the loss function, (4.4) always provides the optimal estimator given the simplicity-preference function (2.6).

**Theorem 1 (Automated Optimal Shrinkage).** Under regularity conditions, suppose a model is over-parameterized as defined by Definition 4.2, the auto-modeling estimator (4.4) has

\[
\theta^{(n)}_{AM} \in \Theta_*
\]  

(4.7)

Meanwhile, if the loss function takes the form (2.2), then for any \( \theta^* \in \Theta_* \),

\[
D_{KL}(\mathbb{P}, \mathbb{P}_{\theta^*_{AM}}) = D_{KL}(\mathbb{P}, \mathbb{P}_{\theta^*})
\]  

(4.8)

The above theorem proves the validity of the estimation obtained by auto-modeling under the over-parameterization assumption. Although conceptually easy to understand, the assumption is generally hard to verify in practice. The corollary below shows that without the over-parameterization assumption, the auto-modeling estimator still satisfies the consistency property, which proves its validity in a more general scenario.
Corollary 4.1 (Consistency). For any \( \theta^* \in \Theta^{(n)} \), define the active set as
\[ \mathcal{A}(\theta^*) := \{ j : \theta^*_j \neq 0 \text{ for } j = 1, \ldots, p \} \]
If \( |\mathcal{A}(\theta^*)| < \infty \) for any \( \theta^* \in \Theta^{(n)} \), the auto-modeling estimator satisfies weakly
\[ \lim_{n \to \infty} \left( D_{KL}(P, P_{\theta_{\text{AM}}^{(n)}}) - D_{KL}(P, P_{\theta^*}) \right) = 0 \]
if the loss function takes the form (2.2) and some regularity conditions hold. Furthermore, if the model error (4.1) goes to zero as \( n \to \infty \),
\[ \lim_{n \to \infty} D_{KL}(P, P_{\theta_{\text{AM}}^{(n)}}) = 0 \]
The proof for Theorem 1 and Corollary 4.1, as well as the regularity conditions for the loss function are given in Appendix or Supplementary Material.

4.2 Imputing True Population: A Bootstrap Ensemble Approach

In practice, the true population distribution \( P \) will not be available. Thus, instead of (4.4), the auto-modeling estimator takes the form
\[ \hat{\theta}_{\text{AM}}(n) = \mathcal{A}_\theta(\hat{P}, Q(n)) \] (4.9)

The Lemma below can be easily obtained with the result given in Corollary 4.1.

Lemma 4.1. With conditions in Corollary 4.1 hold, suppose that \( Q(n) \) converges to \( P \) and that the model error (4.1) goes to zero as \( n \to \infty \). Then,
\[ \lim_{n \to \infty} D_{KL}(P, P_{\theta_{\text{AM}}^{(n)}}) = 0 \]
The proposed approach for imputing the true population \( P \), described in Algorithm 2.1, 2.2 and Figure 1, can be further clarified with the pictorial representation Figure 2 with the auto-modeling operator \( \mathcal{A}_\theta \).

![Figure 2: The proposed bootstrap imputation approach for auto-modeling estimation. \( \hat{P}^{(j)} \) for \( j = 1, \ldots, B \) denotes \( B \) bootstrap population, which is used for \( B \) auto-modeling procedure, each with empirical distribution \( \hat{P} \) as the future observations. The obtained estimations are used to generate samples for the imputation distribution \( Q \), which is seen as the future distribution in the final estimation. The validity of the bootstrap imputation approach is theoretically supported by the theory of bootstrap (Efron and Tibshirani [1994]). Formally, we record the following result.

Theorem 2 (Consistent Imputation). With conditions in Corollary 4.1 hold, suppose that the model error (4.1) goes to zero as \( n \to \infty \). Then,
\[ Q^{(n)} \to P \]
The proof for Theorem 2 is given in Appendix. Combining Lemma 4.1, the validity of the auto-modeling estimator is proved when bootstrap imputation is used. Although future theoretical investigation of the convergence rate for the
method is necessary, the bootstrap approach generally provides satisfactory result in all kinds of applications, as will be introduced in the next section.

It is worth mentioning that our imputation method is closely related to the ensemble approach (Bagging and Stacking), which is thoroughly discussed in statistics and machine learning literature (Breiman [1996]; Wolpert [1992]). Ensemble approach aims at obtaining multiple high-variance base models and combine them in a way to obtain a strong, robust prediction system. Our method, being conceptually similar to the bagging method, requires $B$ base imputation models obtained on each of the bootstrap data set. The $B$ base models are combined in the way that their predictions on the observed data set are used to generate imputation population for obtaining the final model, which shares the same idea of stacking method. However, being different from the ensemble approach, our method only keeps a single model, which facilitates the model inference and interpretation. With the support of the ensemble literature, there is strong confidence that the bootstrap imputation method can indeed create an overdispersed imputation population, which provides robustness for the auto-modeling estimator.

5 Applications

5.1 Simultaneous Estimation of Many-Normal-Means

The many-normal-means problem, which plays a fundamental role in many areas of statistics, is about making inference on the unknown means $\mu_1, \ldots, \mu_n$ from the sample $Y_1, \ldots, Y_n$ with the following model $Y_i \sim N(\mu_i, 1)$, $i = 1, \ldots, n$, where $Y_1, \ldots, Y_n$ are independent of each other (c.f. a recent discussion by Qiu and Wang [2021] and references therein). A way of formulating this problem in the setting of Section 2 where $Y_1, \ldots, Y_n$ is assumed to be a sample from a single population, is to view $\mu_1, \ldots, \mu_n$ as missing values taken from some unknown population. That is, we consider the model

$$
\mu_i \sim \pi^{(n)}_\theta \quad \text{and} \quad Y_i | \mu_i \sim N(\mu_i, 1)
$$

for $i = 1, \ldots, n$. Although more general and alternative non-parametric models for $\pi^{(n)}_\theta$ can be considered, here we take a simple discrete distribution at $m$ unknown points $\eta_1 \leq \eta_2 \leq \ldots \leq \eta_m$, with the probability mass $Pr(\mu = \eta_k) = \alpha_k$, $k = 1, \ldots, m$. It follows that the observed-data likelihood based on $Y_i$ is given by

$$
\frac{1}{\sqrt{2\pi}} \sum_{k=1}^m \alpha_k e^{-(Y_i - \eta_k)^2 / 2}.
$$

In the following simulation studies, auto-modeling framework is used for fitting the discrete distribution model $\pi^{(n)}_\theta$, which provides an approximation to the true distribution. For simplicity-preference function, write $\theta_1 = \eta_1, \theta_k = \eta_k - \eta_{k-1}$ for $k = 2, \ldots, m$ and $\theta_{m+k} = \alpha_k$ for $k = 1, \ldots, m$. We take the $L_1$-penalty on $(\theta_2, \ldots, \theta_m)' \in \mathbb{R}^{m-1}$, that is, $\pi^{(n)}_\lambda(\theta) = \sum_{k=2}^m \lambda_k |\theta_k|$, where $\lambda_k \geq 0$ and $k = 2, \ldots, m$.

With the estimated parameter $\hat{\theta}_1, \ldots, \hat{\theta}_{2m}$, posterior mean of $\mu_i$ given $Y_i$ is taken as the point estimation of $\mu_i$, namely $\hat{\mu}_i = \hat{\mu}_i^{AM} = E_{\mu_1 \sim \pi^{(n)}_\hat{\theta}}(\mu_i | Y_i)$. The mean prediction error (MPE), which has the same expression as averaging out the total squared error, is calculated as

$$
\text{MPE} = \frac{1}{n} \sum_{i=1}^n (\mu_i - \hat{\mu}_i)^2
$$

For comparison with other methods, first consider a more conceptually straightforward estimate of $\mu$ given $Y_i$ by the maximum likelihood estimator (MLE) $\hat{\mu}_i^{MLE} = Y_i$. Stein [1956] first proved that such MLE is inadmissible when $n \geq 3$. Specifically, there exists at least an estimator that dominates MLE in terms of MPE in the form (5.2) when $n \geq 3$. This phenomenon is thereafter known as the Stein’s paradox.

Stein [1956] and James and Stein [1961] proposed an estimator called the James-Stein estimator, which provides a shrinkage for the original sample mean. Such estimator is proved to dominate the original MLE estimator when $n \geq 3$. The James-Stein estimator in the many-normal-means setting is given by

$$
\hat{\mu}_i^{JS} = \bar{Y} + \left[1 - \frac{n - 3}{\sum_{i=1}^n (Y_i - \bar{Y})^2}\right] (Y_i - \bar{Y})
$$

where $\bar{Y} = (1/n) \sum_{i=1}^n Y_i$ is the overall sample mean. The estimator shrinks the MLE estimator of each $\mu_i$ towards the overall sample mean of the observed data.

In the first simulation study, we consider the case in favor of the James-Stein estimator. Assume the true model is $\mu_i \sim N(0, A)$, where $A$ is the scale parameter. Efron and Hastie [2016] shows that the expected MPE of the James-Stein
estimator has the closed form expression
\[
E\left(\frac{1}{n} \sum_{i=1}^{n} (\mu_i - \hat{\mu}_i^{JS})^2\right) = \frac{A}{A+1} + 3 \frac{1}{n} \left(1 - \frac{A}{A+1}\right) \tag{5.4}
\]
Also note that for MLE
\[
E\left(\frac{1}{n} \sum_{i=1}^{n} (\mu_i - \hat{\mu}_i^{MLE})^2\right) = 1 \tag{5.5}
\]
This suggests that when \(n \geq 3\) and \(A = 0\), the James-Stein estimator performs the best such that it will provide the greatest reduction of MPE compared to MLE. To keep \(\mu\) random at the same time, we set \(A = 0.01\), a value that is close to 0.

In the second simulation study, we consider the case when the James-Stein estimator in general does not provide satisfactory results. Assume half of the \(n\) true parameters are simulated by \(\mu_1 \sim N(-2, 0.01)\) and the other half by \(\mu_2 \sim N(2, 0.01)\). This generates a bimodal distribution of the observed samples \(Y\). Ideally, the sample means should shrink towards the two modes, depending on their locations. Since the James-Stein estimator can only shrinks the sample mean toward its overall mean, it will not provide a satisfactory shrinkage in general. More discussion along this line can also be found in Escobar (1994).

In the third simulation study, we consider a normal model example presented in Narasimhan and Efron (2020), which is used as an example for the developed statistical software for zero-inflated and the true \(\mu\) is generated from \(N(-3, 1)\) with probability 0.1. This simulates a scenario where the true model is zero-inflated and the true \(\mu\) are sparse.

For all simulation studies, three different sample sizes, \(n = 10, 20, 50\) are considered. For each case, \(K = 200\) data sets are generated. Auto-modeling, the James-Stein estimator and \(g\)-modeling are applied to each data set and MPE is calculated as in (5.2). The mean of the MPE is taken over the corresponding estimates in \(K\) data sets. Set \(m = n\) for the auto-modeling method. The results are summarized in Table 1.

| Method          | \(\mu \sim N(0, 0.01)\)       | \(\mu_1 \sim N(-2, 0.01)\) | \(\mu_2 \sim N(2, 0.01)\) | \(\mu_1 = 0\) | \(\mu_2 \sim N(-3, 1)\) |
|-----------------|--------------------------------|-----------------------------|-----------------------------|---------------|-----------------------------|
|                 | \(n = 10\)   | \(n = 20\)   | \(n = 50\)    | \(n = 10\)   | \(n = 20\)   | \(n = 50\)    | \(n = 10\)   | \(n = 20\)   | \(n = 50\)    |
| MLE             | 1.022         | 0.972         | 0.985          | 0.990         | 1.009         | 1.003          | 0.971         | 1.021         | 0.983          |
| James-Stein     | 0.300         | 0.167         | 0.066          | 0.876         | 0.850         | 0.826          | 0.521         | 0.516         | 0.482          |
| \(g\)-modeling  | 0.419         | 0.395         | 0.168          | 0.748         | 0.724         | 0.737          | Y             | 0.554         | 0.552         | 0.364          |
| Auto-modeling   | **0.199**     | **0.110**     | **0.054**      | **0.600**     | **0.437**     | **0.356**      | **0.420**     | **0.418**     | **0.312**      |

**Table 1:** Summary MPE results in three simulation studies with different methods.

The results suggest that auto-modeling method performs better than the other two methods in all cases. Specifically, the greatest reduction of MPE by auto-modeling compared to the James-Stein estimator can be seen in the second simulation study example with bimodal distribution samples. Figure 3 visualizes the shrinkage pattern of both methods in one of the simulated data set. It shows that auto-modeling shrinks all of the sample means toward the correct direction. At the same time, the James-Stein estimator is only capable of shrinking the sample means toward the center, regardless of its location, which is not ideal in this case.

### 5.2 Linear regression: the case of \(p > n\)

Consider the classic linear regression setting, with \(p\) predictors and \(n\) observations \((x_i, y_i), i = 1, \ldots, n\). A common fully specified model can be written as
\[
y_i = x_i' \beta + \epsilon_i \quad (y_i \in \mathbb{R}, x_i \in \mathbb{R}^p, i = 1, \ldots, n) \tag{5.6}
\]
where \(x_i = (x_{i1}, \ldots, x_{ip})'\) is a \(p\)-dimensional vector, \(\epsilon_i \sim N(0, \sigma^2)\), and \(\beta = (\beta_1, \ldots, \beta_p)'\).

A typical microarray data set has \(p \gg n\). Usually, there are thousands of genes and less than 100 samples. Effective variable selection method is required in such cases for the selection of significant genes. More ideally, the built prediction model should consist of the gene selection procedure. The leukemia data example and colon data example are used here for demonstrating the effectiveness of auto-modeling in gene selection and prediction with linear regression.

The leukemia data in Golub et al. (1999) consists of 7129 genes and 72 samples. The training set has 38 samples and the remaining 34 samples are used as the test set. The goal is to build a classification model for classifying the acute
leukemias into those arising from lymphoid precursors (acute lymphoblastic leukemia, ALL) or from myeloid precursors (acute myeloid leukemia, AML). Similar to Zou and Hastie (2005), a pre-screening method based on $t$-statistics scores [Tibshirani et al. (2002)] is used to select 2500 most significant genes to make the computation manageable without loss of important information.

The colon data in Alon et al. (1999) consists of 2000 genes and 62 samples (40 tumor and 22 normal colon tissue samples). The 2000 high-intensity genes were obtained by clustering from more than 6500 human genes. In this example, the first 31 samples (19 tumor and 12 normal colon) are used as test data. The goal is to classify new samples into normal colon samples or tumor with the built classification model.

For both data sets, auto-modeling is applied to linear regression for prediction and further variable selection, with simplicity-preference function taking form (2.6). Besides auto-modeling, Lasso (Tibshirani 1996), which applies the $L_1$ penalty term to linear regression, and ridge (Hoerl and Kennard 1970), which applies the $L_2$ penalty are also performed for comparison. The elastic net (Zou and Hastie 2005), which applies the combination of $L_1$ and $L_2$ penalty is also included. 10-fold cross-validation is applied to select the required tuning parameter for these existing methods. The two types of leukemias in the data set are 0-1 encoded and 0.5 is taken as the threshold value for final classification.

| Method       | Test Error | Test MSE | Number of $|\beta| > 1e^{-4}$ | Number of $|\beta| > 0$ |
|--------------|------------|----------|----------------|----------------|
| Lasso        | 2/34       | 0.0586   | 39             | 42             |
| Ridge        | 0/34       | 0.0420   | 2209           | 2500           |
| Elastic Net  | 0/34       | 0.0420   | 2209           | 2500           |
| Auto-modeling| 0/34       | **0.0307** | 107            | 425            |

Table 2: Summary of leukemia data ($p = 2500, n = 38$) classification results. The parameter $\beta$ denotes the standardized coefficients.
The results of leukemia data example are summarized in Table 2. The results show that auto-modeling achieves zero test error with lower test MSE compared to ridge and the elastic net. Furthermore, the latter two methods fail to do valid variable selection in this example. The results of colon data example are summarized in Table 3. Compared to other methods, auto-modeling has lowest test error and does validate gene selection.

With simplicity-preference function (2.6), auto-modeling estimation is equivalent to solving a weighted $L_1$ penalized linear regression problem with automated selection of each $\lambda$. Supported by the underlying philosophy of auto-modeling, this provides a novel but solid interpretation of the penalty term used in many regularized linear regression problems.

### 5.3 Image classification using convolutional deep nets

For an application of the proposed method to deepnets, here we consider a numerical example of image classification with the famous MNIST data set. The MNIST database is a large database of handwritten digits that is commonly used for training various image processing systems (Wikipedia, 2020). The training and test sample sizes are about 60,000 and 10,000, respectively, for each of the handwritten digits 0,...,9. The image size is $28 \times 28$ pixels, with pixel values measured at gray-scale levels from 0 to 255. Thus, for each observation, $x_i$ stands for the image and $y_i$ stands for the label or digit. The classification problem is to predict $y$ given $x$.

Our application takes a well-known convolutional deepnet model, known as convolution neural networks (CNNs). The first four layers form a convolutional net of $K = 16$ channels. Each channel consists of a convolutional layer, a maximum pooling layer, another convolutional layer, and another maximum pooling layer. Each of the two convolutional layers is specified with the four configuration parameters: the number of filters is $K$, the spatial extent $F = 5$, the stride $S = 1$, and zero-padding $P = 0$. The first convolutional layer has input size $28 \times 28 \times 1$, where 1 is the black-white image depth. The max pooling layers both have the spatial extent parameter $F = 3$ and the stride parameter $S = 2$. This convolutional net results in a $16 \times 3 \times 3 = 144$ dimensional output to be feeded into a fully-connected deepnet of 5 layers of 256 with bias/intercept. When necessary, i.e., for the two convolution layers and deepnet layers, all the layers use the smooth ReLU activation function

$$\sigma(x) = \begin{cases} x + \frac{1}{\kappa} \ln (1 + e^{-\kappa x}), & \text{if } x \geq 0 \\ \frac{1}{\kappa} \ln (1 + e^{\kappa x}), & \text{otherwise,} \end{cases}$$

where the constant $\kappa = 100$ is used in our numerical experiments. The final layer is a multivariate logistic regression link that takes the output of the deepnet as covariates and produces the label probabilities. This results in a total number of 309,433 model parameters. The length of the weight vector $w_l$ for each layer, excluding the max-pooling and the output layers, is contained to be unit with a penalty of the form $||w_l||_2 - 1)^2$.

To apply the proposed method for image classification using CNNs, we created our own customized implementation of the block ADAM algorithm in C from scratch on Linux machines, utilizing multicore CPUs via multi-threading. Following Kingma and Ba (2014) and using the notation therein, we set the running parameters of the block ADAM algorithm for the model parameter $\theta$ block as follows. The batch size (of the random sample) was set to 256. The step size or learning rate is set to be $\alpha = 0.0001$. The moving exponential weights for the first two moments are $\beta_1 = 0.9$ and $\beta_2 = 0.999$, respectively. For the simplicity preference parameter $\lambda$ block, we used $\alpha(\lambda) = 0.001\alpha$, $\beta_1(\lambda) = 0.99$, and $\beta_2(\lambda) = 0.9999$. These parameter values were chosen for slower and, thereby, more stable updates of $\lambda$’s.

Our numerical experiments were carried out on a cluster of six nodes with 16 CPU cores on each node. One block ADAM runs on one node machine for estimation and one block ADAM runs on each of the remaining machines for imputation. Each imputation run imputes one observation through socket connections to the estimation run. The estimation run keeps a pool of size of 60,000 for storing the dynamic imputation sample. Each new imputed image and label pair replaces one in the imputation pool at random. Each imputation run restarts with a new double bootstrap sample every 10,000 ADAM iterations, but with the current estimate of $\theta$ and $\lambda$ as the starting values.

The $L_2$-norm simplicity-preference function is used for the experiment reported here. Since classification of new images is considered in this example, test images, not their labels, together with training images are used to create

| Method       | Test Error | Test MSE | Number of $|\beta| > 1e^{-4}$ | Number of $|\beta| > 0$ |
|--------------|------------|----------|----------------|----------------|
| Lasso        | 8/31       | 0.2051   | 33             | 34             |
| Ridge        | 8/31       | 0.1736   | 1871           | 2000           |
| Elastic Net  | 11/31      | 0.2054   | 44             | 46             |
| Auto-modeling| 4/31       | **0.1568** | 381           | 672           |

Table 3: Summary of colon data ($p = 2000$, $n = 31$) classification results. The parameter $\beta$ denotes the standardized coefficients.
input $x$ covariates for imputation. For more over-dispersed imputation, these images can also be modified via random deformation (Simard et al., 2003). To keep it simple, the results reported here were obtained without deformation.

Figure 4: Classification error rates (circle — training, dot — test if stopped at the corresponding iteration) in the MNIST image classification example.

Figure 5: The MNIST image classification example after 500,000 iterations: (a) the scatter plot of classification error rates for the test sample versus those for the training sample, (b) the histogram of the classification error rates for the test sample conditional on that the those for the training sample is zero.

The experiment reported here used the standard bootstrap for imputation. The running classification results are shown in Figure 4. While not fully converged, the sequences of the classification error rates appear to be stable after 500,000 iterations. Classification error rates for the test sample appear to be positively correlated with those for the training sample. Figure 5(a) shows the scatter plot of their values after 500,000 iterations. Figure 5(b) shows the histogram of the classification error rates for the test sample conditional on the those for the training sample being zero, with mean and median close to 0.05%. These results show that when the model is obtained at iterations with the smallest
classification error rate for the training sample, the classification error rate for the test sample is about 0.05%, smaller than the smallest, 0.09%, reported in the literature [An et al. (2020)], in which the ensemble method is used. Moreover, our method results in a single model, which performs much better than the best single model (0.17%) reported in [Assiri (2020)].

It is noted that “Even the seminal MNIST digits dataset, which has served as the bedrock of optical digit recognition for the past 20 years and has been benchmarked in tens of thousands of peer-reviewed ML publications, contains 15 (human-validated) label errors in the test set.” A closer look at the test images that are difficult to classify reveals that such images are distinguishable between two digits, such as 1 and 7, and 9 and 4. This implies that on average, at least half of the 15 mislabeled images would be classified correctly. Thus, a good classifier is expected to do slightly better than 0.08%. This seems to suggest that our method has provided more or less the best possible result on the MNIST data set, no significant improvement can be made further.

The estimates of $\lambda$’s and $\theta$’s are shown in Figure 6. For numerical stability, a small value is used to bound the $\lambda$’s, as shown by the left-most bar in Figure 6(a). Even with the generalized $L_2$-normal penalty, the use of the estimates of $\lambda$’s have effectively shrunk toward zero and resulting effectively very sparse CNN, where about 90% $\theta$—values are zero.

6 Concluding Remarks

In this paper, we proposed a new method for estimation of over-parameterized models from a model building perspective. Philosophically, the key idea is to consider a process of data-driven model building as to find a simple model to fit the future observations, with satisfactory prediction accuracy determined by the sample data. Technically, we introduce the simplicity-preference function $\pi(\cdot)$ with the working parameter or hyperparameter $\lambda$. The working parameter $\lambda$ allows for performing component-wise parameter $\theta_i$ penalization. This hyperparameter $\lambda$ is determined by data in such a way that while standing for simplicity preference, $\pi(\cdot)$ approximates the difference between observed data and future data in terms of log-likelihood functions. For efficient inference in this scenario, a double-process procedure is proposed to fit the over-parameterized models. One process creates future observations with imputation models obtained via the method of bootstrapping. Taking imputations generated by the imputation process, the other fits the over-parameterized models to the sample data. Theoretical results, examples, and applications to the many-normal-means problem, linear regression with $p > n$, and image classification of the MNIST data show that proposed method is promising, offering a potential paradigm shift for estimation of over-parameterized models.

While promising, the proposed method deserves further deep investigations, in addition to those mentioned in the previous sections. These include developments of the method to improve machine learning methods. The target of creating $\pi(\cdot)$ is a Taylor expansion of the difference of the population loss and the sample loss. Thus more efficient models may be obtained by including more higher order than linear but non-negative terms into $\pi(\cdot)$. The function $\pi(\cdot)$

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2 https://www.csail.mit.edu/news/major-ml-datasets-have-tens-thousands-errors
can also be viewed as an adaptive regularization or an adaptive prior in the context of Bayesian analysis. As alternatives to the bootstrap imputation method, other multiple imputation methods can be considered. Multiple imputation is a useful tool for dealing with missing-data problems with a rich literature. Thus, it would be interesting and useful to develop alternative imputation methods for improving computational efficiency and statistical validity and robustness. Equally important, development of efficient computational methods is a key to the ultimate success of the proposed method for produce both valid and efficient big data analysis. Finally, statistical inference, such as conformal prediction (c.f. Cella and Martin (2022) and references therein), can be made possible in the proposed framework.

Appendix: Proofs of Theorems

A.1 Proof of Theorem 1

Let \((X, Y)\) takes values in \(W \subset \mathbb{R}^{q+1}\) and \(\theta \in \Theta \subset \mathbb{R}^p\). Assume the loss function satisfies the regularity condition:

1. for each \(\theta \in \Theta\), \(L(\theta|\cdot)\) is Borel Measurable on \(W\)
2. for each \((X, Y) \in W\), \(L(\cdot|X, Y)\) is continuous on \(\Theta\)
3. \(|L(\theta|X, Y)| < b(X, Y)\) for all \(\theta \in \Theta\), where \(b\) is a non-negative function on \(W\) such that \(E|b(X, Y)| < \infty\)
4. \(\theta_0 = \arg \min_{\theta \in \Theta} E_{(X, Y) \sim \mathbb{P}}[L(\theta|X, Y)]\) exists.

Auto-modeling aims at optimizing \(G_{\hat{\theta}}(\theta, \hat{\lambda})\) given in (2.5), where \(\hat{\lambda}\) is chosen such that at \(\theta = \hat{\theta}\),

\[
\hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{\theta}, \hat{\lambda}}(\theta, \lambda)}{\partial \theta_i} \right| \quad \text{(A.1)}
\]

for \(i = 1, \ldots, p\). This is equivalent to finding \((\hat{\theta}, \hat{\lambda})\) pair such that

\[
\hat{\theta} = \arg \min_{\theta} G_{\hat{\theta}}(\theta, \hat{\lambda}) \quad \text{(A.2)}
\]
as well as (A.1) satisfies at \(\theta = \hat{\theta}\). Note that one can overcome the differentiability problem when using numerical method such as subgradient method for optimization. Thus, we have

\[
\hat{\lambda} = \min_{\lambda} \left| \frac{\partial V_{\hat{\theta}, \hat{\lambda}}(\hat{\theta}, \lambda)}{\partial \hat{\theta}} \right| = \left| \frac{\partial E_{(X, Y) \sim \mathbb{P}}[L(\hat{\theta}|X, Y)]}{\partial \hat{\theta}} \right| - \left| \frac{\partial \left( E_{(X, Y) \sim \mathbb{P}}[L(\hat{\theta}|X, Y)] + \pi^{(n)}(\hat{\theta}) \right)}{\partial \hat{\theta}} \right| \quad \text{(A.3)}
\]

with \(\hat{\theta}\) satisfies (A.2). The last step follows since the optimal point for \(G_{\hat{\theta}}(\theta, \hat{\lambda})\) has 0 derivative (consider sub-derivative when not differentiable).

Note by overparameterization assumption, \(\exists \theta^* \in \Theta_\ast\) such that \(\theta^* \in \Theta_\Lambda\) where

\[
\Theta_\Lambda = \{ \arg \min_\theta G_{\hat{\theta}}(\theta, \lambda) | \lambda \in \Lambda \}
\]

Equivalently, \(E_{(X, Y) \sim \mathbb{P}}[L(\hat{\theta}|X, Y)]\) can be minimized with some \((\theta^*, \lambda^*)\) pair such that (A.2) is satisfied. This suggests that with such choice

\[
\frac{\partial E_{(X, Y) \sim \mathbb{P}}[L(\theta^*|X, Y)]}{\partial \theta^*} = 0
\]

Notice that \(\frac{\partial E_{(X, Y) \sim \mathbb{P}}[L(\hat{\theta}|X, Y)]}{\partial \hat{\theta}} \geq 0\) for any \(\hat{\theta} \in \Theta\), which suggests that both objective functions (A.2) and (A.3) of the Auto-modeling are optimized with such choice. This suggests that \((\theta^*, \lambda^*)\) is a valid solution for Auto-modeling framework.
When the negative log-likelihood function is used as the loss function, by (2.3),

\[ p(X, Y) \rightarrow \pi \]

Thus, it remains to show that for any \( \theta \in \Theta \), that each possible solution \( G \) defined as

\[ \hat{\pi} \]

Indeed gives \( \hat{\pi} \rightarrow \pi \). As long as

\[ V \]

\[ \theta, \lambda \]

\[ A \]

\[ \hat{\lambda} \]

Thus, it is sufficient to show that each possible solution \( \theta \in \Theta \) indeed gives \( \pi(n)(\theta, \lambda) \rightarrow 0 \). By definition, the active set for any \( \theta \in \Theta \) is defined as

\[ \mathcal{A}(\theta) := \{ j : \theta_j \neq 0 \text{ for } j = 1, \ldots, p \} \]

Denote the non-active parameter set as \( \hat{\mathcal{A}}(\theta) \), the complement of \( \mathcal{A}(\theta) \). Decompose the simplicity-preference function as

\[ \pi(n)(\theta, \lambda) = \pi(n)(\theta, \lambda) + \pi(n)(\theta, \lambda) \]

It is only required to show \( \pi(n)(\theta^*, \hat{\lambda}) \rightarrow 0 \) for any \( \theta^* \in \Theta \). This is because \( \theta^*_A = 0 \) indicates \( \pi(n)(\theta^*, \hat{\lambda}) = 0 \). Thus, it remains to show that for any \( \theta^* \in \Theta \) and \( i \in \mathcal{A}(\theta^*) \),

\[ \hat{\lambda} \]

Notice that

\[ V^{(n)}(\theta, \lambda) = E_{(X,Y)}[L^{(n)}(\theta|X,Y)] - E_{(X,Y)}[L^{(n)}(\theta|X,Y)] - \pi(n)(\theta^*, \lambda) \]

\[ = E_{(X,Y)}[L^{(n)}(\theta|X,Y)] - \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta|x_i, y_i) - \pi(n)(\theta^*, \lambda) \]

By assumption, for any \( \theta^* \in \Theta \), \( \theta^*_A \) has finite dimension. Consider only the active set parameters by setting \( \theta_j = 0 \) for \( j \notin \mathcal{A}(\theta^*) \), without loss of generality, one can rewrite the objective function as

\[ V^{(n)}(\theta, \lambda) = E_{(X,Y)}[L^{(n)}(\theta_A|X,Y)] - \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta_A|x_i, y_i) - \pi(n)(\theta_A, \lambda) \]
Since the active parameter space $\Theta_A^*$ is bounded, the complexity of the best model will not increase to infinity. Let $\Theta_A^{n(e)} \rightarrow \Theta_{Alim}$ where $\Theta_{Alim}$ is the limit parameter space. With regularity conditions 1-4 for the loss function in the proof of Theorem 1 hold, the uniform weak law of large numbers (UWLLN) can be applied to the active set. Thus,

$$\max_{\theta \in \Theta_A} \left| E_{(X,Y) \sim \hat{P}}[L^{(n)}(\theta_A|X,Y)] - \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta_A|x_i,y_i) \right| \rightarrow 0 \hspace{1cm} (A.6)$$

This suggests that for $i \in A(\theta^*)$,

$$\hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{P},\hat{P}}^{(n)}(\theta^*,\lambda)}{\partial \theta_i} \right| = \min_{\lambda_i} \left| \frac{\partial V_{\hat{P},\hat{P}}^{(n)}(\theta_A^*,\lambda)}{\partial \theta_i} \right| \rightarrow \min_{\lambda_i} \left| -\frac{\partial \pi(n)(\theta_A^*,\lambda)}{\partial \theta_i} \right| = 0$$

which finishes the proof that $\theta_{AM}^* \in \Theta^{(n)}_A$ as $n \rightarrow \infty$. With similar argument as (A.4), it can be concluded that

$$\lim_{n \rightarrow \infty} \left( D_{KL}(\hat{P},\hat{P}^{(n)}_{\theta_{AM}^*}) - D_{KL}(\hat{P},\hat{P}^{(n)}_{\theta_{A}^*}) \right) = 0$$

It can be seen that if model error $D_{KL}(\hat{P},\hat{P}^{(n)}_{\theta_{AM}^*}) \rightarrow 0$ as $n \rightarrow \infty$,

$$\lim_{n \rightarrow \infty} D_{KL}(\hat{P},\hat{P}^{(n)}_{\theta_{AM}^*}) = 0$$

A.3 Proof of Lemma 4.1

By assumption

$$\hat{\theta}_{A}^{(n)} = \mathcal{Q}_{\theta}^{(n)}(\hat{P},\hat{Q}^{(n)}) \rightarrow \mathcal{Q}_{\theta}^{(n)}(\hat{P},\hat{P}) = \theta_{A}^{(n)}$$

The conclusion follows by Corollary 4.1

A.4 Proof of Theorem 2

Recall that the imputation process aims to solve the objective function

$$E_{(X,Y) \sim \hat{P}}[L^{(n)}(\theta|X,Y)] = G^{(n)}_{\hat{P}}(\theta,\lambda) + V^{(n)}_{\hat{P},\hat{P}}(\theta,\lambda)$$

The bootstrap population, as is introduced in [Efron and Tibshirani 1994], follows asymptotically $\hat{P}^{(n)} \rightarrow \hat{P}$. Also note that $\hat{P}^{(n)} \rightarrow \hat{P}$. Thus, as long as $\pi(n)(\theta,\lambda) \rightarrow 0$, we have

$$G^{(n)}_{\hat{P}}(\theta,\lambda) \rightarrow E_{(X,Y) \sim \hat{P}}[L^{(n)}(\theta|X,Y)]$$

and the solution of Auto-modeling by optimizing $G^{(n)}_{\hat{P}}(\theta,\lambda)$ has $\hat{\theta}_{(b)} \in \Theta^{(n)}_A$ as $n \rightarrow \infty$. Given the model error $\mathcal{Q}_{\theta}^{(n)}(\theta,\lambda)$ goes to zero, this implies no imputation error exists asymptotically. With a similar argument to the proof for Corollary 4.1, it is sufficient to show that each possible solution $\theta^* \in \Theta^{(n)}_A$ indeed gives $\pi(n)(\theta^*,\hat{\lambda}) \rightarrow 0$. With a similar definition of the active set $A$ and non-active set $\bar{A}$, it remains to show that for any $\theta^* \in \Theta^{(n)}_A$ and $i \in A(\theta^*)$,

$$\hat{\lambda}_i = \min_{\lambda_i} \left| \frac{\partial V_{\hat{P},\hat{P}}^{(n)}(\theta^*,\lambda)}{\partial \theta_i} \right| \rightarrow 0 \hspace{1cm} (A.7)$$

Notice that

$$V_{\hat{P},\hat{P}}^{(n)}(\theta^*,\lambda) = E_{(X,Y) \sim \hat{P}}[L^{(n)}(\theta|X,Y)] - E_{(X,Y) \sim \hat{P}}[L^{(n)}(\theta|X,Y)] - \pi(n)(\theta^*,\lambda)$$

$$= \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta|x_i,y_i) - \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta|x_i,y_i) - \pi(n)(\theta^*,\lambda)$$
By assumption, for any $\theta^* \in \Theta^{(n)}$, $\Theta_{\bar{A}}^*$ has finite dimension. Consider only the active set parameters by setting $\theta_j = 0$ for $j \notin \bar{A}(\theta^*)$, without loss of generality, one can rewrite the objective function as

$$ Y^{(n)}_{\hat{P}, \hat{P}}(\theta^*, \lambda) = \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta_A | x_i, y_i) - \frac{1}{n} \sum_{i=1}^{n} L^{(n)}(\theta_{\bar{A}} | \bar{x}_i, \bar{y}_i) - \pi^{(n)}(\theta_{\bar{A}}, \lambda) $$

Since the active parameter space $\Theta_{\bar{A}}^*$ is bounded, the complexity of the best model will not increase to infinity. Let $\Theta_{\bar{A}}^{(n)} \to \Theta_{\bar{A}lim}^*$ where $\Theta_{\bar{A}lim}^*$ is the limit parameter space. Regularity conditions for the loss function suggests that $E(L(\theta(X,Y)) < \infty$ for any $\theta \in \Theta$. For any fixed $\theta_A$, the following weak convergence law can be obtained with the result in [Bickel and Freedman (1981)]:

$$ \sqrt{n} \left( \frac{1}{n} \sum_{i=1}^{n} L(\theta_A | x_i, y_i) - \frac{1}{n} \sum_{i=1}^{n} L(\theta_{\bar{A}} | \bar{x}_i, \bar{y}_i) \right) \Rightarrow N(0, \sigma^2) $$

where $\sigma^2 = E(L(\theta_A(X,Y)) - E(L(\theta_{\bar{A}}(X,Y)))$. Since the choice of $\theta_A$ is arbitrary and is bounded by $\Theta_{\bar{A}lim}^*$, the uniform convergence in probability of the loss function for the bootstrap sample is proved. This suggests that for $i \in \bar{A}(\theta^*)$,

$$ \hat{\lambda}_i = \min_{\lambda_i} \frac{\partial Y^{(n)}_{\hat{P}, \hat{P}}(\theta^*, \lambda)}{\partial \theta_i} = \min_{\lambda_i} \left| \frac{\partial Y^{(n)}_{\hat{P}, \hat{P}}(\theta^*, \lambda)}{\partial \theta_i^*} \right| $$

$$ \Rightarrow \min_{\lambda_i} \left| - \frac{\partial \pi^{(n)}(\theta^*, \lambda)}{\partial \theta_i^*} \right| = 0 $$

which concludes $\hat{\theta}(i) \in \Theta^{(n)}$ as $n \to \infty$. When model error (4.1) goes to zero,

$$ D_{KL}(\hat{P}, Q^{(n)}) \to D_{KL}(\hat{P}, \hat{P}^{(n)}_{\theta^*}) = 0 $$

or equivalently, $Q^{(n)} \to \hat{P}$. 

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