Estimation with GANs

Master's Thesis

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1 Introduction

Welcome to my thesis! It is based on the paper Kaji, Manresa, and Pouliot (2023).

2 Method

2.1 Background

Consider the problem of estimating the parameters of a structural economic model. For $k \in \{1, ..., K\}$, let

$$Y_k = f_{\Theta}(X_k, Z_k;), \tag{1}$$

where Y_k is a vector of outcome variables influenced by a vector of noise variables Z_k . The strength and functional form of the relationships between the variables is defined by a function f and its parameters Θ .

A common approach to this problem is maximum likelihood estimation, that is, to find $\hat{\theta}$ such that

$$\hat{\theta} = \arg \max_{\theta \in \Theta} \mathcal{L}_n(\theta; \boldsymbol{y}) . \tag{2}$$

However, for some more sophisticated economic models, it is not easy or even possible to calculate the likelihood function.

This motivates further approaches, such as simulation methods, which attempts to infer θ based on a simulation of the true data. Most notable among these is perhaps the simulated method of moments.

The question naturally arises of how to judge whether the simulated distribution comes sufficiently close to the real distribution. This is one motivation for adversarial estimation.

2.2 Adversarial estimation

The basic idea of adversarial estimation is to structure the parameter estimation around two auxiliary models, called the *generator* and the *discriminator*. They "play against each other" based on a parameter estimate $\hat{\theta}_t$ which gets updated iteratively. The generator $G(\hat{\theta}): Z \to O$ creates simulated data based on a guess of the true parameter value $\hat{\theta}$. The discriminator $D_t: O \to [0,1]$ is a classifier that returns the probability of a given observation being real

rather than coming from the generator. If loss is some objective function that measures the distance between the fake and real samples, the adversarial estimator solve the problem

$$\hat{\theta_{adv}} = \underset{\theta \in \Theta}{\operatorname{arg \, min \, max}} \underset{D \in \mathcal{D}_n}{\operatorname{loss}}(D(X_i), D(G(\theta))). \tag{3}$$

Note that this game has a clear Nash-Equilibrium

This method is a variant of "Generative Adversarial Networks", first proposed by I. J. Goodfellow et al. (2014) (later published as I. Goodfellow et al. (2020)). There, two neural networks take the role of generator and discriminator and instead of estimating a parameter vector, noise is transformed into some output, such as an image. While GANs achieved great success in image generation and related tasks, they are not directly suitable for structural estimation. One reason is that the functional form of the generator network is usually very complex, with nodes being fully connected and activation functions being used. Relatedly, the exact architecture of a neural network is usually not chosen to be economically (or at all) interpretable, but rather as an imprecise "art" based on predictive performance. Therefore, one essential contribution of Kaji, Manresa, and Pouliot (2023) is to impose that the generator has the structure of an economic model. This model being fully specified by θ is what makes adversarial estimation meaningful. It wouldn't be if θ were a long list of the weights and biases in a multi-layered neural network.

An implementation of 3 looks, generally, like algorithm 1.

Algorithm 1 Adversarial estimation

Set necessary hyperparameters and initial values

Sample real observations

while Stopping criterion does not hold do

Generate fake observations from the current generator

Train the discriminator given the fake observations

Calculate the loss

Update $\hat{\theta}$

end while

There are various ways to fill in the details of this algorithm. The stopping criterion might be a convergence criterion of the generator's optimization problem, or simply a sufficiently high number of repetitions being reached. The discriminator might take various forms, which I discuss below. There are two canonical choices for the loss function, which I discuss afterwards. The updates of the generator can be done with a gradient descent algorithm if it is differentiable or at least smooth enough that calculating numerical gradients will not lead an optimizer astray. Otherwise, they should be performed with a gradient-free optimization procedure.

Algorithm 1 in Kaji, Manresa, and Pouliot (2023) illustrates one way to fill out the details of 1. They use convergence as a stopping criterion, a (not necessarily trained to completion)

neural network discriminator, cross-entropy loss, and update the generator using a version of the popular Adam algorithm (Diederik (2014)), which requires setting a range of hyperparameters. Their simulation code shows another way. There, they compare a range of estimators (including neural networks trained to completion) and update the generator using a gradient-free approach.

Now I discuss some of these terms in detail.

2.3 Types of discriminators

MLE? Oracle Logistic regression SMM? II? Neural nets

2.4 Losses

- 2.4.1 Cross-entropy loss
- 2.4.2 Wasserstein loss

3 Simulation

3.1 The Roy model

The authors simulate estimation of the Roy model, a discrete choice model which has intractable likelihood for certain parameter values.

First, I reproduce parts of the author's simulation in the scientific Python stack, more precisely, using the packages numpy, scipy, and scikit-learn (Harris et al. (2020), Virtanen et al. (2020), and Pedregosa et al. (2011), respectively). My code is available

The replication package can be downloaded from the journal website. It contains the author's simulation code, written in Matlab. As the authors state in the readme file, the simulations for the Roy model are contained in the files main_roy.m (Figures 6, 7) and main_case.m (Figures 8, 9, and Table I). They draw on functions in other files to simulate data and calculate losses.

Both main files share a general structure: After setting parameters of the simulation itself (e.g. sample sizes, number of simulation runs) and the Roy model, the values of loss functions are calculated along a linear grid and then rendered to created Figures 6 and 8. Thereafter, real and fake observations are generated and the estimation is performed on them. It is implemented as a constrained minimization of a loss function which in turn calculates the discriminators. The constraints are bounds on the parameters of the Roy model, on which the authors do not futher elaborate, but which are likely added for computational efficiency. Where necessary, an additional nonlinear constraint enforces that the guesses of the minimizer stay within the support of the roy model.

3.2 Implementation details

3.2.1 Discriminators

The authors' code for the neural network discriminator is in NND.m. It uses Matlab's patternnet and train. The scientific Python stack comes with limited support for neural networks, but I can sufficiently approximate the author's discriminator using sklearn.neural network.MLPClassifier.

Following the authors, I create a net with 1 hidden layer containing 10 nodes, followed by the tanh activation function. Inspecting sklearn's source code reveals that a logistic output activation function is automatically set. Because the conjugate-gradient descent algorithm is not available to train MLPClassifier, I use the Adam algorithm (Diederik (2014)). It is popular for training neural networks and achieves comparable results in my case.

MLPClassifier's default convergence criteria cause my code to raise warnings about non-convergence of the discriminator nets. This is not completely mitigated even by setting max_iter (the maximum number of iterations of the optimizer) to 2000 (10 times the default value), at the cost of a longer runtime. Nevertheless, the networks converge well enough under the default settings. Leaving max_iter at 200, but increasing tol, the tolerance of the convergence criterium, five- or tenfold mitigates the warnings but results in flatter and less smooth loss functions.

The authors also set the normalization and regularization parameters of patternnet. Since these are handled differently in MLPClassifier, I do not translate this adaption.

My simulations show that these modifications do not significantly alter the shape of the loss curves.

3.2.2 Generators

For the outer optimization loop that trains the generator, the authors use the third-party fmin-searchcon function (D'Errico (2024)). This is a wrapper function that adds support for bounds and nonlinear constraints to Matlab's built-in fminsearch, which employs the Nelder-Mead simplex algorithm (Lagarias et al. (1998)) to minimize a function without computing gradients. I employ scipy.optimize.minimize, which natively supports the Nelder-Mead algorithm with bounds and nonlinear constraints. I set an option to perform a version of the Nelder-Mead algorithm that's adapted to higher-dimensional problems, which shows improved convergence in my simulation.

I employ the mp module from Python's standard library to parallelize simulation runs on an HPC cluster (cf. A).

3.3 Wasserstein

To demonstrate the effect of adding the Wasserstein loss, I program another simulation using pytorch (Ansel et al. (2024)), a popular and highly developed neural network library. The library GeomLoss (Feydy et al. (2019)) allows me to add an approximation of the Wasserstein loss to it. Besides the Wasserstein loss, I also add several other best practices taken from Athey et al. (2021).

4 Conclusion

This section concludes.

Appendix A Acknowledgement of system use

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Selbstständigkeitserklärung

Ich versichere hiermit, dass ich die vorstehende Masterarbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, dass die vorgelegte Arbeit noch an keiner anderen Hochschule zur Prüfung vorgelegt wurde und dass sie weder ganz noch in Teilen bereits veröffentlicht wurde. Wörtliche Zitate und Stellen, die anderen Werken dem Sinn nach entnommen sind, habe ich in jedem einzelnen Fall kenntlich gemacht.

16. September 2024

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