Estimation with GANs

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1 Introduction

This thesis is based on the paper Kaji, Manresa, and Pouliot (2023).

2 Background

2.1 Structural estimation

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. It is also intuitive that one approach to this involves classification. In machine learning, a popular tool for classification are neural networks, which I introduce next.

2.2 Neural networks

Definition

Training

3 Adversarial estimation

The basic idea of adversarial estimation is to structure the parameter estimation around two auxiliary models, called the *generator* and the *discriminator* (or *critic*). The generator $G(\hat{\theta})$: $Z \to O$ creates simulated data based on a guess of the true parameter value $\hat{\theta}$. Given the real and the simulated data, the discriminator returns objective function for the generator, which I will call *loss*. This loss function can be any divergence or distance between the distributions of the real and simulated data, inleuding functions that are directy analytically tractable. In the classic GAN case involving neural networks, the loss function is the result of the discriminator solving a maximization problem:

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

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.

3.1 Examples of discriminators

All the following discriminators have in common that for a data point *x* they return a probability that it is from the real rather than the simulated data. How this probability is then turned into an objective for the generator will be discussed in the next subsection.

Recall the unique Nash equilibrium from If the true densities p_0 and $p_{\theta}(x)$ are known, we get the *oracle discriminator*.

Definition 1 (Oracle discriminator). The oracle discriminator assigns

$$D_{\theta}(x) := \frac{p_0(x)}{p_0(x) + p_{\theta}(x)} \tag{4}$$

to every $x \in .$

Kaji, Manresa, and Pouliot (2023) call this the *oracle discriminator*. Of course, p_0 and $p_{\theta}(x)$ are unkown in practice. Also, this discriminator is only optimal in the Nash equilibrium as off-equilibrium, it neglects to update from the prior proabilities p_0 and $p_{\theta}(x)$. Nevertheless, it is useful as a benchmark in simulations and has an interesting theoretical property: If the simulated sample size $m \to \infty$, θ_{oracle} approaches θ_{MLE} .

A simple statistical method for classification is logistic regression. In line with the simulation study in Kaji, Manresa, and Pouliot (2023), I consider a version that regresses on some collection of features of the data points and moments of the data.

Definition 2 (Logistic discriminator). Let Λ be a sigmoid function with values in (0, 1), and x^{mom} an $(i + j) \times k$ -matrix of features and moments of the data calculated for each data point. Let $(\beta_0, \ldots, \beta_k \in \mathbb{R}^{k+1})$ be coefficients of a logistic regression run with x^{mom} as a regressor and an output vecor Y consisting of 0s and 1s for the simulated and true observations. Then the **logistic discriminator** assigns

$$D(x) = \Lambda(\beta_0 + \sum_{k=1}^{K} \beta_k x_k^{mom})$$
 (5)

to every $x \in .$

Note that this classifier has to be calculated anew after each update of θ . While this calculation will usually be fast on modern computers, the same is not necessarily true of the potentially more powerful neural network discriminator. Therefore, neural networks are often not trained to completion in practice and we different training procedures might result in different discriminators.

Definition 3 (Neural network discriminator). Define a classifier neural network $\mathcal{N}: \mathcal{X}^k \to [0,1]$ by:

$$\mathcal{N}(x) = \sigma_L(W_L \sigma_{L-1}(W_{L-1} \cdots \sigma_1(W_1 x + b_1) \cdots + b_{L-1}) + b_L), \tag{6}$$

where $x \in \mathbb{R}^n$ is the input vector, L is the number of layers, W_i are weight matrices, b_i are bias vectors, σ_i are activation functions. Let θ_{train} be a collection of hyperparameters that specify the training of a neural network, such as a loss function, an intial guess, a number of training steps, a training algorithm, and a list of hyperparameters of the latter. Call $\mathcal{N}(\theta_{train})$ the network \mathcal{N} after it has been trained according to θ_{train} . Then the **neural network discriminator** assigns

$$D(x) = \mathcal{N}(\theta_{train})(x) \tag{7}$$

to every $x \in .$

To understand more deeply the loss landscape which a neural network discriminator builds for the generator, we must consider the loss function on which it is trained.

3.2 Generator objectives

3.2.1 Jensen-Shannon divergence

The classical way to turn the proabilities D(x) into an objective for the generator is the following:

Definition 4 (Cross-entropy loss). The empirical cross-entropy loss (CE) is:

$$\frac{1}{n} \sum_{i=1}^{n} \log D(X_i) + \frac{1}{m} \sum_{i=1}^{m} \log (1 - D(X_{i,\theta})).$$

A discriminator that maximizes the cross-entropy loss thereby calculates the Jensen-Shannon divergence (plus a constant) for the generator to minimize.

Theorem 5 (I. J. Goodfellow et al. (2014)). · · ·

A neural network discriminator that is not trained to completion returns an approximation of the Jensen-Shannon divergence. In practice, only such an approximation is often used, for two reasons: First, the training a neural network to completion multiple times for every gradient calucation of the generator's optimizer can be very computationally costly, especially given that GANs in practice are often large neural networks and are applied to high-dimensional data sets. Second, an imprecise estimate of the gradient often still leads to convergence.

However, even the Jensen-Shannon divergence calculated by an optimal discriminator has a crucial disadvatage: The divergence is maximal if p_G and p_0 have disjoint support. Therefore, there are regions of the loss landscape where even the optimal CE-discriminator provides a gradient of zero in every direction at every point to the generator. If the generator "ends up" in such a region or the initial guess is there, algorithm 1 is unlikely to converge. Luckily, there are ...

3.2.2 Wasserstein-p distance

Using the so-called Wasserstein-1 distance as an optimization target for the generator was first proposed by Arjovsky, Chintala, and Bottou (2017).

Definition 6 (Wasserstein-p distance). For two probability distribution \mathbb{P}_0 and \mathbb{P}_G , let $\Pi(\mathbb{P}_0, \mathbb{P}_G)$ be the set of all joint distributions $\gamma(x, y)$ whose marginals are \mathbb{P}_r and \mathbb{P}_q . Then for $p \ge 1$,

$$W_p(\mathbb{P}_0, \mathbb{P}_G) = \inf_{\gamma \in \Gamma(\mathbb{P}_0, \mathbb{P}_G)} \left(\mathbf{E}_{(x, y) \sim \gamma} d(x, y)^p \right)^{1/p},$$

is the Wasserstein-p distance (also Wasserstein p-distance) between \mathbb{P}_0 and \mathbb{P}_G .

A natural interpretation of this equation comes from the field of optimal transport. It quantifies how much probability mass has to be moved how far in order to transfer \mathbb{P}_0 into \mathbb{P}_G , or vice versa, assuming that this transport is done optimally. Inspired by this image, the Wasserstein-1 distance is also called *Earth-Mover distance*.

The Wasserstein distances deliver a measure of the distance between two distributions that is strictly monotone even if they are non-overlapping. However, since they require a solution to the optimal transport problem, they can be demanding to calculate, especially in high-dimensional spaces. In the context of GANs, it is natural to consider approximating it using a neural network. To this end, the following fact is helpful:

Theorem 7 (Kantorovich-Rubinstein duality).

$$W_1\left(\mathbb{P}_0, \mathbb{P}_G\right) = \sup_{\|f\|_{L} \le 1} \mathbb{E}_{x \sim \mathbb{P}_0}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_G}[f(x)]$$
 (8)

This dual representation of the Wasserstein-1 distance paves the way to approximating it using a neural network. The network estimates the function f and is often called critic instead of discriminator since it does not return a probability anymore. Unfortunately, it is not trivial to regularize a neural network to obey the Lipschitz constraint. Arjovsky, Chintala, and Bottou (2017) clamp the weights of the neural network to lie in a compact space. They themselves describe this approach as "clearly terrible", since there is no principled way to chose the clipping parameter and setting it too big or too small comes with difficult trade-offs.

Gulrajani et al. (2017) propose to penalize the norm of the gradient of the critic with respect to its input. This solution has been more widely accepted and is also used by Athey et al. (2021).

Of course, it is also possible to approximate the Wasserstein-1 distance without training a neural network. Since the Wasserstein distance is the solution to an optimal transport problem, it can be derived using a "Pseudo-auction algorithm". For differentiability, this algorithm can than be approximated using a smoothed "soft-auction" algorithm. The divergence resulting from this algorithm is called the *Sinkhorn divergence*.

4 Simulation

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

4.1 The Roy model

The Roy model models a set of agents chosing which sector to work in in each of two time periods. At the start of the game, nature determines the wages offered to each agent, by the following formulas: In the first time period, each agent i observes the (natural logarithms of the) wages $\log w_{i11}$ and $\log w_{i12}$ offered to them in the two sectors. Knowing their own discount factor β and the parameters γ_1 and γ_2 , they solve the dynamic programming problem and pick a sector for the first period. In the second period, they observe the wages $\log w_{i21}$ and $\log w_{i12}$ and pick a sector.

The researcher observes the realized wages $\log w_1$ and $\log w_2$ and as well as the corresponding sector choices $d_1, d_2 \in 1, 2$.

4.2 General simulation structure

First, I reproduce parts of the authors' 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

I program another simulation using PyTorch (Ansel et al. (2024)), a popular and highly developed neural network library for Python. Among the advantages of Pytorch is that it offers support for training neural networks on GPUs Additionally, the library GeomLoss (Feydy et al. (2019)) builds on PyTorch. Its SampleLoss function provides the Sinkhorn approximations of the Wasserstein-1 and -2 distances. It is also optimized for running on GPUs by virtue of being built on KeOps (Charlier et al. (2021)).

For my scientific Python code, I use the mp module from Python's standard library to parallelize simulation runs on an HPC cluster (cf. A). I generate plots using Matplotlib (Hunter (2007)).

The replication package of Kaji, Manresa, and Pouliot (2023) can be downloaded from the journal website. It contains the authors' 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. The grid describes seven- or eight-dimensional "cross-hairs", where one parameters is varied while the others remain fixed at the true value. Thereafter, real and fake observations are generated and an intial guess in generated. Then, the the Roy model is estimated using multiple methods, which are implemented as a constrained minimizations. 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.

```
Algorithm 2 Initial guess in main_roy.m
```

```
Input: True parameter vector \theta, lower and upper bounds L, U, the support of the Roy model \mathcal S while \theta_{0,p} \notin \mathcal S, for each parameter p of \theta to be estimated: do

Sample noise u_p \sim \mathcal N(0,0.2)

Set \theta_{0,p} := \theta_p + u_p

Clip \theta_{0,p} := \min(\max(\theta_{0,p}, L_p), U_p)

end while
```

In main_roy.m, the authors plot cross-sections of the loss landscapes generated by the Oracle and neural network discriminator as well as the loss implied by MLE. Then, they generate the intial guess θ_0 using 2. Following simple maximum likelihood estimation with θ_0 as an intial value, they perform adversarial estimation with:

- the Oracle discriminator, using the result of MLE as intial value
- the Logistic discriminator, using the result of the previous step as initial value
- the neural network discriminator, again using the result of the Oracle step as intial value

They also estimate the Roy model using Indirect Infernce and optimally-weighted SMM, but don't use the results.

In main case.m,

4.3 Implementation details

4.3.1 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 authors' 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.

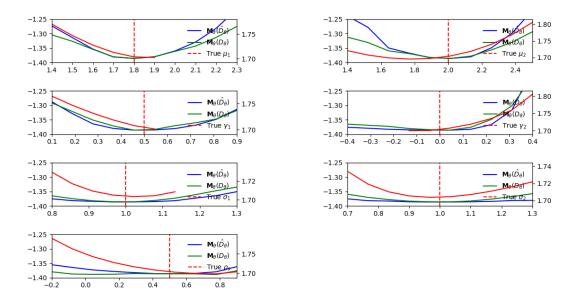


Figure 1. Replication of Figure 6 in Kaji, Manresa, and Pouliot (2023)

4.3.2 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.

4.4 Cross-sections of the loss landscape

Figures 1 and 2 match Figures 6 and 8 in Kaji, Manresa, and Pouliot (2023), confirming that my replication in the scientific Python stack, including of the neural network discriminator is sufficiently close to the original.

Figure 3 shows a variant of 2 plotted over wider intervals. It is striking that for some parameters, the loss is flat when moving to far away from the optimal value. Partly, this can be explained by the discrete choice nature of the Roy model. Consider for example μ_1 . If it becomes to small relative to mu_2 while γ_1 and γ_2 are held constant, the agents stop chosing sector 1. Since only their chosen sectors and wages are observed, in such cases there are no observations that help to narrow down the vale of μ_1 (except to bound it from above). Similar

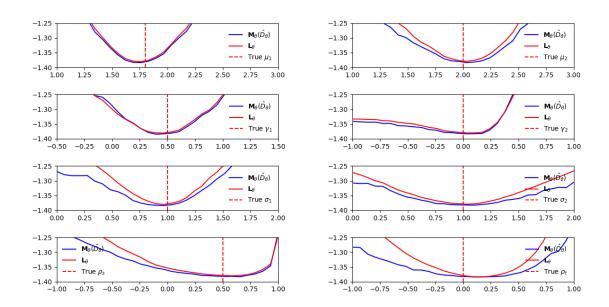


Figure 2. Replication of Figure 8 in Kaji, Manresa, and Pouliot (2023)

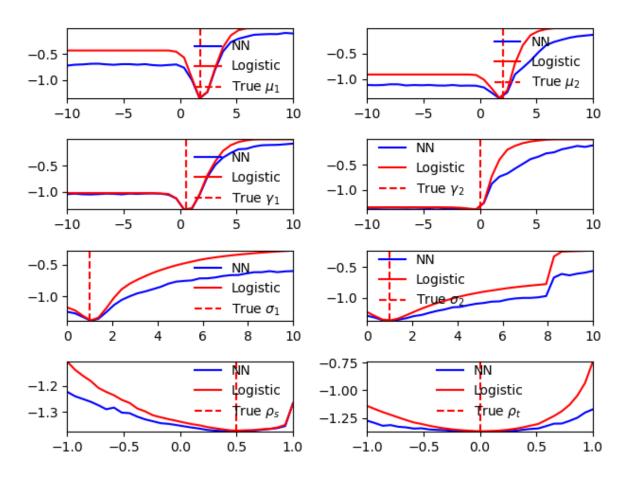


Figure 3. Losses cross-sections plotted over wider intervals

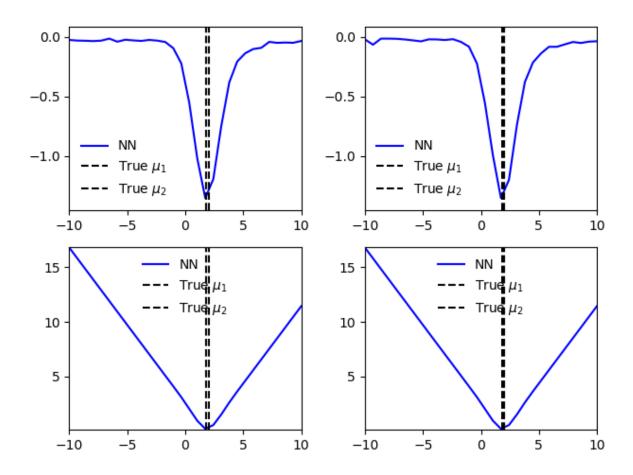


Figure 4. Diagonal loss cross-sections. Rows: Jensen-Shannon divergence, Wasserstein-1. Columns: $(\mu_1, \mu_2), (\mu_1, -\mu_2)$.

arguments explain the flatness towards the tail of the cross-hairs for all four location parameters μ_1 , μ_2 , γ_1 , and γ_2 .

Recall from section 3.2.1 that there is another reason for the loss-function to become flat, at at least for the neural network estimator with cross-entropy loss. Namely, the constant Jensen-Shannon divergence for disjoint distributions. To isolate the effect, I rotate part of the cross-hairs to look at the loss along the diagonal (μ_1, μ_2) . This way, the fake distribution can become disjoint from the real distribution without affecting the agents' choices. ¹

Figure 4 shows the results: In the top row, a neural network discriminator approximates the JS divergence. The the bottom row, the Wasserstein-1 distance as approximated by the Sinkhorn divergence is plotted. The left column shows clearly that the Jensen-Shannon divergence becomes constant when (μ_1, μ_2) is small or big enough that the distributions become disjoint, while the Wasserstein-1 distance provides constant gradients. The right column plots

^{1.} There is a small distortion because $\mu_1 = 1.8 \neq 2.0 = \mu_2$.

the diagonal $(\mu_1, -\mu_2)$: disjointness is also realized in this case for large absolute values of (μ_1, μ_2) .

4.5 Estimation

5 Conclusion

This section concludes.

Appendix A Acknowledgement of system use

The author gratefully acknowledges the granted access to the Marvin cluster hosted by the University of Bonn.

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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.

22. September 2024

Marvin Benedikt Riemer