

# Architecture Learning of Deep Neural Networks for Counterfactual Inference

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## Abstract

We propose a novel approach for automatically inferring appropriate architectures of deep neural networks for the task of counterfactual inference over observational data. The individualised causal effect of an intervention or treatment is modelled in terms of a multi-task learning problem using a deep neural network which consists of a number of layers that are shared among the factual and counterfactual outcomes and a number of outcome-specific layers. Our approach enables automatically selecting an appropriate architecture (i.e. number of shared and outcome-specific layers) by exploiting inferred characteristics of the dataset such as the propensity score, the skewness of the data, and the complexity of the different outcome functions. We conduct experiments on a synthetic dataset allowing us to parametrize and fully control the characteristics of the data before applying our approach to a real-world observational study for which we infer the characteristics in order to derive an appropriate architecture. As shown in the experiments, our method outperforms the state-of-the-art.

## Introduction

The technological advancements of recent years have resulted in an increasing availability of data in various fields such as healthcare, education, and economics. This data can be used to make predictions concerning unseen data points on the basis of statistical models. When dealing with observational studies, we are often particularly interested in the task of predicting the individualised treatment effect that certain intervention has on a given subject or context. In the case of electronic health records, for instance, a dataset typically consists of a set of patients each with individual features, a treatment assignment indicator (i.e. whether or not they received the treatment), and an observed outcome which we call the *factual outcome*. The quantity we are interested in is the *counterfactual outcome* (i.e. the outcome had the patient received a different treatment assignment) because it allows us to compute the individualised treatment effect helping us make informed decision during treatment planning.

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Classical works have focused on estimating average treatment effects through variants of propensity score matching (Rubin, 2005; Austin, 2011; Abadie and Imbens, 2016; Rosenbaum and Rubin, 1983; Rubin, 1973). More recent works tackled the problem of estimating individualised treatment effects using representation learning (Johansson et al., 2016; Shalit et al., 2017), Bayesian inference (Hill, 2011), and standard supervised learning (Wager and Athey, 2015).

Recent works have shown that the problem can be effectively framed in terms of a multi-task learning problem using deep neural networks (Alaa et al., 2017). The network has a set of layers that are shared among both the factual and the counterfactual outcomes and a number of outcome-specific layers. However, the questions of how to select an appropriate architecture (i.e. the number of shared layers, and the number of outcome-specific layers) may drastically influence the expressiveness and computational complexity of the model and remains an open challenge. While there are various general approaches for model selection and architecture learning in neural networks, they do not make use of the specific nature of causal inference.

In this paper, we propose a novel approach for automatically learning appropriate architectures of deep neural networks for the task of counterfactual inference over observational data. This is achieved by exploiting inferred characteristics of the dataset such as the propensity score, and the "shared complexity" among the different outcomes and the difference between the outcome surfaces. For instance, if one of the outcomes follows a much more complex function than the other, this should be reflected in a potentially asymmetric architecture which utilises a higher number of outcome-specific layers for the more complex outcome.

## Problem Formulation

We represent each subject  $i$  in our population with a  $d$ -dimensional feature vector  $X_i \in \mathcal{X}$ , and two *potential outcomes*  $Y_i^{(1)}, Y_i^{(0)} \in \mathbb{R}$  which are drawn from a distribution  $(Y_i^{(1)}, Y_i^{(0)}) \mid X_i = x \sim \mathbb{P}(\cdot \mid X_i = x)$ . This way, the *individualised treatment effect* for subject  $i$  can be expressed as

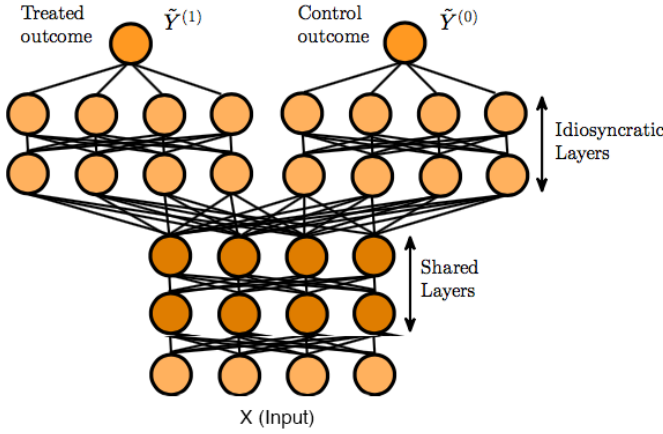


Figure 1: DRAFT: Architecture of a Deep Counterfactual Network (DCN). Objective is to learn appropriate values for number of different layers (here  $L_s = L_{i,0} = L_{i,1} = 2$ ).

$$T(x) = \mathbb{E}[Y_i^{(1)} - Y_i^{(0)} \mid X_i = x]. \quad (1)$$

Given this definition, the objective is to approximate the function  $T(x)$  using an observational dataset  $\mathcal{D}$  consisting of  $n$  independent samples. Each sample is comprised of a tuple  $\langle X_i, W_i, Y_i^{(W_i)} \rangle$ , where  $X_i$  represents the subject's features,  $W_i \in \{0, 1\}$  the treatment assignment indicator, and  $Y_i^{(W_i)}$  and  $Y_i^{(1-W_i)}$  the respective *factual* and *counterfactual* outcome. The treatment assignment is a random variable depending on the subjects' features, i.e.  $W_i \not\perp X_i$ . The assignment reflects a domain-specific policy which can be captured in terms of the probability  $p(x) = \mathbb{P}(W_i = 1 \mid X_i = x)$  called the *propensity score*.

We are following the approach of (Alaa et al., 2017) and are using a *deep counterfactual network* (DCN) to infer  $T(x)$  from  $\mathcal{D}$ . The DCN treats the problem as a multi-task learning problem using a deep neural network with an architecture illustrated in figure 1. The network uses a number  $L_s$  of shared layers, a number  $L_{i,0}$  of idiosyncratic (outcome-specific) layers for the *treated outcome*, and a number  $L_{i,1}$  for the *control outcome*. We are interested in learning an appropriate architecture of the DCN, in particular, coming up with suitable values for  $L_s$ ,  $L_{i,0}$ , and  $L_{i,1}$ .

### Architecture Learning

- \* How does architecture learning work in general?
- \* What are the main existing methods for this?

- \* What is our approach?
- \* Hyper-parameter search that is informed by propensity score and different metrics of the data

### Relevant Characteristics

Briefly describe ...

- (a) **Skewness** \* What do we mean by that?  
 Depending on propensity score.  
 \* How do we get that the PS?  
 \* How should it be reflected in the layers?  
 \* How does it influence the architecture?  
 \* Qualitatively? Quantitatively?  
 \* out1 / total, out2 / total

- (b) **Complexity of Response Surfaces** \* What do we mean by that?  
 \* What does it depend on?  
 \* How do we measure it?  
 \* How should it be reflected in the layers?  
 \* How does it influence the architecture?  
 \* Qualitatively? Quantitatively?  
 \* shared / total or out1 / total, out2 / total ?

- (c) **Interdependence between Features** \* What do we mean by that?  
 \* What does it depend on?  
 \* How do we measure it?  
 \* How should it be reflected in the layers?  
 \* How does it influence the architecture?  
 \* Qualitatively? Quantitatively?  
 \* shared / total

### Deriving a suitable Architecture for the DCN

- \* Once we are able to quantify these characteristics, what do we do with it?
- \* What is the relationship between these characteristics and an appropriate architecture?

### Experiments

The experiments are conducted on two different datasets. Firstly, we use a synthetic model which allows us to parametrise and fully control the characteristics mentioned in the previous section. This gives us the power to investigate how the different characteristics influence the performance of the learnt architecture. Secondly, we run the experiments on the *UNOS* dataset (consisting of information regarding patients who underwent an organ transplantation) to show how our approach generalises to a real-world dataset for which we do not have access to the characteristics directly but have to infer them from the data in order to learn a suitable architecture. In both cases, we compare the performance of a DCN whose architecture was learnt by our approach to a generic DCN and a number of other baseline approaches and architectures.

As we are dealing with counterfactual inference, we generally do not have access to the ground truth counterfactual outcomes, making it difficult to evaluate the performance of our predictions on real-world data. As a consequence, we adopt a semi-synthetic experimental setup (Hill, 2012; Johansson et al., 2016) for which we use the original covariates and treatment assignments but simulate the

outcomes according to a specific response surface described in detail below.

Since it is our objective to learn an appropriate architecture by exploiting characteristics of the data, the number of (shared and outcome-specific) layers varies across the different datasets. However, throughout both networks we are using a fully-connected architecture with 200 hidden units in all layers (ReLU activation) and we evaluate the performance in terms of the mean squared error (MSE) of the estimated treatment effect. The datasets are split into a training set (80%) and test set (20%) and evaluated exclusively on the test set, averaging over 100 experiments for which new outcomes are drawn each time.

## Synthetic Model

**Data Generation** For the synthetic model, we draw  $n = 1000$  samples in the form of a tuple  $\langle X_i, W_i, Y_i \rangle$  for each subject  $i$ . The tuple  $X_i = (x_{i,0}, x_{i,1}, \dots, x_{i,24})$  consists of  $d = 25$  covariates for each subject which are independently drawn from a uniform distribution, i.e.

$$x_{i,0}, x_{i,1}, \dots, x_{i,24} \stackrel{iid}{\sim} \mathcal{U}(0, 1)$$

keeping each covariate strictly non-negative. For the treatment assignment indicator  $W_i \in \{0, 1\}$ , we define

$$\tilde{p}(X_i) = \frac{1}{1 + \exp(-\alpha \sum_{x_j \in X_i} x_j)}$$

$$W_i \sim \text{Bernoulli}(\tilde{p}(X_i))$$

where  $\tilde{p}(X_i)$  represents the subject's propensity score and the parameter  $\alpha \in \mathbb{R}^0$  gives us a way to control the imbalance between the treated and untreated subjects. For  $\alpha = 0$ , we get  $\tilde{p}(X_i) = 0.5$  corresponding to a maximum balance between number of treated and untreated subjects whereas an increasing alpha shifts the distribution towards a higher proportion of treated subjects. We compute both outcomes  $Y^{(0)}, Y^{(1)} \in \mathbb{R}$  as

$$Y_i^{(0)} = f_0(X_i) + \mathcal{N}(0, 1)$$

$$Y_i^{(1)} = f_1(X_i) + \mathcal{N}(0, 1)$$

which are governed by their corresponding outcome functions  $f_0$  and  $f_1$  defined as

$$f_1(X_i) = \sum_{x_j \in X_i} \lambda_j^{(1)} x_j + \beta^{(1)} \cdot \exp\left(\sum_{x_j \in X_i} \mu_j^{(1)} x_j^2\right)$$

$$f_0(X_i) = \sum_{x_j \in X_i} \lambda_j^{(0)} x_j + \beta^{(0)} \cdot \exp\left(\sum_{x_j \in X_i} \mu_j^{(0)} x_j\right).$$

Each outcome function consists of a linear part governed by the coefficients in the vectors  $\lambda^{(0)}$  and  $\lambda^{(1)}$  respectively, and an outcome-specific polynomial part inside the exponential function governed by the coefficients in the vectors  $\mu^{(0)}$  and  $\mu^{(1)}$ . In the case of  $f_1$  this is a quadratic function

Table 1: (Draft) Performance on Synthetic Dataset

Algorithm	MSE
k-NN	$5.30 \pm 0.30$
Causal Forest	$3.86 \pm 0.20$
BART	$3.50 \pm 0.20$
BNN	$2.45 \pm 0.10$
NN-4	$2.88 \pm 0.10$
DCN	$2.58 \pm 0.06$
DCN-LA	$2.31 \pm 0.05$

whereas for  $f_0$  we are using a linear function. The parameters  $\beta^{(0)}, \beta^{(1)} \in \mathbb{R}^0$  let us control the weight of the outcome-specific polynomial part in comparison to the common linear part.

The vectors  $\lambda^{(1)}, \mu^{(1)}$  for the treated outcome function  $f_1$  are drawn based on the data generation process designated as the "Response Surface B" setting in (Hill, 2012). For the outcome function  $f_0$  of untreated subjects, we draw the vectors  $\lambda^{(0)}, \mu^{(0)}$  from a normal distribution centred around their corresponding treated counterpart, i.e.

$$\lambda_i^{(0)} \sim \mathcal{N}(\lambda_i^{(1)}, \sigma) \quad \mu_i^{(0)} \sim \mathcal{N}(\mu_i^{(1)}, \sigma),$$

with a standard deviation  $\sigma$ . This way, we can use the parameter  $\sigma \in \mathbb{R}^0$  to control the similarity between the two outcome surfaces. Finally, we can set  $Y_i = W_i \cdot Y_i^{(1)} + (1 - W_i) \cdot Y_i^{(0)}$  representing our *factual outcome* for subject  $i$ . The other (i.e. counterfactual) outcome is not used in the training set but needed later for evaluation purposes.

In summary, we receive a synthetic model which is parametrised by  $\alpha, \beta^{(0)}, \beta^{(1)}$ , and  $\sigma$  each corresponding to a different characteristic we are interested in: The parameter  $\alpha$  defines the skewness of the treatment assignment (i.e. the portion of treated vs. untreated subjects),  $\beta^{(0)}$  and  $\beta^{(1)}$  define the emphasis of the outcome-specific parts of the equation in relation to their common linear part, and  $\sigma$  determines the overall similarity between the two outcome surfaces.

**Draft: Results and Discussion** Table 1 shows the results of our evaluation of the learnt architecture (DCN-LA) in comparison with other existing methods.

*Details of the experiment (total number of layers, epochs)*

*Description of the other methods*

*Discussion of impact of parameters*

*Graph: Impact of sigma as shown in figure 2*

*Graph: Impact of  $\beta_0$  and  $\beta_1$*

*Discussion of results*

## UNOS Dataset

In order to show how our approach generalises in a real-world scenario, we are running the experiments on the UNOS dataset.

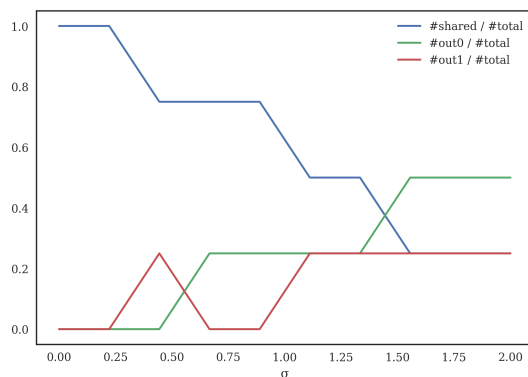


Figure 2: DRAFT (idealised): Influence of similarity parameter  $\sigma$  on the learnt optimal architecture.

### Draft: About the dataset

*Source and meaning of UNOS*

*Description of dataset (number of samples, covariates, etc.)*

*Relevant statistics*

*Treatment assignment and outcome*

### Draft: Results and Discussion

*Description of how the characteristics are inferred from the dataset*

*Description of how the architecture is learnt using the characteristics*

*Discuss results table*

*Show graph and influence of different parameters*

Table 2: (Draft) Performance on UNOS Dataset

Algorithm	MSE
k-NN	$5.30 \pm 0.30$
Causal Forest	$3.86 \pm 0.20$
BART	$3.50 \pm 0.20$
BNN	$2.45 \pm 0.10$
NN-4	$2.88 \pm 0.10$
DCN	$2.58 \pm 0.06$
DCN-LA	$2.31 \pm 0.05$

## Conclusions and Future Research

Counterfactual inference over observational data is of great importance in various areas such as healthcare, education, and economics. Deep neural networks are highly suitable for the task and represent the state-of-the-art as they are able to capture complex relations in the outcome surfaces. However, it remains an open challenge of how to select an appropriate architecture for models. This is true in particular in the case of *deep counterfactual networks* which treat

the problem as a multi-task learning problem with different numbers of shared and outcome-specific layers.

Our approach addresses this issue and provides an effective way to automatically learn a suitable architecture by inferring relevant characteristics from the data and incorporating them into the model selection. As shown in the experiments, our approach outperforms the state-of-the-art.

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