

# Goodness of Causal Fit

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## Abstract

We propose a Goodness of Causal Fit (GCF) measure which depends on Pearl “do” interventions. This is different from a measure of Goodness of Fit (GF), which does not use interventions. Given a DAG set  $\mathcal{G}$ , to find a good  $G \in \mathcal{G}$ , we propose plotting  $GCF(G)$  versus  $GF(G)$  for all  $G \in \mathcal{G}$ , and finding a graph  $G \in \mathcal{G}$  with a large amount of both types of goodness.

# 1 Introduction

Frequently, when students first encounter Bayesian Networks (bnets) and Causal Inference (CI) (Refs.[1], [3]), they experience serious doubts about the usefulness of this theory, because they believe finding the underlying model (i.e., DAG) for most realistic physical situations is too difficult or impossible. I think that part of the problem is that these students are assuming, perhaps unconsciously, that there exists a unique DAG that fits Nature perfectly, and a mind-boggling number of possibilities to sift through to find that DAG. Rather than looking for a unique DAG, I think a better strategy is to write down a set  $\mathcal{G}$  of likely DAGs, and to calculate for each DAG in  $\mathcal{G}$ , a measure called Goodness of Causal Fit (GCF). Then use the DAGs with the highest GCF scores.

The goal of this paper is to propose a GCF measure. Such a measure is of course not unique, and someone may propose in the future a measure that is better than ours.

When designing a GCF measure, it is important to keep in mind the First Axiom<sup>1</sup> of CI: The data is model-less. In the First Axiom, when we say “data”, we are referring to what is commonly called a dataset. A dataset is a table of data, where all the entries of each column have the same units, and measure a single feature, and each row refers to one particular sample or individual. Datasets are particularly useful for estimating probability distributions and for training neural nets. In the First Axiom, when we say “model”, we are referring to a DAG (directed acyclic graph) or a bnet (Bayesian Network= DAG + probability table for each node of DAG).

You can try to derive a model from a dataset, but you’ll soon find out that you can only go so far. The process of finding a *partial* model from a dataset is called structure learning (SL). SL can be done quite nicely with Marco Scutari’s open source program **bnlearn** (Ref[2]). The problem is that SL often cannot narrow down the model to a single one. It finds an undirected graph (UG), and it can determine the direction of some of the arrows in the UG, but it is often incapable, for well understood fundamental—not just technical—reasons, of finding the direction of *all* the arrows of the UG. So it often fails to fully specify a DAG model.

Let’s call the ordered pair (dataset, model) a **dataset++**. Then what the First Axiom is saying is that a dataset is model-free or model-less (although sometimes one can find a partial model hidden in there). A dataset is not a dataset++.

Graphs which contain both directed and undirected edges are called **partially directed (PD) graphs**. **bnlearn** takes a dataset as input and returns a PD graph  $G_{pd}$ . Given a PD graph  $G_{pd}$ , let  $\mathcal{G}(G_{pd})$  be the DAG set  $\mathcal{G}$  which is generated by giving directions to all undirected edges of  $G_{pd}$  in all possible ways. We will refer to  $\mathcal{G}(G_{pd})$  as the **DAG set completely generated by  $G_{pd}$** . and to any  $\mathcal{G}' \subset \mathcal{G}(G_{pd})$  as a **DAG set incompletely generated by  $G_{pd}$** . Once we define below our GCF measure, we will apply it to sets of the type  $\mathcal{G}(G_{pd})$  as an example.

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<sup>1</sup>This is just my whimsical name for it.

It's clear that any measure of GCF will have to involve interventions such as the “do” intervention (see Refs. [1] and [3]) invented by Pearl et al for CI. Without interventions like “do”, it is impossible to distinguish causally the DAGs in a set  $\mathcal{G}(G_{pd})$ .

Henceforth, random variables will be indicated by underlining.

## 2 Goodness of Fit

Before trying to define a GCF measure, it is instructive to review the closely related, well established, measures of Goodness of Fit (GF).

Consider two probability distributions  $PO(x)$  and  $PE(x)$ , where  $x \in S_{\underline{x}}$ . By a GF measure, we mean a measure of the difference between  $PO$  and  $PE$ . Usually  $PO$  is the observed probability distribution and  $PE$  is the expected, theoretical one.

Three popular measures of the difference between  $PO$  and  $PE$  are:

1. The **Kullback-Liebler divergence**:

$$D_{KL}(PO \parallel PE) = \sum_{x \in S_{\underline{x}}} PO(x) \ln \frac{PO(x)}{PE(x)}. \quad (1)$$

2. The **Pearson divergence** (aka **Pearson Chi-squared test statistic**):

$$D_{\chi^2}(PO \parallel PE) = \sum_{x \in S_{\underline{x}}} \frac{[PO(x) - PE(x)]^2}{PE(x)} = \sum_{x \in S_{\underline{x}}} \frac{PO^2(x)}{PE(x)} - 1. \quad (2)$$

It's easy to show using  $\ln(1 + \delta) = \delta + \mathcal{O}(\delta^2)$  that if  $\left| \frac{PO(x)}{PE(x)} - 1 \right| \ll 1$  for all  $x \in S_{\underline{x}}$ , then

$$D_{KL}(PO \parallel PE) \approx D_{\chi^2}(PO \parallel PE) \quad (3)$$

3. The **Euclidean distance squared**:

$$D_E(PO, PE) = \sum_{x \in S_{\underline{x}}} [PO(x) - PE(x)]^2 \quad (4)$$

Note that of these 3 measures, only  $D_E(PO, PE)$  is symmetric in  $PO$  and  $PE$ .

Given any bnet  $G$  with full probability distribution <sup>2</sup>  $P_G(x.)$  and a probability distribution<sup>3</sup>  $\tilde{P}(x.)$  derived empirically from a dataset, let

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<sup>2</sup>We define  $x.$  to be a vector with components  $x_i$

<sup>3</sup>Empirical distributions will be denoted by  $P$  with a tilde over it.

$$D(G) = \sum_{x.} \tilde{P}(x.) \ln \frac{\tilde{P}(x.)}{P_G(x.)} \quad (5)$$

$$= D_{KL}(\tilde{P}(\underline{x}.) \parallel P_G(\underline{x}.) ) \quad (6)$$

We define **Goodness of Fit (GF)** of the bnet  $G$  by

$$GF(G) = \ln \frac{1}{D(G)} \quad (7)$$

### 3 GCF example 1

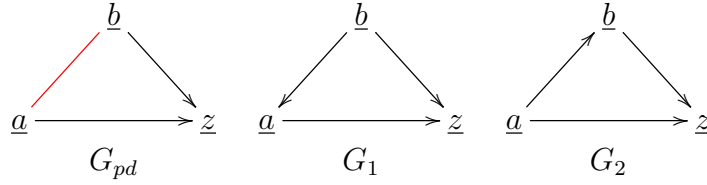


Figure 1:  $\mathcal{G}(G_{pd}) = \{G_1, G_2\}$ . The partially directed graph  $G_{pd}$  generates the DAGs  $G_1$  and  $G_2$  by giving directions to all undirected edges of  $G_{pd}$  in all possible ways. (In this case, there is only one undirected edge in  $G_{pd}$ .)

For the first example of our measure of GCF, we consider  $\mathcal{G}(G_{pd}) = \{G_1, G_2\}$  given by Fig.1. We will assume the following:

- First, we assume that we have collected a dataset from which we have extracted a full empirical distribution  $\tilde{P}(z, a, b)$ . From  $\tilde{P}(z, a, b)$ , we assume that the following have been calculated.  $\tilde{P}(z, b|a)$   $\tilde{P}(z, a|b)$   $\tilde{P}(a)$ ,  $\tilde{P}(b)$ .
- Second, we assume that a dataset has been collected for which  $\underline{a}$  was held fixed to each of the possible values  $a \in S_{\underline{a}}$  of  $\underline{a}$ . Furthermore, we assume that the distribution  $\tilde{P}(z, b|do(\underline{a}) = a)$  has been calculated from that dataset.
- Third, we assume that a dataset has been collected for which  $\underline{b}$  was held fixed to each of the possible values  $b \in S_{\underline{b}}$  of  $\underline{b}$ . Furthermore, we assume that the distribution  $\tilde{P}(z, a|do(\underline{b}) = b)$  has been calculated from that dataset.

We will refer to  $\tilde{P}(z, b|do(\underline{a}) = a)$  and  $\tilde{P}(z, a|do(\underline{b}) = b)$  as **empirical do-probability distributions**.

Now define

$$H_a = \sum_{z,b} \tilde{P}(z, b|a) \ln \frac{\tilde{P}(z, b|a)}{\tilde{P}(z, b|do(\underline{a}) = a)} \quad (8)$$

$$= D_{KL}(\tilde{P}(z, b|a) \parallel \tilde{P}(z, b|do(\underline{a}) = a)) \quad (9)$$

$$H_{\underline{a}} = \sum_a \tilde{P}(a) H_a \quad (10)$$

$$= E_a[H_a] \quad (11)$$

and

$$H_b = D_{KL}(\tilde{P}(z, \underline{a}|b) \parallel \tilde{P}(z, \underline{a}|do(\underline{b}) = b)) \quad (12)$$

$$H_{\underline{b}} = \sum_a \tilde{P}(b) H_b \quad (13)$$

$$= E_b[H_b] . \quad (14)$$

We will refer to  $H_{\underline{x}}$  for any node  $\underline{x}$  as a **hospitality**. Note that the hospitality for node  $\underline{x}$  is zero if node  $\underline{x}$  has no incoming arrows (i.e., is “inhospitable”), and becomes positive if node  $\underline{x}$  does admit some incoming arrows (i.e., is “hospitable”).

Note that if the truth is  $G_2$  with  $\underline{a} \rightarrow \underline{b}$ , then

$$H_a = 0 \text{ for all } a \text{ so } \underbrace{H_a}_0 \leq H_b \quad (15)$$

and whereas if the truth is  $G_1$  with  $\underline{b} \rightarrow \underline{a}$ , then

$$H_b = 0 \text{ for all } b \text{ so } H_{\underline{a}} \geq \underbrace{H_b}_0 . \quad (16)$$

Hence, no matter what the truth is, the arrow connecting nodes  $\underline{a}$  and  $\underline{b}$  always points towards the larger of the 2 hospitalities (i.e., the arrow “seeks the most hospitable node”)

If  $H_{\underline{a}} \leq H_{\underline{b}}$ , then define  $GCF(G_1) = -1$  and  $GCF(G_2) = +1$ .

If  $H_{\underline{b}} \leq H_{\underline{a}}$ , then define  $GCF(G_1) = +1$  and  $GCF(G_2) = -1$ .

## 4 GCF example 2

For the second example of our measure of GCF, consider  $\mathcal{G} = \{G_1, G_2, G_3\}$  given by Fig.2.

Which of the hospitalities  $H_{\underline{x}_2}$ ,  $H_{\underline{x}_1}$  and  $H_{\underline{x}_3}$ , is smallest, middle and highest, depends on the empirical do-probability distributions. For definiteness, suppose the sizes of these hospitalities are related as follows:



Figure 2:  $\mathcal{G} = \{G_1, G_2, G_3\}$ .  $\mathcal{G}$  is a set of observationally equivalent (OE) graphs. These are graphs that have the same value for GF, and are therefore indistinguishable by means of GF alone. For more info about OE graphs, see Chapter entitled “Observationally Equivalent DAGs” in Ref.[3]. Note that  $\mathcal{G}(G_{pd})$  includes one more DAG, the one in which node  $\underline{x}_1$  is a collider.

$$H_{\underline{x}_2} \leq H_{\underline{x}_1} \leq H_{\underline{x}_3} . \quad (17)$$

For any two hospitalities  $H_{\underline{a}}$  and  $H_{\underline{b}}$ , define the distance

$$d_{\underline{b}, \underline{a}} = |H_{\underline{b}} - H_{\underline{a}}| \quad (18)$$

If we abbreviate  $\underline{x}_j$  by  $j$  when used as a subscript, we can define the GCF for each of the graphs in  $\mathcal{G}$  by:

$$GCF(G_1) = \frac{-d_{2,1} + d_{1,3}}{d_{2,1} + d_{1,3}} \quad (19a)$$

$$GCF(G_2) = \frac{d_{2,1} + d_{1,3}}{d_{2,1} + d_{1,3}} = 1 \quad (19b)$$

$$GCF(G_3) = \frac{-d_{2,1} - d_{1,3}}{d_{2,1} + d_{1,3}} = -1 \quad (19c)$$

## 5 GCF in general

Eqs.(19) are a special case of the following formulae.

For any two hospitalities  $H_{\underline{a}}$  and  $H_{\underline{b}}$ , define the **hospitality distance** by

$$d_{\underline{b}, \underline{a}} = |H_{\underline{b}} - H_{\underline{a}}| . \quad (20)$$

For any  $G_i \in \mathcal{G}$ , define the **edge reward function** by

$$\rho_{G_i}(\underline{a}-\underline{b}) = \begin{cases} +1 & \text{if edge } \underline{a}-\underline{b} \text{ in } G_i \text{ points towards larger of } H_{\underline{a}} \text{ and } H_{\underline{b}}. \\ -1 & \text{otherwise} \end{cases} \quad (21)$$

Finally, suppose that  $\mathcal{G}$  is either incompletely or completely generated by a PD graph  $G_{pd}$  with undirected edges  $\{\underline{a}_k-\underline{b}_k\}_{k=0,1,\dots,nk-1}$ . Then define the GCF of graph  $G_i \in \mathcal{G}$  by

$$GCF(G_i) = \frac{\sum_{k=0}^{nk-1} \rho_{G_i}(\underline{a}_k-\underline{b}_k) d_{\underline{a}_k, \underline{b}_k}}{\sum_{k=0}^{nk-1} d_{\underline{a}_k, \underline{b}_k}}. \quad (22)$$

Note that  $-1 \leq GCF(G_i) \leq 1$ .

If the DAG set  $\mathcal{G}$  contains only one DAG  $G$ , define  $GCF(G) = 1$ , because all directions of arrows in  $G$  are known.

Call an undirected graph a **frame** and define the **frame of a DAG** to be the frame that one obtains by turning all the edges of the DAG from directed to undirected ones.

So far, we have applied our measure of GCF to a DAG set  $\mathcal{G}$  which is either completely or incompletely generated by a PD graph  $G_{pd}$ , or is a singleton set. But what if we want a GCF that can score every DAG in a DAG set  $\mathcal{G}$  that contains DAGs with different frames but the same nodes? In that case, let  $F$  be the frame which is the union of all edges in all  $G \in \mathcal{G}$ . For each edge  $\underline{a}-\underline{b}$  of  $F$ , if all the  $G \in \mathcal{G}$  give the same direction to that edge, then give that direction to that edge in  $F$ . After doing this for all edges of  $F$ , call  $G_{pd}$  the resulting PD graph. Modify each  $G \in \mathcal{G}$  by adding to it undirected edges that occur in  $G_{pd}$  but not in  $G$ . At this point, we have reduced our seemingly more complicated problem to the original one in which  $\mathcal{G}$  is an incompletely generated set of  $G_{pd}$ .

So let  $\mathcal{G}$  be an arbitrary DAG set. Our GCF measure is not enough to decide the best possible  $G$  in  $\mathcal{G}$ , because there might be several graphs with  $GCF \approx 1$ . For this reason, we recommend plotting  $GCF(G)$  versus  $GF(G)$  for all  $G \in \mathcal{G}$ . Then choose a  $G$  with a large amount of both types of goodness. It might even be advantageous to average over a small subset of DAGs in  $\mathcal{G}$  that have large amounts of both types of goodness. This would be similar to averaging over an ensemble of decision trees to get a random forest. A plot of  $GCF(G)$  versus  $GF(G)$  agrees with the spirit of the First Axiom and dataset++s, because also in those, we acknowledge a separation between the dataset (GF) and model (GCF) degrees of freedom.

## References

- [1] Judea Pearl. *Causality: Models, Reasoning, and Inference, Second Edition*. Cambridge University Press, 2013.
- [2] Marco Scutari. bnlearn. <https://www.bnlearn.com/>.

- [3] Robert R. Tucci. Bayesuvius (book). <https://github.com/rrtucci/Bayesuvius/raw/master/main.pdf>.