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(Article begins on next page)

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On the approximation of the Shapley value via machine learning in transportation network cooperative games

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This paper is dedicated to the memory of our colleague and friend Yuval Hadas, who sadly passed away after the submission of the manuscript. We will remember Yuval as an enthusiastic researcher and a very kind person, a pleasure to work with and spend free time with.

Abstract. The Shapley value, a well-established concept in cooperative game theory, serves as a metric for assessing the significance of each player in a transferable utility game. Recently, it has found application in gauging the importance of individual nodes or arcs within a network. However, in this context, the exact evaluation of the Shapley value is often computationally expensive, particularly in the case of extensive networks. This study delves into the challenge of approximating the Shapley value in a transferable utility game defined on a network, wherein the characteristics of the network are parameterized by a variable of interest (e.g., the traffic demand). We examine the smoothness of the Shapley value with respect to this parameter and leverage such smoothness to theoretically justify the adoption of machine-learning techniques for its approximate computation. Additionally, we present potential extensions for further research in this area.

Keywords: Transferable-Utility Games, Shapley Value, Approximate Computation, Wardrop Equilibrium, Machine Learning.

1 Introduction

A basic question in network analysis is the following: how "important" is each node/arc in a network? Analyzing the "importance" of nodes/arcs can assist decision-makers in identifying weak components, detecting and preventing failures, controlling fire

outbreaks in extensive wilderness areas, improving connectivity (for instance, in terms of travel time, costs, reliability, access, and flow), etc.

To quantify, e.g., the relative importance of nodes in a network, one possible approach uses the concept of *centrality*. The following are some classical *measures of centrality* of a node i in a network:

- *Degree centrality* relies on the concept of node degree, computed based on the adjacency matrix of the network.
- *Closeness centrality* is computed as one over the summation of the lengths of the shortest paths between node i and all the other nodes.
- *Betweenness centrality* is based on the number of shortest paths between any pair of other nodes via or not necessarily via the intermediate node of interest i.
- *Eigenvalue centrality* is based on the idea that a node i being connected to other nodes with higher scores is given more importance.

However, classical measures of centrality present several limitations:

- They do not consider how the network behaves if any subset of nodes is removed from the network.
- The *Origin-Destination (OD)* demand is not typically considered.
- Some transportation-related properties (e.g., arc capacity, route choice, and congestion) are not easily captured.

Alternative measures of node centrality based on cooperative game theory can deal with the issues reported above. Their definitions can also be extended easily to assess centrality of arcs, differently from most classical measures of node centrality (a variation of betweenness centrality holds for edges and is the *edge betweenness centrality*, see Girvan and Newman, 2002). Applications range, e.g., from movement analysis (Kolykhalova et al., 2020) to traffic networks (Passacantando et al., 2021a) and wildfire fighting (Qayyum et al., 2024).

In this work, we discuss advantages and limitations of one such game-theoretical measure, based on a solution concept from cooperative game theory (the Shapley value). Then, we justify theoretically its approximation by machine-learning techniques, after analyzing its smoothness with respect to a parameter of interest (the traffic demand).

2 Transportation Network cooperative (TNc) games

In this section, we briefly summarize a measure of centrality, based on the framework of *Transportation Network cooperative (TNc) games* (see, e.g., Hadas, Gnecco, and Sanguineti, 2017; Passacantando et al., 2021a, 2021b), which solves the issues reported

in the Introduction (although it introduces some other computational issues, as discussed later).

- In the TNc framework, a subset of the nodes (or arcs) of the network is considered as the set of players in a *Transferable Utility (TU) cooperative game model* (see the Appendix for a reminder on TU games).
- The value (utility) of each subset (coalition) of the set of all players (*grand coalition*) is defined in such a way to represent a wide range of transportation attributes, such as the total travel time.
- A suitable solution concept from cooperative game theory is applied to rank the nodes (or arcs) (e.g., the *Shapley value*, which measures the expected marginal utility provided by each player to a randomly formed coalition of players: see the Appendix for its definition). This provides a measure of the centrality of nodes (or arcs) in the network.

The key advantage of this approach is that nodes (or arcs) are ranked by considering how they contribute to the utilities of all possible subsets of nodes (or arcs).

3 Computational issues related to the evaluation of the Shapley value in TNc games

Nevertheless, the exact evaluation of the Shapley value for TNc games poses relevant computational issues:

- In general, the computational effort increases exponentially with the number of players (although, in some special cases, this does not occur, see, e.g., Michalak et al., 2013; Kolykhalova et al., 2020). One possible way to reduce such a computational effort is to restrict the set of players to some special nodes or arcs of interest (Gnecco, Hadas, and Sanguineti, 2021, 2022).
- Such an effort is even larger when considering TNc games in which players are arcs and the utility function measures congestion (Passacantando et al., 2021a, 2021b). Indeed, in this case, the utility of each coalition is not given directly. Instead, as an additional step, one has to solve a suitable optimization problem or variational inequality for every coalition, to find its utility (see Section 4.1).
- The computational effort is further increased by the presence of parameters (e.g., the traffic demand).

An approximate evaluation of the Shapley value in a TNc game can be obtained using a *Monte Carlo approach*, which replaces the expectation in the definition of the Shapley value (given in the Appendix) with an empirical average. This is done, e.g., by the ApproShapley algorithm reported in Castro et al. (2009) for generic TU games, and by its extension to TNc games, discussed in Gnecco, Hadas, and Sanguineti (2021). Theoretical guarantees (unbiasedness and bounds on the variance of the Monte Carlo

estimate of the Shapley value) can also be obtained (Gnecco, Hadas, and Sanguineti, 2021).

4 Contributions of the work

In the following, we discuss an alternative approximate evaluation of the Shapley value, based on machine learning (Section 4.2). It can be used when the Shapley value is a smooth function of a parameter (which is analyzed in Section 4.1). As discussed in Section 4.3, this approximation could also be combined with the Monte Carlo approach.

4.1 Analysis of Lipschitz continuity of the Shapley value as a function of the traffic demand

For certain TNc games, the *Shapley value* is a *Lipschitz continuous function* (with Lipschitz constant L) *of a parameter* d (e.g., the *traffic demand* in TNc games modeling congestion). In particular, it is a function of bounded variation on any bounded and closed interval I (see Figure 1 for an example).

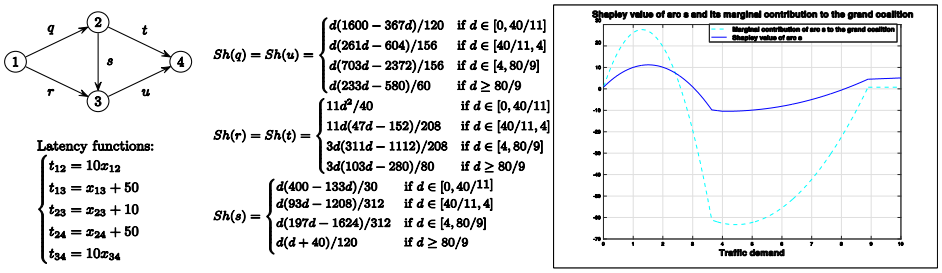

Fig. 1. ***Left***: Example of a transportation network with latency functions on the arcs (*Braess' network*) from Passacantando et al. (2021a). ***Middle***: Shapley value (expressed in this case in closed form) of each arc as a function of the traffic demand d from node 1 to node 4 (see Passacantando et al., 2021a, and the following paragraphs for the definition of the utility function). ***Right***: Shapley value and marginal contribution to the grand coalition of the specific arc s. Note: in this TNc game, the set of players is made by all the arcs in the network.

As detailed in Section 4.2, such smoothness can motivate the use of machine learning for Shapley value approximation.

The utility function in the family of TNc games considered in Passacantando et al. (2021a) is obtained by solving several *user equilibrium traffic assignment problems* (Correa and Stier-Moses, 2011), one for each coalition of players, which corresponds to a suitable subnetwork of the original network.

Specifically, we consider a directed graph $G = (V, A)$, where V is the set of nodes, $A \subseteq V \times V$ is the set of arcs and $C \subseteq V \times V$ is a set of Origin-Destination (OD) pairs. For any OD pair $c \in C$, we denote by d_c the corresponding traffic demand, K_c the set of

paths joining it and y_c^k the flow on a generic path $k \in K_c$. A path flow vector $y \geq 0$ is feasible if it satisfies the traffic demands, i.e., $\sum_{k \in K_c} y_c^k = d_c$ holds for any $c \in C$. For any arc $(i,j) \in A$, x_{ij} denotes the flow on (i,j), while t_{ij} is the latency (or travel time) function on the arc (i,j) which is assumed to be a function only of the flow x_{ij} on arc (i,j), and to be continuous and increasing. The travel time on each path $k \in K_c$, denoted by T_c^k, is defined as the sum of travel times on the arcs of such a path. We denote by a_{ij}^{kc} the element in position kc (with $c \in C, k \in K_c$) of the incidence matrix of G related to the arc $(i,j) \in A$, so that arc flows x and path flows y are linked by the following equation:

$$x_{ij} = \sum_{c \in C} \sum_{k \in K_c} a_{ij}^{kc}\, y_c^k\,, \qquad \forall (i,j) \in A.$$

In this framework, we consider a TNc game where the set N of players is a subset of A. The graph associated with a generic coalition $S \subseteq N$, denoted by $G(S) \coloneqq \big(V, S \cup (A \backslash N)\big)$, contains the arcs of coalition S and the arcs that are not players of the game. We define $\mathcal{F}$ as the set of coalitions $S \subseteq N$ such that for each OD pair $c \in C$ there exists at least one path in $G(S)$ connecting c. For any coalition $S \in \mathcal{F}$, a feasible path flow vector $y(S)$ is called a *selfish Wardrop equilibrium* (or *user equilibrium*) in the network $G(S)$ if for any OD pair $c \in C$ and path $k \in K_c$ one has

$$T_c^k(y(S)) \begin{cases} = \lambda_c \;\; if \; y_c^k > 0, \\ \geq \lambda_c \;\; if \; y_c^k = 0, \end{cases}$$

where λ_c is the *equilibrium disutility* for the OD pair c.

Finding a selfish Wardrop equilibrium $y(S)$ amounts to solving the following *convex optimization problem* (Morandi, 2023):

$$\begin{aligned} &\text{minimize} \sum_{(i,j) \in S \cup (A \backslash N)} \int_0^{x_{ij}} t_{ij}(\omega) d\omega \\ &\text{subject to:} \\ &x_{ij} = \sum_{c \in C} \sum_{k \in K_c} a_{ij}^{kc}\, y_c^k\,, && \forall (i,j) \in S \cup (A \backslash N), \\ &d_c = \textstyle\sum_{k \in K_c} y_c^k\,, && \forall c \in C, \\ &x_{ij} \geq 0, && \forall (i,j) \in S \cup (A \backslash N), \\ &y_c^k \geq 0, && \forall c \in C, \forall k \in K_c. \end{aligned} \tag{1}$$

The total travel time at the equilibrium is defined as:

$$TT(S) \coloneqq \sum_{c \in C} \sum_{k \in K_c} T_c^k(y(S))\, y_c^k(S) = \sum_{(i,j) \in S \cup (A \backslash N)} t_{ij}\big(x(S)\big)\, x_{ij}(S).$$

It is worth noting that this total travel time is well-defined since the arc equilibrium flow x exists and is unique, as being the latencies of the arcs continuous and increasing functions of the respective flows (Correa and Stier-Moses, 2011). Moreover, it is worth mentioning that the convex optimization problem (1) arises as a particular case of a more general *variational inequality* approach (Patriksson, 2015), also applicable to the situation in which the latency function of each arc depends on the flows on other arcs.

We define the utility function v: $2^N \rightarrow R$ of the TNc game by considering two cases:

- If the empty coalition $\emptyset \in \mathcal{F}$, then $v(S) := TT(\emptyset) - TT(S)$ for any $S \subseteq N$.
- If the empty coalition $\emptyset \notin \mathcal{F}$, then

$$v(S) := \begin{cases} [\max_{S' \in \mathcal{F}_m} TT(S')] - TT(S) & if\ S \in\ \mathcal{F}, \\ 0 & if\ S \notin\ \mathcal{F}, \end{cases} \qquad \forall S \subseteq N,$$

where $\mathcal{F}_m$ is the subset of *minimally connected* coalitions, i.e., the ones for which the removal of any player makes the resulting coalition not belong to $\mathcal{F}$.

If the latency functions t_{ij} are continuously differentiable for any arc $(i,j) \in A$, then the arc equilibrium flow $x(S)$, for any coalition $S \subseteq N$, is a Lipschitz continuous function of the vector d of traffic demands (Lu, 2008). Loosely speaking, such smoothness result depends on the fact that a small variation of the demands produces a correspondingly small change in the feasible region and in the optimal solution of the optimization problem. Therefore, the total travel time at equilibrium, the utility function of each coalition, and the Shapley value of each arc are also Lipschitz continuous functions of the traffic demands.

4.2 Motivation for the application of supervised machine learning to Shapley value approximation

Under the previous Lipschitz continuity property (with constant L), in the univariate case (i.e., when $|C| = 1$ and $d_c = d$, likewise in the example of Figure 1), one can approximate the Shapley value of each arc on any bounded and closed interval I by using a *one-hidden-layer feedforward neural network* with a *sigmoidal activation function* σ (i.e., a bounded, differentiable, and real function defined for all real input values, having non-negative derivative at each point, and exactly one inflection point) and M computational units, obtaining a *sup-norm approximation error* on I smaller than or equal to $\frac{c(I) \cdot L}{M}$, where $c(I) \geq 0$ depends only on the length of the interval I and on the choice of σ. Such a neural network has the following form:

$$f_M(d) = \sum_{m=1}^{M} c_m \sigma(a_m \cdot d + b_m), \qquad (2)$$

where $a_m,\ b_m,\ c_m \in \mathbb{R}$ $(m = 1, \ldots, M)$ are parameters to be optimized during the training of the network.

The result above follows by an application of Theorem 1 in Gao and Xu (1993) on nonlinear approximation of univariate functions of bounded variation by this kind of neural networks.

This result suggests the application of *supervised machine-learning methods* to approximate each Shapley value function $f(d)$ by using a neural network of the form (2) and a training set made of a finite number of pairs of the form $(d_p, f(d_p))$, $p = 1, \dots, P$.

As an example of application, Figure 2 compares, as functions of the traffic demand d from node 1 to node 4, the Shapley value $Sh(s)$ of arc s in the example reported in Figure 1 with its approximations obtained by training two one-hidden-layer feedforward neural networks of the form (2) on the interval $I = [0,10]$. The first neural network has $M = 3$ computational units, whereas the second neural network has $M = 12$ computational units. The square loss has been used as loss function for training, whereas the training inputs have been chosen as $d_p = (p-1)/5$, for $p = 1, \dots, P = 51$ (which correspond with the positions of the circles in the figure). In both cases, training has been performed by batch gradient descent implemented by backpropagation, with learning rate equal to 0.01, and 10000 training epochs. Before the application of each neural network, for scaling reasons the input d has been mapped linearly onto the interval $[0,1]$, and the weights of all the computational units (i.e., a_m, b_m, and c_m) have been initialized by realizations of random variables, uniformly and independently distributed on the interval $[-1,1]$. Then, the predictions coming from the two trained neural networks have been plotted on the interval I using a finer discretization with respect to the training set. The results reported in the figure show a clearly better performance of the network with the largest number of computational units.

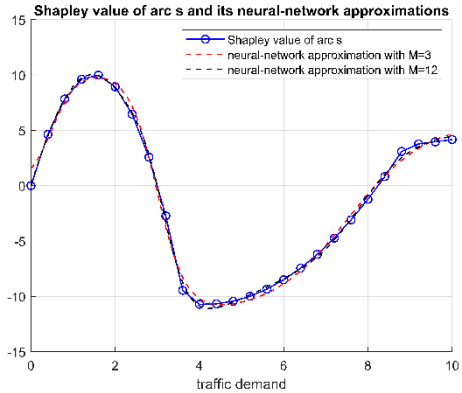

Fig. 2. Shapley value of arc s in the TNc example from Passacantando et al. (2021a), and its neural-network approximations obtained with $M = 3$ and $M = 12$ computational units, respectively.

4.3 Possible extensions of the analysis

The average error on the training set in Section 4.2 could be related to a corresponding *estimation error* by using either *deterministic learning theory* (Cervellera and Muselli, 2011) or *statistical learning theory* (Vapnik, 1998).

The following is a possible way to combine the Monte Carlo approach briefly presented in Section 3 with the machine-learning approach of Section 4.2: one could consider the case in which a Monte Carlo approximation of the Shapley value of each arc is available on the training set, instead of the Shapley value itself. In other words, in this more general case the training set would be noisy, i.e., the training pairs would have the form $(d_p, f(d_p) + \varepsilon_p),\ p = 1, \dots, P$, being the ε_p realizations of independent random variables. These would be not necessarily identically distributed, due to their different associated values of the parameter d. Also in this more general situation, results from statistical learning theory could be used to bound from above the estimation error. Such a bound could be combined with an upper bound on the *approximation error* of the Shapley value such as the one presented in Section 4.2 with the final aim to determine an upper bound on the *generalization error*, following the general statistical learning theory approach of Niyogi and Girosi (1996).

Higher-order smoothness of the Shapley value with respect to the vector of demands could be needed to extend the bound on the sup-norm approximation error of Section 4.2 to the multivariate case. However, smoothness higher than Lipschitz continuity is not expected to hold in general, because a change in the vector of demands could also change the set of active constraints at optimality for some of the optimization subproblems (1), possibly resulting in loss of differentiability (likewise in the example reported in Figure 1).

5 Conclusions

We have examined the Lipschitz continuity of the Shapley value for a class of parameter-dependent TU cooperative games on graphs. Then, we have exploited such a property to motivate the use of machine-learning techniques for the approximate computation of the Shapley value.

Variations of the results (e.g., other conditions under which the Shapley value is a smooth function of some parameters) are expected to hold for families of TU cooperative games on graphs: for instance, the cases in which the selfish Wardrop equilibrium considered in Section 4.1 is replaced either by the *Nash equilibrium* of a *noncooperative game model* in which the players are groups of users (Krylatov, Zakharov, and Tuovinen, 2020) or by the *system optimum* (see, e.g., Correa and Stier-Moses, 2011), which involves a social planner. Such cases could be analyzed under the *parametric variational inequality* approach investigated in Passacantando and Raciti (2023). A further interesting case concerns players that represent *joints of the human body* or *individuals in a group of people*, and the Shapley value is used as a *measure of*

the importance of such players for TU cooperative game models (parametrized by time) that capture the *group motion behavior* via suitable movement features (Kolykhalova et al., 2020).

Appendix: Transferable Utility (TU) games and Shapley value

A *Transferable Utility (TU) cooperative game* (Maschler, Solan, and Zamir, 2020) is a pair (N, v), defined as follows: $N = \{1, \dots, n\}$ is the set of players and is called the grand coalition. $S \subseteq N$ denotes a coalition. For each $S \in 2^N$, $v(S)$ denotes the utility that can be achieved by the players in S. For the empty coalition, one has $v(\emptyset) = 0$. In this class of games, there is the possibility of transferring utilities from one player to any other one without incurring any loss. If player i contributes nothing to the value of any extended coalition, then it should receive 0 in a fair allocation of the utility of the grand coalition. If player i positively contributes to at least one coalition S (and contributes non-negatively in all the other cases), then it should receive more than 0. The Shapley value represents indeed a fair way to allocate the utility of the grand coalition within the set of players (the reader is referred, e.g., to Maschler, Solan, and Zamir, 2020, for its complete axiomatic characterization), and has the following expression:

$$Sh(i) = \sum_{S \subseteq N} \left[\left(v(S) - v(S \setminus \{i\}) \right) \frac{(|S|-1)!(n-|S|)!}{n!} \right], \qquad \forall\, i \in N. \tag{3}$$

Equation (3) can be interpreted as the expected marginal utility of player i, when she joins the coalition formed by all the players that precede her in a random permutation of the set of players (all the permutations being equally likely).

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