

# A Novel Application of Tensor Networks for the Investigation of Design Optimization Tools in the Marine Domain

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## ABSTRACT

*Traditional optimization methods often struggle to map the unique interactions between design variables, operational constraints, and performance objectives. Tensor networks, a mathematical framework rooted in quantum physics, address this challenge by providing a tool to model state relationships within multidimensional data structures. In the context of bulk carrier synthesis and optimization, tensor networks enable the simultaneous analysis of multiple constraints and their interactions via a state space representation. A state space representation offers a holistic understanding of the optimization landscapes by providing insights that add to traditional optimization analysis techniques. This paper presents a methodology for converting the optimization problem into multiple tensor network representations, details the implementation of tensor network algorithms, and showcases implementation results. The findings underscore the capacity of tensor networks to provide a deep, data-driven understanding of complex optimization landscapes, thus enabling novel decision-making opportunities.*

## KEY WORDS

Tensor Networks, Early-Stage Design, Optimization, Concept Design Tools, Informed Decision Making

## INTRODUCTION

In recent years, optimization techniques have emerged as indispensable tools in the pursuit of efficient, autonomous, eco-friendly, and high-performance marine solutions. This conference paper delves into the multifaceted challenges faced when applying optimization methodologies in the nascent stages of marine design. From the intricate dance between hydrodynamics and structural integrity to the intricacies of incorporating sustainability criteria, this paper illuminates the complexities that must be navigated by designers and engineers in this dynamic and evolving field.

The maritime industry stands at the precipice of transformation, driven by the demands for greater efficiency, sustainability, autonomy, and performance in marine vessels. As designers and engineers embark on the challenge of designing the next generation of vessels, they are increasingly turning to optimization techniques to guide their decisions from the very inception of a project. However, this endeavor is not without its challenges, as optimizing marine designs at the early stages presents a unique set of challenges. Engineers and designers, driven by the promise of improved efficiency, cost-effectiveness, and innovation, often embrace optimization results with unwavering trust. However, this “blind faith” in optimization outcomes may have unintended consequences that warrant careful consideration.

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Traditional optimization methods and optimization analysis methods often struggle to comprehensively map the complex interactions between design variables, operational constraints, and performance objectives Papalambros and Wilde (2000) Marler and Arora (2004). No current methods exist for mapping populations of solutions in relation to design variables, objectives, or constraint activation across a solution space. The case study presented in this manuscript aims to help provide a framework for understanding how to better formulate and understand the results of optimization in early-stage design. The methodology and framework presented in this manuscript employ tensor networks and concepts from ontological commitment.

There has been limited research utilizing the philosophy-based side of ontologies within engineering, but there can be crucial implications for marine design. One concept that is of great interest in this domain is ontological commitment. Ontological commitment is a concept from philosophy that pertains to assertions of existence and entities of kinds of entities Juben (1998). In the context of engineering and design, ontological commitment refers to the assumptions and pre-conditions about the fundamental nature of the design variables, objects, functions, and relationships that comprise the design. Ontological commitment in this context yields the possibility to enable the understanding of potential design implications associated with the integration of the multiple contextual views of design artifacts within a singular framework. To enable the use of ontologies and ontological commitment in the marine domain, tensor networks show promising capability as a framework. Tensor networks, a mathematical framework rooted in quantum physics, have found promising utility in diverse domains due to their ability to capture intricate patterns and correlations within large, highly entangled datasets, such as those seen in the marine domain Klishin (2020). The main question addressed by this research is how one understands a-priori the encoded and non-encoded relations and inter-dependencies that exist within design tools from an ontological lens. In the case of this research, an encoded relation is one captured by a direct relation of input variables or objectives in relation to constraints or intermediate functions. A non-encoded relation is a relation that may exist between variables, constraints, intermediate functions, or objectives that is not directly codified in the formulation of a problem. A tensor network framework is able to capture the impact of non-encoded and encoded relations by having the ability to investigate all possible couplings in n-dimensions.

While networks and network science have proven to be invaluable tools, in most cases researchers are simply analyzing networks that already exist with some innovative modifications and representations. However, within the naval design domain, standard networks (e.g., social networks) do not exist. For this reason, naval design researchers have been forced to create unique novel network frameworks and associated novel network metrics, tailored to specific naval design problems. As with other naval design research, a critical step is the proper abstraction and creation of not only a ship-centric ontological framework but also the methods needed to populate the network. How one structures the nodes, edges, layers, and population will determine the framework's ability to uncover the desired insights. Based on the challenges presented by the problem, tensor networks show promise in their ability to provide insights. Tensor networks address the challenge of investigating optimization tools by providing a powerful framework to unravel intricate relationships within multidimensional data structures.

This manuscript presents a novel tensor network framework for investigating optimization codes, which is used in the presented case study. The case study presented in this manuscript is based on the Sen and Yang Bulk Carrier multi-objective optimization problem Sen and Yang (1998). The problem is well studied and provides a simple example to investigate the capabilities of tensor networks while providing novel insights. The Sen and Yang Bulk Carrier Optimization is governed by three objectives, six design variables, 13 constraints, and 34 intermediate functions. In the performed case study, both optimization-based data and Monte Carlo-based data from the model were analyzed using the novel tensor network framework. The novel framework developed provided several insights detailed later in this paper. These insights included the ability to investigate constraint activation, the nature of constraints and regions of binding, and the ability to identify regions of viability within the solution space.

The investigation completed in this case study provides a few important insights for the marine domain. First, as engineers and designers, one must recognize that one's design tool predicts the resulting trade space. The way one defines inputs and objectives directly impacts and commits the resulting solution space of the problem. Second, one must investigate what assumptions or constraints bind a design space. This will help ensure that the solutions from an early-stage design optimization tool have a meaningful impact on the designs made and prevent later design re-work. Third, the case study shows that it is critical to investigate whether one's inputs and their ranges and constraints are reasonable. Fourth, it is essential to

know if the preferred solution is valid and robust. Finally, the case study presented provides a framework to evaluate the crucial question of can a design tool give the designer what they want relative to a specified objective.

## BACKGROUND

The following sections detail the necessary background for the case study presented in this manuscript.

### Ontological Commitment

The notion of ontological commitment stemming from the realm of metaphysics has not found widespread application within the field of engineering design, especially not directly or overtly. In metaphysics, ontological commitment refers to the necessity of positing certain entities for a theory or system to be deemed valid or true Rayo (2007). In the context of engineering design, ontological commitment holds relevance concerning the presumptions and prerequisites that underlie a design. This concept is formally defined as “a relation that holds between persons or existence assertions, on the one hand, and specific entities or kinds of entities, on the other” Jubien (1998). This implies that “assertions of the existence of specific entities or kinds of entities are the intuitive source of the notion of an ontological commitment” Jubien (1998).

In simpler terms, ontological commitment signifies the recognition that one assigns significance to something by inferring belief within an established domain or context, and its validity hinges on its connection to some notion of prior existence. There are numerous instances illustrating ontological commitments. For instance, within the realm of physics, the field is ontologically committed to the existence of entities such as atoms, quarks, and space-time. To expand on this, physics theory is ontologically committed to the concept of electrons, meaning that the authenticity of physics demands the existence of electrons, adhering to specific behavioral patterns.

Another perspective on ontological commitment is that it discloses the “demands imposed on the world” Rayo (2007). Nevertheless, despite extensive discussions in philosophy, the term “ontological commitment” is not commonly utilized in engineering design as a technical term or framework. Engineering primarily concerns itself with practicality and concrete outcomes, prioritizing tangible requirements over abstract metaphysical considerations.

However, the notion of ontological commitment does hold relevance in engineering design in the sense that the design process often entails decisions regarding which types of entities should be included or excluded from a design. In certain instances, engineers or designers may need to make assumptions or commitments about the nature of reality or the existence of specific entities to develop a functional design. For instance, in the field of software engineering, choices about the inclusion of particular data structures or classes in a program may carry ontological implications. Similarly, in the design of complex systems, decisions about the incorporation of various components or subsystems may involve ontological commitments. Nonetheless, in both scenarios, the language and concepts employed to address these matters typically belong to the engineering domain, rather than being derived from metaphysics.

Two critical concepts within ontological commitment are explicit and implicit ontological commitment. The concepts are directly a bi-product of the modern efforts to try to quantify all entities involved in a commitment and were originally presented by Peacock and Krämer and expanded upon by Österblom Peacock (2011) Krämer (2014) Österblom (2017). Explicit ontological commitments are defined by the entities that are claimed to exist that are directly stated in the statement of a theory or statement Peacock (2011) Österblom (2017). Put simply, “a theory is explicitly ontologically committed [to an entity] if it contains some sentence that means there are X” Krämer (2014) Österblom (2017). Explicit ontological commitment is a pretty clear notion and covers any direct statement of existence. To cover the commitments that are not directly stated or directly related to a theory or statement, there is implicit ontological commitment. Implicit ontological commitment is defined by two criteria. The first of the criteria for determining implicit ontological commitments is “the theory could not be true unless X existed,” and the second is “the theory is committed to X and not explicitly committed to X” Peacock (2011) Österblom (2017). One important aspect to note about ontological commitments is that they are an

“unavoidably modal notion” Österblom (2017). Specifically, this means with implicit ontological commitment, it is not necessarily always clear whether an entity is involved in the commitment of a statement or theory or not. A more in-depth discussion of the use of ontological commitment in the marine domain can be found in a previous conference paper written by the author Arrigan et al. (2022).

Within the domain of naval architecture, there is a multitude of ontological commitments that go into a ship’s design. For example, one can explore the ontological commitment to ship stability, which is inherently acknowledged as a paramount design principle. This is exemplified by the explicit prioritization of a positive, non-zero metacentric height (GM), which serves as a fundamental criterion for a vessel’s ability to right itself after being heeled by external forces. The acceptance of this constraint reveals a naturally embedded ontological commitment to ensuring the stability of a ship, a necessity for operational safety and seaworthiness. Consequently, the solution space for ship design is inherently limited to configurations that yield a positive, non-zero GM. In this case, there is an explicit commitment to ships with positive, non-zero GMs and an implicit commitment to their stability. Digging deeper into the components that contribute to the calculation of GM, which includes the distance from the keel to the center of buoyancy (KB), the distance between the metacenter and center of buoyancy (BM), and the distance from the keel to the center of gravity (KG), one stumbles upon a series of implicit commitments. These pertain to the various elements and design choices that influence KG, such as weight distribution, onboard systems, and cargo loading protocols, which themselves are circumscribed by a myriad of other constraints and linguistic stipulations. Simultaneously, KB and BM are predominantly dictated by the engineered geometry of the hull. Thus, there are clearly ontological commitments in ship design regarding stability. In this context, they can be classified as high-order commitments due to the layering of explicit and implicit first-order commitments that make up the ontological commitment of stability.

## STATISTICAL PHYSICS

Statistical physics is a branch of quantum physics concerned with understanding the behavior of large-scale systems based on the interactions between their individual components largely via tensor networks Huang (2009). Tensor networks are networks of  $n$ -dimensional arrays, referred to as tensors. Tensor networks can be utilized as a powerful tool for investigating highly correlated and entangled, complex systems. Tensor networks efficiently represent all possible combinations of components’ states and their connections to other components and their respective states. This ability directly allows one to rapidly query the state space and obtain probability distributions across different components and their respective states through performing contractions and studying the statistical properties of their collective behavior. In the marine domain, tensor networks have just started to be used and are in the nascent stages of being introduced to their many use cases. Currently, within the marine domain, tensor networks have been used to shed new light on the problem of ship arrangements and routing Klishin (2020) Klishin et al. (2019). Additionally, tensor networks are being used for decoupling diagnostic decision-making from the scale of the state space to enable self-adaptive health monitoring Manohar and Singer (2022).

In the view of the authors, tensor networks enable a strong framework for investigating optimization codes as one can easily investigate the impact of individual or multiple components across certain or changing states. Traditional optimization analysis methods, design of experiments, and sensitivity analysis struggle to comprehensively map the complex interactions between design variables, operational constraints, and performance objectives. Tensor networks provide a powerful tool to unravel intricate relationships within multidimensional data structures since it is native for data to be represented as high-dimensional tensors in the tensor network. Tensor networks enable the simultaneous analysis of multiple constraints, design variables, and their interactions simultaneously and offer a holistic understanding of the optimization landscape. Furthermore, tensor networks allow for the identification of constraint activation regions, shedding light on the conditions under which specific constraints come into play. This ability directly provides the design process with insights that would otherwise remain hidden. To fully understand the results presented from the case study detailed in this manuscript, it is critical to lay out the technical details of a few important statistical physics and tensor network-based concepts.

Statistical physics largely utilizes the Variation Principle of Maximum Entropy Cimini et al. (2019). This principle states that the probability distribution best representing the current state of (knowledge on) a system maximizes Shannon entropy subject to the context of any prior information on the system itself. In more common terms this means that the lowest en-

ergy is the most probable. In quantum mechanics, the ground state of a system is the state in which the quantum mechanical Hamiltonian operator has its lowest eigenvalue Klishin (2020). The wave function corresponding to the ground state contains information about the probability distribution of finding a particle in various positions and momentum states. This same idea applies to tensor networks where one can obtain position and state probability information from a given network. Within statistical physics there are two primary information structures: partition functions and tensor networks Klishin (2020). The partition functions describe the statistical properties of a system and can be manipulated to obtain statistical properties, such as probability distributions, about the system Klishin et al. (2019). The partition function directly provides a connection between the microscopic properties of individual particles and the macroscopic properties of the entire system. It is defined as the sum of the Boltzmann factors (meant to obtain the Boltzmann Distribution), which are exponential functions of the system's energy at each state. In work done by Klishin et al., they developed a method for integrating a partition function into a tensor network such that the tensor network can be modified and contracted to evaluate the partition function and learn statistical information about the system Klishin et al. (2019) Klishin (2020). The partition function  $\mathcal{Z}$  sums over all possible system state configurations  $\alpha$ . The energy of the system in configuration  $\alpha$  is given by the objective function  $\mathcal{O}_i(\alpha)$ . The partition function is defined below.

$$\mathcal{Z} = \sum_{\alpha} e^{-\sum_i \lambda_i \mathcal{O}_i(\alpha)} \quad (1)$$

From this partition function, the probability of specific configurations can be derived. By taking the specific configuration  $\alpha$ , it can be extracted from the equation and normalized as in Eq. 2. This gives the probability of the system being in configuration  $\alpha$ .

$$p_{\alpha} = \frac{1}{\mathcal{Z}} e^{-\lambda \mathcal{O}(\alpha)} \quad (2)$$

In the above formulation  $\lambda$  is  $\frac{1}{T_{Critical}}$ . In statistical physics, the critical temperature of the system represents when phase transition occurs. The value selected for the critical temperature, or in this case  $\lambda$ , is essential. A lower value of  $\lambda$  suggests that the behavior of a system is more random. A higher value of  $\lambda$  suggests that the behavior of a system is more known. A value around the transition point suggests the behavior of the system is largely unknown. In terms of a probability distribution, a lower  $\lambda$  suggests a more uniform distribution, and a higher  $\lambda$  suggests a centered or skewed distribution. A second important component of the partition function is the objective function  $\mathcal{O}_i(\alpha)$ . The objective function  $\mathcal{O}_i(\alpha)$  returns the system's energy while at state configuration  $\alpha$ .  $\mathcal{O}(\alpha)$  is equivalent to the system's Hamiltonian at configuration  $\alpha$ . The objective function can be configured for varying goals. For the case study presented in this manuscript, the objective function was configured to favor extreme high or low displacements.  $\lambda$  could also be thought of as a configuration pressure, favoring more random or known behavior of the system. Fundamentally, the objective function defines state-to-state relationships via the energy between states. This is the point where the Principle of Maximum Entropy comes into play since the lowest objective state will have the highest probability.

The second information structure of statistical physics is tensor networks. Tensor networks are networks of tensors where the edges between tensors represent contractions, which are summations over a shared index Ran et al. (2022). The first important concept to understand in relation to tensor networks is the concept of rank. Rank refers to the order of the tensor. A rank zero tensor is a scalar, a rank one tensor is a vector, a rank two tensor is a matrix, and so on. Since contractions represent a summation over a shared index between two tensors, a tensor network represents a series of mathematical operations. Therefore, by encoding a partition function into a tensor network, contracting the tensor network evaluates the partition function Klishin (2020). As an example, consider the contraction between two two-rank tensors  $A_{ij}$  and  $B_{jk}$  over a shared index  $i$ . The result of the contraction is a new two-rank tensor,  $C_{ik}$ .

$$A_{ij}B_{jk} = A_{i1}B_{1k} + A_{i2}B_{2k} + \dots + A_{in}B_{nk} = C_{ik} \quad (3)$$

Within this partition-encoded tensor network, there are two types of tensors. The first type of tensors are those which represent particles in the system and their states. The second type of tensor is a coupling tensor which represents all state-to-state energy combinations between two particles in the system. In the tensor network, particle tensors are connected to other particle tensors via an intermediary coupling tensor if those two particles directly impact one another. The states represented within the particle tensors and the energy represented within the coupling tensors are determined by their use case. The values utilized in these tensors will be detailed in the later sections of this manuscript.

When the tensor network is contracted, the result is a probability distribution over that system's state space. There are two other critical concepts related to contractions that should also be mentioned. To obtain statistical information about a system via a tensor network, there are two critical concepts related to contractions that need to be presented. These are the concepts of external legs and anchors. In addition to being able to perform contractions of the tensor network, to aid querying one can add external legs and or anchors. An external leg artificially adds a rank to a tensor to prevent it from being fully summed in the partition function. If there are no external legs on a tensor network, a contraction of the tensor network yields a single number. Multiple external legs can be added to a network. A single external leg will yield a marginal probability relative to the node it was placed and multiple external legs will result in a joint probability relative to the respective nodes. Similar to external legs, none, one, or multiple anchors can be added to a tensor network. Anchors condition the system on being in a specific state. Thus, the specified configuration is held constant over partition function summation. This in turn yields a conditional probability for the system conditioned on a specific state or multiple states.

To wrap up this brief introduction to statistical physics and tensor networks, it should be noted that tensor networks require three pieces of information to be constructed. The first is a logical network of nodes of a system. The second is the state space of these nodes. Finally, there needs to be an objective function that describes the cost or energy of the system being in specific configurations.

## Sen and Yang Bulk Carrier Problem Formulation

The following section details the formulation of the Sen and Yang Bulk Carrier optimization. Sen and Yang (1998). Additional information may also be found in Yang et al. (1990) and Yang and Sen (1996).

### *Inputs and Intermediate Functions*

The model defines six inputs: length ( $L$ ), beam ( $B$ ), draft ( $T$ ), depth ( $D$ ), speed ( $V$ ), and block coefficient ( $C_B$ ).

Using these inputs, the model defines a host of intermediate functions:

$$\begin{aligned} \text{annual cost} &= \text{capital charges} + \text{running cost} \\ &\quad + \text{voyage cost} + \text{RTPA} \end{aligned} \tag{4}$$

$$\text{capital charges} = 0.2 \times \text{ship cost} \tag{5}$$

$$\begin{aligned} \text{ship cost} &= 1.3 \times (\text{steel mass})^{0.85} \\ &\quad + 3500 \times \text{outfit mass} + 2400 \times P^{0.8} \end{aligned} \tag{6}$$

$$\text{steel mass} = 0.034 \times L^{1.7} \times B^{0.7} \times D^{0.4} \times C_B^{0.5} \tag{7}$$

$$\text{outfit mass} = L^{0.8} \times B^{0.6} \times D^{0.3} \times C_B^{0.1} \tag{8}$$

$$\text{machinery mass} = 0.17 \times P^{0.9} \tag{9}$$

$$P = \Delta^{2/3} \times V^3 \times \frac{1}{b(C_B) \times \frac{V}{(g \times L)^{0.5}} + a(C_B)} \tag{10}$$

$$\Delta = 1.025 \times L \times B \times T \times C_B \tag{11}$$

$$\text{running cost} = 40000 \times DW^{0.3} \tag{12}$$

$$DW = \Delta - \text{light ship mass} \tag{13}$$

$$\tag{14}$$

$$\begin{aligned}
\text{voyage cost} &= \text{fuel cost} + \text{port cost} & (15) \\
\text{fuel cost} &= 1.05 \times \text{daily consumption} \times \text{sea days} \times \text{fuel price} & (16) \\
\text{daily consumption} &= P \times 0.19 \times 0.024 + 0.2 & (17) \\
\text{sea days} &= \frac{\text{round trip miles}}{24 \times V} & (18) \\
\text{round trip miles} &= 5000 \text{ (nautical miles)} & (19) \\
\text{fuel price} &= 100 \text{ (pounds/ton)} & (20) \\
\text{port cost} &= 6.3 \times DW^{0.8} & (21) \\
RTPA &= \frac{350}{\text{sea days} + \text{port days}} & (22) \\
\text{port days} &= 2 \times \left( \frac{\text{cargo deadweight}}{\text{cargo handling rate}} + 0.5 \right) & (23) \\
\text{cargo deadweight} &= DW - \text{fuel carried} - \text{crew, stores, and water} & (24) \\
\text{fuel carried} &= \text{daily consumption} \times (\text{sea days} + 5) & (25) \\
\text{crew, stores, and water} &= 2.0 \times DW^{0.5} & (26) \\
\text{cargo handling rate} &= 8000 \text{ (tons/day)} & (27)
\end{aligned}$$

where  $RTPA$  is round trips per annum,  $DW$  is deadweight, and  $g$  is the gravitational constant ( $g = 9.8065 \text{ m/s}^2$ ). The functions  $a(C_B)$  and  $b(C_B)$  are regression equations based on Froude Number and a coefficient referred to as the *Admiralty Coefficient*, detailed in the original paper. Functions  $a(C_B)$  and  $b(C_B)$  are defined as follows:

$$a(C_b) = \eta_1 \times C_B^2 + \eta_2 \times C_B + \eta_3 \quad (28)$$

$$b(C_b) = \zeta_1 \times C_B^2 + \zeta_2 \times C_B + \zeta_3 \quad (29)$$

$$\eta = [4977.06, -8105.61, 4456.51] \quad (30)$$

$$\zeta = [-10847.2, 12817, -6960.32] \quad (31)$$

## Objectives

The model defines three objectives:

$$\text{transportation cost} = \frac{\text{annual cost}}{\text{annual cargo}} \quad (32)$$

$$\text{light ship mass} = \text{steel mass} + \text{outfit mass} + \text{machinery mass} \quad (33)$$

$$\text{annual cargo} = \text{cargo deadweight} \times RTPA \quad (34)$$

$$\Omega_1 = \min(\text{transportation cost}) \quad (35)$$

$$\Omega_2 = \min(\text{light ship mass}) \quad (36)$$

$$\Omega_3 = \max(\text{annual cargo}) \quad (37)$$

## Constraints

The model defines dimensional and displacement constraints:

$$L/B \geq 6 \quad (38)$$

$$L/D \leq 15 \quad (39)$$

$$L/T \leq 19 \quad (40)$$

$$T \leq 0.45 \times DW^{0.31} \quad (41)$$

$$T \leq 0.7 \times D + 0.7 \quad (42)$$

$$DW \geq 3000 \quad (43)$$

$$DW \leq 500000 \quad (44)$$

Powering constraints:

$$C_B \geq 0.63 \quad (45)$$

$$C_B \leq 0.75 \quad (46)$$

$$V \geq 14 \quad (47)$$

$$V \leq 18 \quad (48)$$

$$\frac{V}{(g \times L)^{0.5}} \leq 0.32 \quad (49)$$

Stability constraint:

$$GM \geq 0.07 \times B \quad (50)$$

where

$$GM = KB + BM - KG \quad (51)$$

$$KB = 0.53 \times T \quad (52)$$

$$BM = \frac{(0.085 \times C_B - 0.002) \times B^2}{T \times C_B} \quad (53)$$

$$KG = 1.0 + 0.52 \times D \quad (54)$$

## CASE STUDY DATA

The following sections detail the data collected and used for the case study presented in this manuscript. Included in the table below are the selected limits that were used with the Sen and Yang Bulk Carrier problem for this study.

**Table 1: Lower and Upper Bounds Defined for Case Study**

Design Variable	Lower Bound	Upper Bound
Length (m)	195	500
Draft (m)	10	27
Depth (m)	13	46
Block Coefficient	0.63	0.75
Beam (m)	24	80
Speed (kts)	14	18



In the case study presented in this manuscript, the states of the tensor network were determined to be a change in the dimension of a meter, a change in speed of a meter per second, and a change in the block coefficient of one hundredth. Some cases were run for the case study where each of the design variables was given 100 different possible states over the range of the lower and upper bound.

In this work, point-wise mutual information was utilized in the creation of the tensor networks for the case study presented. The point-wise mutual information takes the form as shown below.

$$PMI(a, b) = \log\left(\frac{P(a, b)}{P(a) * P(b)}\right) \quad (55)$$

The point-wise mutual information represents comparing the joint probability of  $P(a, b)$  occurring to the marginals of  $P(a)$  and  $P(b)$ . In this case study, the point-wise mutual information was used as a surrogate for the energy needed in tensor building and contracting the tensor networks. For the investigated case, the objective function was defined following the formulation below.

$$\mathcal{O}(\alpha) = e^{PMI(\alpha) \times Cost(\alpha)} \quad (56)$$

$$Cost(\alpha) = e^{-\frac{Displacement(\alpha)}{1,000,000}} \quad (57)$$

$$Displacement(\alpha) = L(\alpha) \times B(\alpha) \times T(\alpha) \times C_b(\alpha) \quad (58)$$

In the above equations,  $\alpha$  represents a given state configuration. The displacement is averaged based on the data points in each respective state configuration. The state configurations are determined by the number of states for each node. In this case, the states are as defined earlier in this section.

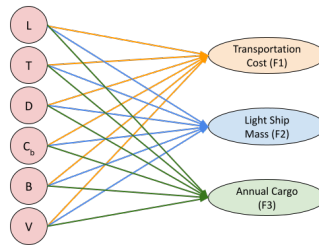
Two methods for developing data for this case study were used. The first approach used was to output the iterations of a multi-objective optimization of the Sen and Yang bulk carrier. The optimization was formulated using the equations detailed in this manuscript and using MATLAB's built-in fminimax optimizer. The algorithm for the optimizer is gradient-based. The data from the optimizer is comprised of multiple runs from multiple initial starting conditions, some including those mentioned in the original formulation. The other data set developed for this case study was a Monte Carlo simulation of the Sen and Yang Bulk Carrier Optimization. The Monte Carlo simulation was run with the upper and lower bounds detailed in this manuscript. These were also used as the upper and lower bounds for the optimization. The Monte Carlo simulation was run for 1,000,000 iterations. The data sets are comprised of the values of the inputs, output, constraints, and every intermediate function value for each iteration of the optimization or the Monte Carlo. In both data sets only the feasible solutions were considered for this initial case study. It was noted from looking at the results including the in-feasible solutions that the trends seen did not largely vary from those seen in the feasible solutions.

## DEVELOPED CASE STUDY NETWORKS FOR INVESTIGATING RELATIONS

To investigate a priori the encoded and non-encoded relations and inter-dependencies that exist within the Sen and Yang Bulk carrier design tool multiple tensor networks were formulated. The formulation used for the case study presented in this manuscript is similar to some of the work done by Klishin et al (2019). In this case study, each variable or node in the tensor networks presented later in this manuscript represents a rank one tensor acting as a possible state vector. The tensor networks formulated were developed to be able to easily place external legs and anchors on important variables within the tool. Based on the input tensor network to the framework, the data was populated for the network to enable necessary calculations and queries. The following sections delve into the four networks developed and their states.

## Input to Output Network

The first of the four networks developed sought to investigate one of the most fundamental relations that exist, the relation of the input variable to the output final objective values. In the developed bipartite network, the input variables are on the left and each is connected to each of the relevant output objectives that they impact. In this case, each input is connected to each of the outputs. This can be seen in the developed network below.

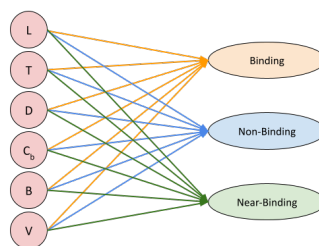


**Figure 1:** Developed Tensor Network for Investigating Input Output Relations

In the developed network above, the states for each of the nodes were defined as a change in the value of the input variable or the output objective.

## Input to Constraint Status Network

The second network developed sought to begin to capture some of the more hidden relations in the tool. The bipartite network consists of the input variables on the left and three nodes on the right indicating a constraint status of non-binding, near binding, or binding. In this case, the values of each constraint in the data were pre-processed to determine the associated node to which each belonged. In this case study near binding was defined to be a value of  $\epsilon$  away from the binding value. Each constraint was re-arranged so that when the constraint was bound or violated the value would become zero or greater than zero. For the presented data,  $\epsilon$  was determined using best judgment as an engineer. In this case,  $\epsilon$  was defined to be 0.5 for when a constraint was near binding.

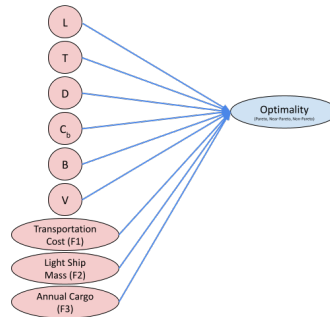


**Figure 2:** Developed Tensor Network for Investigating Constraint Status (Non-Binding, Near Binding, Binding)

In the developed network above, the states for each of the input nodes were defined as a change in the value of the input variable. For the status nodes of non-binding, near binding, or binding, the states were determined to be the number of constraints falling under non-binding, near binding, or binding for each data point.

## Input to Solution Status Network

The third network developed again sought to capture some of the relations that are not typically apparent in a tool. The bipartite network consists of the input variables and the output objectives on the left and one node on the right for the solution status.

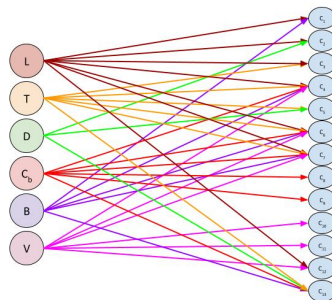


**Figure 3:** Developed Tensor Network for Investigating Solution Status (Non-Pareto, Near Pareto, Pareto)

In the developed network above, the states for each of the input and output objective nodes were defined as a change in the value of the variable. For the solution status node, only three possible states were defined, non-Pareto, near Pareto, or Pareto referring to the optimality of the solution. In this case, the values of output objectives in the data were pre-processed to determine if a solution was non-Pareto, near Pareto, or Pareto. In this case study, near Pareto was defined to be a value of  $\epsilon$  away from the Pareto front. For the presented data,  $\epsilon$  was determined using best judgment as an engineer.

## Input to Constraint Network

The final network developed sought to capture some of the relations in terms of constraint activation that are not typically apparent in a tool. The bipartite network consists of the input variable nodes on the left and constraint nodes on the right. Each of the input nodes is connected to each of the relevant constraints that they impact.



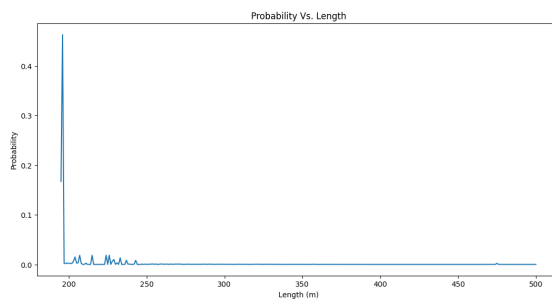
**Figure 4:** Developed Tensor Network for Investigating Constraint Activation over the Solution Space

In the developed network above, the states for each of the input nodes were defined as a change in the value of the variable. For the constraint nodes, each of the nodes had the possible states of non-binding, near binding, or binding. In this case, the values of each constraint in the data were pre-processed to determine the associated state for each of the constraint nodes. As stated above, near binding was defined to be a value of  $\epsilon$  away from the binding value. For the presented data,  $\epsilon$  was determined using best judgment as an engineer.

# RESULTS

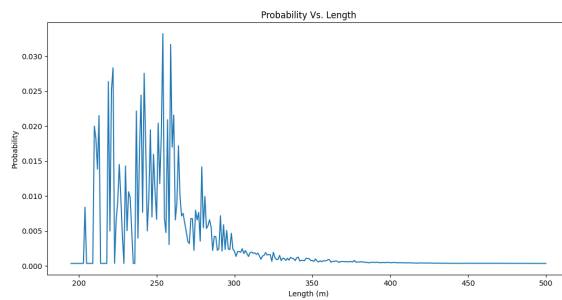
The following section details the results from performing queries in the developed networks with different external legs. Numerous more contractions were performed, not detailed in this manuscript, to further validate the findings. The contraction results presented in this manuscript are intended to provide insight into the tool and to demonstrate the capabilities of tensor networks in relation to optimization.

One of the first sets of contractions performed was done to help begin to understand the results of a tensor network contraction and to be able to easily check the result against one's instincts as a naval architect. The contraction was done on the input to output relation network and an external leg was placed on length. In evaluating the contraction, the tensor network objective was defined to maximize or minimize displacement. As a naval architect, with a simple ship like a bulk carrier, one would expect if one minimizes displacement, they would get a very short ship close to the minimum, and if one maximizes displacement, they would get a long ship close to the maximum. Included below are the contraction results for the queries. In this case, a higher probability indicates a higher likelihood of a ship with that given length.



**Figure 5:** Input Output Tensor Network Contraction Result from Gradient-Based Optimization Data with Objective of Minimizing Displacement with External Leg on Length

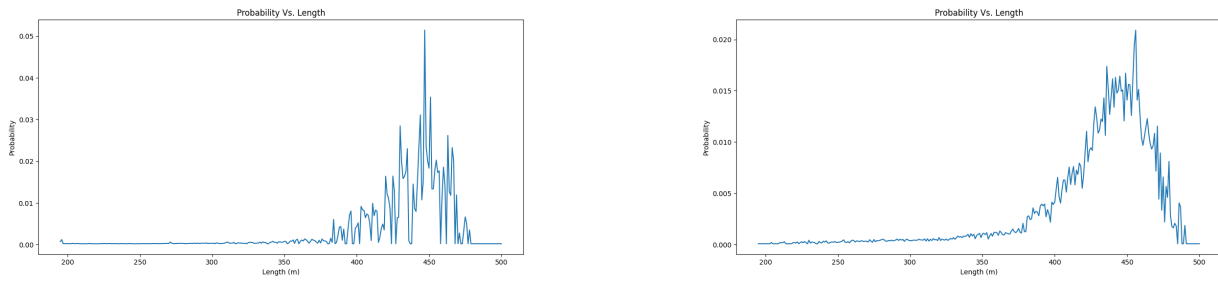
As expected, the results from performing the contraction indicate that the smallest ship is the most probable. The contraction from the Monte Carlo data set shows some interesting dynamics. The reason for the lack of a single line as in the above figure is due to the Monte Carlo data set having a more limited number of feasible solutions in the shorter length range. However, it can be noted that the trends and behavior between the data are the same and that the Monte Carlo data has a higher level of fidelity due to the increased number and range of coverage of the points. This behavior can be seen in the figure below.



**Figure 6:** Input Output Tensor Network Contraction Result from Monte Carlo Data with Objective of Minimizing Displacement with External Leg on Length

Further, one can investigate the results of maximizing the displacement instead of minimizing it. Included below again are

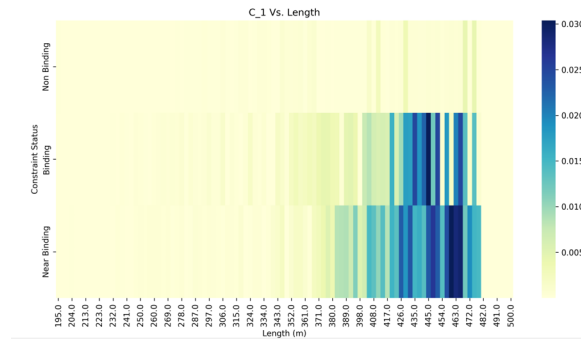
figures of the same contraction from the optimization data set and the Monte Carlo data set.



**Figure 7:** Input Output Tensor Network Contraction Result from Gradient-Based Optimization Data with Objective of Maximizing Displacement with External Leg on Length (Left) and Input Output Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Leg on Length (Right)

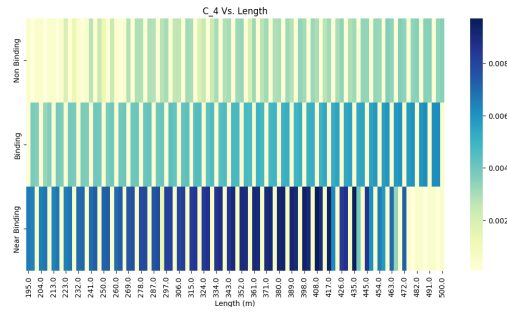
One can see from these contractions that the trends and behavior between the data are the same and that the Monte Carlo data has a higher level of fidelity. Additionally, one interesting behavior can be noted. As a naval architect, one would expect if one maximizes displacement they would get a long ship close to the maximum length. However, this is not the case in either of the contractions. In both, the most probable lies approximately 50 meters shorter than the maximum length. This result does not logically make sense. To investigate the reasoning for this, several other contractions using the other developed tensor networks were performed.

The next set of contractions performed to investigate the findings from maximizing the displacement was looking at the constraint activation across the solution space. One would naturally think that based on the behavior seen above one of the constraints is probably binding. Included below is a sample contraction of the constraint activation network with multiple external legs. The contraction shows the relation of the constraint state of non-binding, near binding, or binding to the entire state space. In the following contractions, the color bar on the right of the plot indicates the probability value for the contraction. In this case, the displacement was maximized and again similar behavior to the previous set of contractions can be seen. The constraint referred to in the contraction is the length-to-beam constraint detailed in Eq. 38.



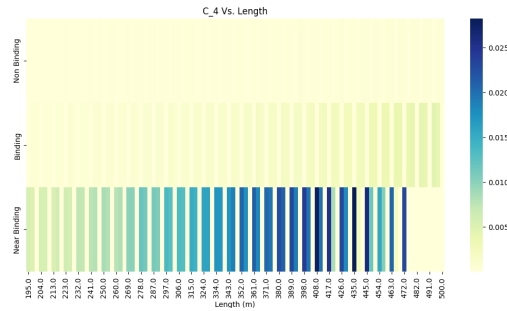
**Figure 8:** Constraint Activation Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Legs on Constraint 1 and Length

From the figure above, it can be noted that over the majority of the state space, the constraint is non or near binding but not binding. While the above figure supports the conclusions, it does not provide insight into the behavior of solutions when maximizing displacement. To provide insight, more contractions were performed. Some interesting results were found from the draft constraints over the solution space. The following contractions are of the same contraction of the constraint activation network just with different external legs. The constraint referred to in the contraction is the draft constraint detailed in Eq. 41.



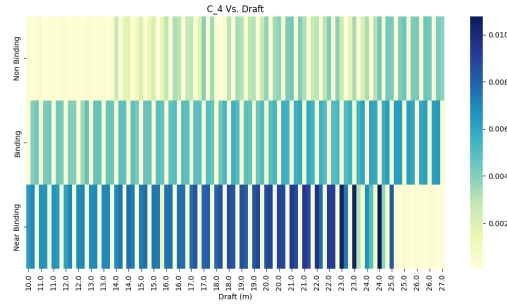
**Figure 9:** Constraint Activation Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Legs on Constraint 4 and Length with  $\lambda = 1$

In the above contraction, one can notice the behavior of interest. In the contraction's result, it looks like a barcode for each of the states of the constraints. To investigate the meaning of the result, the value of  $\lambda$  was increased to see if the critical temperature had an impact. The figure below demonstrates the results.



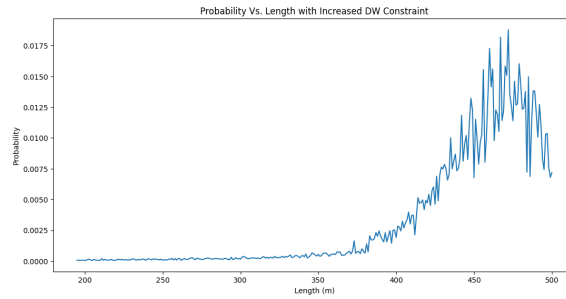
**Figure 10:** Constraint Activation Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Legs on Constraint 4 and Length with  $\lambda = 3$

From the figure above it can be seen that the lower probability values become more muted and the same behavior of the near binding and binding states can be observed. Largely, a higher value of  $\lambda$  suggests that the behavior of a system is more known. In terms of the probability distribution seen, the higher  $\lambda$  highlights the underlying or grounding behavior of the contraction. In addition to performing the contraction with an external leg on length, the same contraction was performed with an external leg on draft.



**Figure 11:** Constraint Activation Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Legs on Constraint 4 and Draft with  $\lambda = 1$

The results from the contraction in the figure above can largely be seen showing the same behavior as that from the contraction of the same constraint but in relation to the length. Upon further investigation, one can notice that at each small range of states for the length and the draft, the constraint is going from non-binding to near binding and then to binding. This is the reason for not being able to achieve large vessels with the tool. What is happening is that as the design tool tries to increase the size of the vessel, the deadweight increases and causes the draft constraint to bind. This in turn forces smaller vessels and is exaggerated at that upper limit. It can also be noted that a second draft constraint also exists in the code seen in Eq. 42. However, this constraint is not dominant and does not impact the solutions in the same way as in Eq. 41. The origins of this constraint are largely unknown and it is assumed that it is most likely from older regression data of bulk carriers when the code was developed. In the Sen and Yang bulk carrier tool, deadweight is known to be the main driving variable, and as a result, directly impacts the allowable size of the vessel through the draft constraint. To check this, the deadweight limit was increased to see if the solution space changed. To see the change, a Monte Carlo data set was created for the increased deadweight limit. A contraction was then performed on the input to output relation network and an external leg was placed on length. The following figure can directly be compared to Fig. 7.

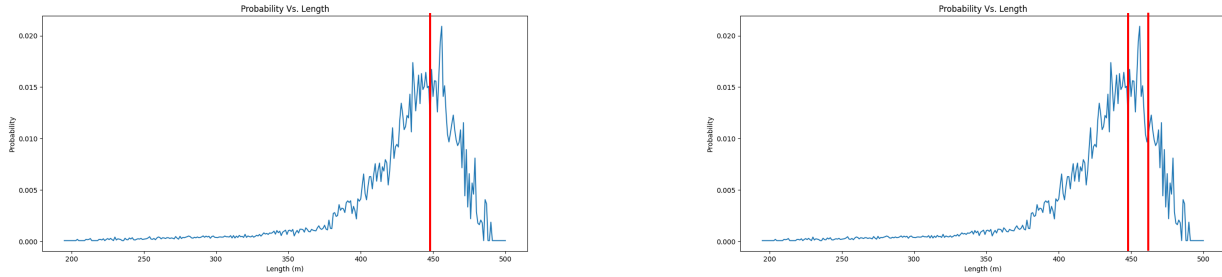


**Figure 12:** Input Output Tensor Network Contraction Result from Monte Carlo Data with Objective of Maximizing Displacement with External Leg on Length with Deadweight Constraint Upper Limit Increased to 800,000

From performing the contraction above and increasing the deadweight constraint upper limit to 800,000 tons, it can be seen that the peak shifted to the right. The peak value sits around 473 m in length which is a large increase from that of the contraction with the deadweight constraint upper limit set to 500,000 tons. This shows that it is a combination of the deadweight and the draft constraint that is limiting the size of the vessel. In other words, the model is ontologically committed to deadweight and the draft constraint in Eq. 41. Without tensor networks, discovering this behavior and the reasoning would be extremely difficult and time-consuming, whereas with tensor networks, performing the contractions only takes seconds.

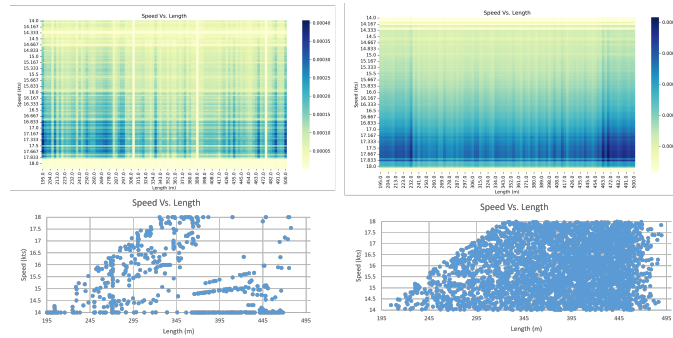
# DISCUSSION

The following section provides a discussion of the results presented above. To verify the results in Fig. 7 the Sen and Yang bulk carrier model was run as a single objective optimization with each of the three objectives in the formulation presented in this manuscript having equal weighting. The optimization was run five times using multiple different optimization algorithms in MATLAB. The results are included in the figure below. The red lines indicate the solution from the optimizer plotted in Fig. 7 or in the case of the genetic algorithm the range of optimal solutions found.



**Figure 13:** Feasible Length from Running fmincon Equal Weighting Single Objective Sen and Yang Bulk Carrier Optimization (Left) and Feasible Length Range from Running GA Equal Weighting Single Objective Sen and Yang Bulk Carrier Optimization (Right)

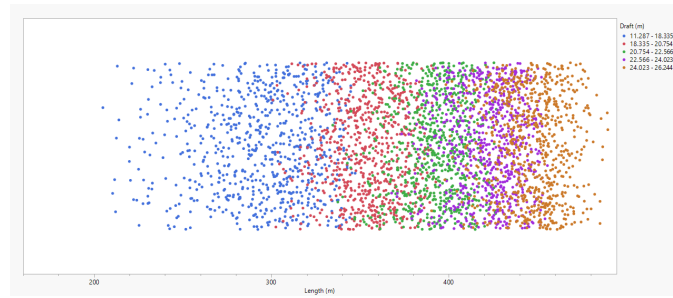
In both of the cases presented above, the single objective optimization with the objective of maximizing displacement provided solutions close to that found from the tensor network contractions. These results from running the tool as a single objective optimization support the findings in the result section and validate the peak value found. In the results presented in the section above most of the contractions were performed on the data set from the Monte Carlo simulation instead of the optimization data. It was found that both data sets had the same behavior and that the Monte Carlo just provided higher fidelity. The figure below shows this between the two data sets.



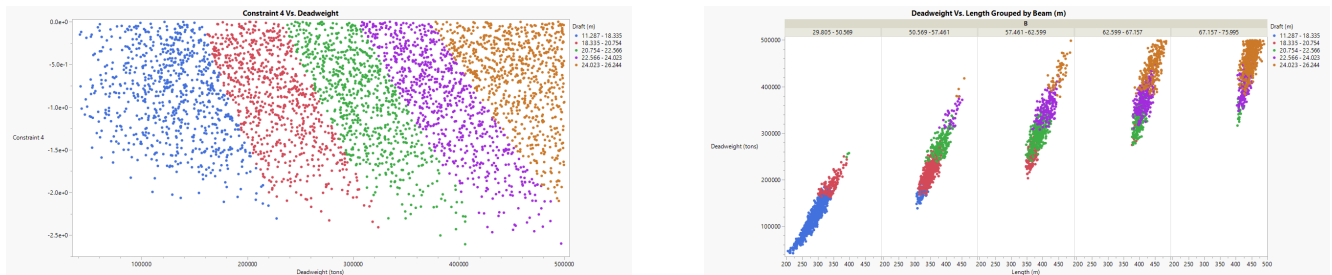
**Figure 14:** Comparison of Tensor Network Contraction Result and Data from Monte Carlo and Gradient-Based Optimization Data with Objective of Maximizing Displacement with External Legs on Length and Speed

From the figure above it is clear that the Monte Carlo data set provides a better picture of the solution space. Many of the gaps seen in the optimization data are filled from the Monte Carlo data. Another interesting point to note is that when looking at the data plotted on its own, the trends seen in the data support the conclusions derived from the tensor network contractions.





**Figure 15:** Population of Feasible Solutions Plotted Over Length Solutions Overlaid by Draft



**Figure 16:** Draft Constraint Eq. 41 Versus Deadweight Overlaid by Draft (Left) and Deadweight Versus Length Grouped by Beam Overlaid by Draft (Right)

From the three figures included above, very distinct populations of solutions can be seen in relation to the length, draft, and deadweight. This suggests constraint or function is heavily impacting feasible solutions. This result can especially be seen in Fig. 16 where there is almost no mixing of different draft populations. One would largely expect there to be mixing in the solutions. These plots support the conclusions found from the contractions presented in the results section of this manuscript.

Through the results found and detailed from the presented case study some interesting insights can be made when looking at the case study from an ontological lens. From the presented results, one can directly see that the optimization model for the bulk carriers is highly committed to deadweight and the identified draft constraint. What this means is that the solutions of the model are predicated on these commitments. This was directly shown by how the set of solutions changed when the deadweight was increased. In the case of the draft constraint discussed earlier in this manuscript, there is an explicit commitment to the constraint from its inclusion in the model, but there is also an implicit commitment to the unknown origin or meaning of the constraint. These simple commitments to the deadweight and the discussed draft constraint significantly impact the optimization and the results that are possible to be obtained from the optimization. The insights from this analysis are more than what one could get from a Design of Experiments analysis and it is much more efficient in terms of finding the information necessary to be able to make similar conclusions.

## CONCLUSIONS

In conclusion, the application of tensor networks to the Sen and Yang bulk carrier model has shed light on the intricate relationships between design variables, operational constraints, and performance objectives that are often challenging for traditional optimization methods to capture. The results from the case study highlight the unique capabilities of tensor networks, rooted in quantum physics, to effectively model state relationships within multidimensional data structures.

The analysis of the bulk carrier synthesis and optimization through tensor networks has allowed for the simultaneous examination of multiple constraints and their interactions using the state space representation. This holistic approach has proven invaluable in unraveling hidden relations within the Sen and Yang model, particularly when attempting to maximize displacement while navigating the complex behavior of the draft constraint.

The presented methodology, which involves converting the optimization problem into multiple tensor network representations and implementing tensor network algorithms, demonstrates the practical efficacy of this approach. The implementation results not only showcase the capacity of tensor networks to provide a deep, data-driven understanding of complex optimization landscapes but also emphasize their potential to uncover novel decision-making opportunities.

As one reflects on the outcomes of this study, it becomes evident that tensor networks offer a promising avenue for addressing the challenges posed by intricate and interconnected optimization parameters in the maritime industry. By providing insights that complement traditional optimization analysis techniques, tensor networks contribute to a richer understanding of optimization landscapes. The findings presented in this paper serve as a catalyst for further exploration of tensor network methodologies in tackling complex optimization challenges across diverse domains. Ultimately, this research opens new horizons for innovative decision-making support processes and underscores the transformative potential of tensor networks in the realm of optimization. There are many opportunities for future work in creating general, easily applicable frameworks for diverse optimizations and engineering design tools.

## **DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN WRITING**

*Statement:* During the preparation of this work the author(s) used ChatGPT 3.5 to help improve language and readability. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

## **CONTRIBUTION STATEMENT**

**CWA:** Conceptualization; data curation, methodology; software; writing – original draft. **ADM:** conceptualization; software; writing – review and editing **MDC:** conceptualization; supervision; writing – review and editing **DJS:** supervision; writing – review and editing.

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