Studying Lagrangian theories with machine learning: a toy model

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The central element of any physical theory, namely the Lagrangian density, is studied with the aid of Machine Learning, by developing a map from the Lagrangian space to \(n\)-dimensional real space. The representation of the Lagrangian as a feature vector allows to construct and train a fully-connected, multi-layer, feed-forward neural network, towards discriminating between “healthy” and “non-healthy” Lagrangians, namely Lagrangians that lead to second-order equations of motion and those which do not, without explicitly performing the extraction of equations of motion. By suitably labeling the training data-sets, one can employ further criteria, resulting to a trained network that could decide for more complex cases. Exploring various possible correspondences between an arbitrary Lagrangian to a \(n\)-vector, in an effort for a general description is deemed very fruitful. Apart from practical applications, the aforementioned direction could also lead to new results regarding data pre-processing techniques.

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I. INTRODUCTION

After a century of theoretical research in the construction of physical theories, we know that the action, and thus the corresponding Lagrangian density, is the cornerstone quantity, since it gives rise to the equations of motion by employing the least-action principle. During the last century rapid progress in the direction of a unified description of electromagnetic, weak and strong nuclear forces within the standard model of particle physics Lagrangian is established. However, the inclusion of gravity in this picture is notoriously difficult, resulting to a number of different approaches (see [1, 2] for a review and [3] for a wider perspective of the problem). One interesting approach is to study higher-order corrections to the Einstein-Hilbert action of general relativity, which result to a renormalizable and thus quantizable gravitational theory, [4]. A serious drawback in this approach is that the existence of higher derivatives in the Lagrangian is known to cause problems, such as the existence of unphysical states, the so-called ghosts. Thus, one is indeed interested in Lagrangians that possess terms with higher-derivatives, but which are ghost-free and have equations of motion that are of second order, which are generally called “healthy” Lagrangians. Searching for healthy Lagrangians is usually done by hand, or at most by using a computer algebra system and is a tedious procedure.

The ubiquity of massive data volumes, coupled with scalable training techniques, novel learning algorithms and immense computational power, has been an important factor for the practical success of (deep) machine learning (ML). From a predictive accuracy standpoint, deep learning algorithms are nowadays considered the state of the art in numerous applications, while deep learning’s success has been the primary reason for a fresh look at the transformative potential of artificial intelligence (AI) as a whole during the past decade. This success has also made a long-standing dream, that of automated, data-driven scientific discovery, seem within reach. From early approaches in biology and the life sciences, [5], to more recent ones in a wide range of scientific fields [6], AI-assisted scientific discovery is pursued towards understanding experimental findings, inferring causal relationships from observational data, or even acquiring novel scientific insights and building new explanatory theories. At the same time, however, and despite recent successes and optimism, a transparency barrier is imposing severe limitations on the applicability of the AI potential in scientific discovery. It is now widely acknowledged that the inability to understand, explain and trace back to a cause the predictions/inferences of black-box machine learning models is responsible for their

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lack of accountability and for end user’s lack of trust in such models in mission-critical applications and high-stakes decisions. In fields where understanding, as opposed to merely predicting, is the basic requirement, such as that of scientific discovery and automated explanatory theory building, the opaqueness of state-of-the-art machine learning is a serious handicap.

On the other hand, a consensus is emerging within the machine learning community for the existence of a trade-off between interpretability and predictive performance, especially in problems featuring highly unstructured data sources, as is often the case in natural sciences. In such cases, the inner workings of simpler machine learning models are transparent at the cost of lower performance, while highly complex models are more accurate, at the cost of interpretability. Explainable AI, [7], attempts to shed light into the complexities of state-of-the-art machine-generated models without compromising their performance. It is attracting significant attention and numerous approaches have already been proposed, involving e.g. the use of focus mechanisms in deep neural networks to highlight regions of the network involved in certain inferences and potentially identify relevant features, [8], or by identifying such features via studying the effects of input perturbations to the output. Other approaches rely on dissecting the object (e.g. an image) to be classified into a set of prototypical parts and then combining evidence from such prototypes to explain the final classification, [9]. The idea behind this paper is to automate the search for a healthy Lagrangian possessing higher-derivatives using Machine Learning (ML).

In this paper, we are interested in studying how efficient an artificial neural network can be in classifying a given Lagrangian to “healthy” and “non-healthy”, after training, without extracting the equations of motion. The manuscript is organized as follows. In Section II we provide a concise presentation of the Lagrangian formalism and we also present our algorithms for creating Lagrangians. In Section III we describe in detail the ML algorithms and architectures we employ, while in Section IV we present and discuss our results. Finally, in Section V we draw our conclusions and we point out directions for further work.

II. DESCRIPTION OF PHYSICAL THEORIES

A framework that allows systematical study of a physical theory is the Lagrangian formalism. The latter comes from classical physics and it was first formulated from Joseph-Louis Lagrange in late 18th century. Along with its generalizations to include various fields and curved space-time is the cornerstone of modern physics. Let us begin our discussion within the context of classical mechanics. Given the action functional

$$S[q, t_1, t_2] = \int_{q(t_1)}^{q(t_2)} L(q, \dot{q}, ..., q^{(n)}) dt,$$

where $t_1, t_2$ are two time instances and $q$ is the fundamental quantity that describes our physical system and specifically the position over time of the particle under study. The corresponding equations of motion arise by applying the Hamilton’s principle, namely the evolution of the physical system is such that the action is stationary, (for a thorough presentation of classical mechanics, see [10]). In other words, the trajectory that the particle will follow between $q(t_1)$ and $q(t_2)$ is such that the action functional derivative is zero, i.e. $\delta S = 0$. This requirement produces the equation of motion as [10]

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) + ... + (-1)^n \frac{d^n}{dt^n} \left( \frac{\partial L}{\partial q^{(n)}} \right) = 0.$$

In the latter we omitted the arguments of the Lagrangian for brevity. The Lagrangian to obtain the Newtonian mechanics is $L = T - V(q)$, where $T$ is the kinetic energy of the system, i.e. $T = 1/2 m \dot{q}^2$. Since the late 18th century were this formalism was first proposed, it has been generalized to include classical and quantum fields, as well as to handle in a unified way time and positions in the context of Einstein’s theory of gravity [11, 12]. Today the procedure of constructing a new physical theory is essentially the process of constructing new Lagrangians containing the desired physical properties.

A. Ostrogradsky’s instability

As a starting point in constructing a Lagrangian, one can consider any function of positions and velocities that is smooth enough. In this procedure there exists a number of theoretical requirements, such as the verification of specific symmetries. However, as Ostrogradsky showed first [13], there exists an additional powerful constraint that does not allow Lagrangians with higher order time-derivatives. This requirement arises from the fact that in such case the corresponding Hamiltonian is not bounded, which implies that the total energy of the system is unbounded.
In order to avoid this Ostrogradsky instability the equations of motion of a physical system need to have up to second order equation of motion. A sufficient condition for that is if the Lagrangian has terms up to first order in derivatives, nevertheless this is not necessary since as Horndeski showed \cite{14} one may have higher-order terms in a Lagrangian in a suitable combination that the resulting higher-order time derivatives in the equations of motion cancel out, resulting to second-order ones. Hence, this implies that discriminating if a given Lagrangian is healthy or not, requires the extraction of the equations of motion and their subsequent elaboration, a procedure that in case of complicated Lagrangians is not trivial. That is why it becomes of great interest the construction of a machine learning procedure that could discriminate if a given Lagrangian is healthy or not without the need to perform the variation and the extraction of equation of motion.

B. Describing a Lagrangian

A Lagrangian could in principle contain scalar quantities that are functions of higher dimensional objects for instance the electromagnetic Lagrangian contains the tensor $F_{\mu\nu}$, while the Einstein-Hilbert Lagrangian of general relativity posses contractions of the Riemann tensor. In order to give a Lagrangian as input to a neural network it is necessary to translate it in a form that the network can handle, i.e. to describe it as a set of features. Formally, a function $\phi : \mathcal{L} \to \mathbb{R}^n$ is to be found in order to provide the feature vectors, where $\mathcal{L}$ is the Lagrangian’s space.

We limit ourselves to classical mechanics, in a sense that the fundamental quantity involved in the Lagrangian is the position of a moving body, $\chi(t)$ as a function of time. Position along with its time derivatives constitute the set of physically interesting entities. Within our modelling, all physical parameters such as mass are set to unity. Moreover, the parameters are measured in proper units, so to maintain the standard physical interpretation of potential energy. Some simple representations are provided in the following.

- A first approach is to use the standard kinetic term, $K = 1/2 \, m \dot{\chi}(t)^2$, and a more general potential. The potential is considered to be

$$V_{01}(\chi(t), \dot{\chi}(t), \ddot{\chi}(t)) = \alpha_4 \chi(t)^{\alpha_4} \dot{\chi}(t)^{\alpha_4},$$

and the corresponding set of numbers to describe this Lagrangian is $\mathbf{f} = [\alpha_0, ..., \alpha_7]$. Using the standard expression for the kinetic energy implies that $[\alpha_0, \alpha_1, \alpha_2, \alpha_3] = [0.5, 0.0, 2.0, 0.0]$. By using eq. (2) it is easy to observe that the essential requirement for a Lagrangian of the form (3) to be free of the Ostrogradski instability is to have $\alpha_4 = 0$ or $\alpha_4 = 1$. The aforementioned representation could generalized by considering more potentials of the form of (3).

$$V_{02}(\chi(t), \dot{\chi}(t), \ddot{\chi}(t)) = \sum_{i=1}^{n} \alpha_{i0} \chi(t)^{\alpha_{i1}} \dot{\chi}(t)^{\alpha_{i2}} \ddot{\chi}(t)^{\alpha_{i3}},$$

and the corresponding feature vector to describe this Lagrangian is $\mathbf{f} = [0.5, 0.0, 2.0, 0.0, ..., \alpha_{n0}, \alpha_{n1}, \alpha_{n2}, \alpha_{n3}]$, with dimension $4n$.

- Another approach is to further assume that every potential that describes a certain class of phenomena will be $C^2$ at least within a certain subspace. From the latter, the corresponding Taylor series always exists, thus an adequate description of a general potential energy is its Taylor coefficients around the point $(\chi_0, \dot{\chi}_0, \ddot{\chi}_0)$. The most general Taylor expansion reads

$$V_0(\chi, \dot{\chi}, \ddot{\chi}) = \sum_{j=0}^{\infty} \left\{ \frac{1}{j!} \left( \chi - \chi_0 \frac{\partial}{\partial \chi} + (\dot{\chi} - \dot{\chi}_0) \frac{\partial}{\partial \dot{\chi}} + (\ddot{\chi} - \ddot{\chi}_0) \frac{\partial}{\partial \ddot{\chi}} \right)^j \right\} V(\chi', \dot{\chi}', \ddot{\chi}') \bigg|_{(\chi' = \chi_0, \dot{\chi}' = \dot{\chi}_0, \ddot{\chi}' = \ddot{\chi}_0)}.$$

By keeping terms up to 2nd order and re-arranging we obtain the following

$$V_{b1}(\chi, \dot{\chi}, \ddot{\chi}) = a_0 + a_1 \chi + a_2 \dot{\chi} + a_3 \ddot{\chi} + a_4 \chi^2 + a_5 \chi^2 + a_6 \chi^2 + a_7 \chi \dot{\chi} + a_8 \chi \ddot{\chi} + a_9 \chi \dddot{\chi},$$

where $a_i$ are real numbers and the corresponding feature vector is $\mathbf{f} = [0.5, 0.0, 2.0, 0.0, \alpha_{0}, ..., \alpha_{9}]$. Obviously, $a_0$ and $a_0$ do not play any role, while the governing parameter is $a_6$. By including terms up to the 3rd order, we obtain the potential $V_{b2}$ as

$$V_{b2}(\chi, \dot{\chi}, \ddot{\chi}) = a_0 + a_1 \chi + a_2 \dot{\chi} + a_3 \ddot{\chi} + a_4 \chi^2 + a_5 \chi^2 + a_6 \chi^2 + a_7 \chi \dot{\chi} + a_8 \chi \ddot{\chi} + a_9 \chi \dddot{\chi} + a_{10} \chi^3 + a_{11} \chi^3 + a_{12} \chi^3 + a_{13} \chi \ddot{\chi} + a_{14} \chi \dddot{\chi} + a_{15} \chi \ddddot{\chi} + a_{16} \chi^2 \chi + a_{17} \chi^2 \dddot{\chi}. \quad (7)$$
| No | $V$ | Parametrization(s) | Description |
|----|-----|-------------------|-------------|
| 1  | 0   | $a, b$            | free particle |
| 2  | $\frac{1}{2} k r^2$ | $a, b$ | mass connected with pendulum with constant $k$ |
| 3  | $G_{1/m} a^m$ | $a, b$ | mass within gravitational field |
| 4  | $4 \epsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6$ | $a_2, b$ | Lennard-Jones potential, [15] |
| 5  | $\epsilon \left( \frac{\sigma}{r} \right)^6$ | $a, b$ | soft-sphere potential, [15] |
| 6  | $m \cos(r)$ | $b$ | non-linear oscillator |
| 7  | $D \left( e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right)$ | $b$ | Morse potential, [15] |

TABLE I: Some classical potentials are presented along with their representation ability in order to assess the generality of the parametrizations employed.

We mention again the term with coefficient $\alpha_{17}$ is total derivative. In principle, a series expansion could be performed on different bases, i.e Legendre, Laguerre and Hermite polynomials.

In this work we will use only parametrization $V_a$, as we are interested to study the potential of training a neural network to discriminate between “healthy” and “non-healthy” theories.

There exist numerous descriptions with regard to certain classes of Lagrangians, although finding a description valid for an arbitrary Lagrangian is left for a future study. In Table I some classical Lagrangians are presented along with the proper map to construct the relevant feature vectors.

### III. MODEL AND ALGORITHMS

In order to classify a Lagrangian as healthy or not, we are using fully-connected feed-forward neural networks and supervised learning.

#### A. Neural Network setup

A neural network perform mappings from an input space to an output space. In our case the input space contains the feature vectors of the Lagrangians and the output space contains the two categories. The basic structural element of a neural network is the layer, that is a group of neurons. The neurons of each layer connect to those of the next and these connections are called synapses. The first layer of the network is called input layer, the last layer is called output layer and all the layers in between are called hidden layers. The architecture mentioned above describes a typical fully connected neural network as shown in Fig. 1. The term feed-forward implies a network that its synapses do not form a cycle, in contrast with e.g the recurrent neural networks, [16]. Formal definitions of the aforementioned terms regarding feed-forward neural networks could be found at [17].

In order to understand how the mapping is happening we need to break down the network to its components. The neurons of the first layer activate as we input a feature vector (corresponding to a Lagrangian). Activation means that a neuron calculate a value and “feeds” it to the next layer. As we mentioned above, in a fully-connected net, all the neurons of a layer are connected to all neurons of the previous one through synapses. Each synapse contains a real number called weight that indicates how much the activation of the previous layer specific neuron, affects the activation of the neuron in the next layer. Furthermore, each neuron contains a real value called bias, that indicates a threshold, over which a neuron will meaningfully pass its value over to the next layer (fire). The activation of a neuron is described as

$$
\alpha_j^l = \sigma \left( \sum_k w_{jk}^l \alpha_{k}^{l-1} + b_j^l \right),
$$

where $w_{jk}^l$ is the weight of the synapse that connects the $k^{th}$ neuron of the $(l-1)^{th}$ layer to the $j^{th}$ neuron in the $l^{th}$ layer. Moreover, $b_j^l$ is the bias of the $j^{th}$ neuron. The function $\sigma$ is the sigmoid function, $\sigma(x) = 1/(1+\exp(x))$.

When a neural network is created all its weights and biases values are random initialized. Therefore, in order for our network to be able to classify correctly a given Langragian, its values need to be adjusted. Specifically these values need to be adjusted in a way so that when a healthy Lagrangian is fed into the network, it will output a real number close to 1 and on the other hand in the case of the non-healthy Lagrangian, it will output a number close to 0.
FIG. 1: The structure of a fully - connected neural Network is presented. The input and output layers have n neurons, while there are k hidden layers, each one consisting of n neurons.

| Epoch | Accuracy | Precision(s) | Recall | $F_1$ | Log. Loss |
|-------|----------|--------------|--------|-------|-----------|
| 500   | 0.529    | 0.103        | 0.817  | 0.642 | 0.666     |
| 1000  | 0.521    | 0.117        | 0.980  | 0.680 | 0.629     |
| 1500  | 0.567    | 0.130        | 0.997  | 0.723 | 0.611     |
| 2500  | 0.588    | 0.136        | 0.999  | 0.740 | 0.599     |
| 3500  | 0.600    | 0.139        | 1.000  | 0.750 | 0.583     |
| 6000  | 0.617    | 0.145        | 1.000  | 0.763 | 0.537     |

TABLE II: Values of different metrics during epochs of training for the fully-connected, feed-forward neural network with architecture 8-16-16-1. Note that early epochs are affected by the initial random selection of weights.

In order to adjust those weights and biases we employed the backpropagation algorithm, described further later in the next subsection.

B. Training

In order to construct the training data set, a Monte Carlo approach is employed. The i-th iteration of the process consists of constructing a random vector of length n. Subsequently, by using a symbolic algebra system, that is *sympy*, [18], the Euler-Lagrange equations (2), are employed to extract the equations of motion. Further, the equations are checked for the existence of time derivatives of order higher than 2. If there are only second derivatives in the equations of motion, the random vector is labelled as “healthy”, else it is labelled “Non-Healthy”. The above procedure is repeated N times. Some characteristic subsets of the $a_i$ space are presented in Fig. 2.

The total training data set constitutes of 2000 “healthy” and 2000 “non-healthy” feature vectors. The training strategy of backpropagation,[17], consists of splitting the total dataset in batches with 400 elements each, i.e resulting 10 batches. When all the elements of a batch are fed into the network, the average cost is computed using the quadratic cost function. The average cost backpropagates through the network fixing its weights and biases. The same process needs to be done for each batch in order for an epoch of training to be completed. Before an epoch of training all the training set is scrambled, resulting in set of different batches. Different values of the learning rate, $\eta$, are employed in an effort to avoid local minima while also maintain steep learning curve. All the steps above describe the iterative process of gradient descend.
FIG. 2: Some 3d-subspaces of the parameter space for Lagrangians of the generic form $\mathcal{L} = T - \alpha_4 \chi^\alpha \chi^\beta \chi^\gamma$. The circular marker corresponds to "non-healthy" Lagrangians while the triangular one to "healthy".

C. Validation

After training the network, 10 data sets are produced, each of them consisting of 10000 feature vectors and they are given to the network for classification. In this point another hyper-parameter is introduced, namely the threshold, that determines how a number in the continuum set $[0, 1]$ is projected to the set $[0, 1] \cap \mathbb{N}$. Assessing the ability of the trained network to classify correctly data that has not encountered before is essential in order to avoid over-fitting. The latter term describes the situation in which the neural network performs very well in the training data and poorly in the testing data, (for a formal discussion of over-fitting within a statistical context see [19]). Towards this purpose, a number of metrics is utilized. Accuracy measures the relative ability of a given network to provide correct predictions, that is

$$\text{Accuracy} = \frac{\text{True Positives} + \text{True Negatives}}{\text{Total Predictions}}. \quad (9)$$

It is straightforward to apply this metric, however there are some caveats. A characteristic example is that a model that classifies all input data as positive, applied to a dataset consisting of 95 positive and 5 negative samples, gives 0.95 accuracy score.

Precision is the metric that expresses the proportion of the actual positive data, over the data items that were classified by our model as positives:

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}. \quad (10)$$

Similarly, recall is the metric that expresses what proportion of the actual positive data, was classified correctly by our model:

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}. \quad (11)$$

Combining recall and precision by means of the harmonic mean results the $F_1$ metric:

$$F_1 = \frac{2 \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}. \quad (12)$$
Up to this point, the numerical value of a network prediction does not used explicitly, as only the classification result is considered. In order to take into account the numerical value of the network, another metric is defined, namely the Logarithmic Loss. Although in principle one could choose just any metric, Log Loss is motivated from information theory, and in particular from Kullback-Leibler information [20]:

\[ F_1 = \frac{2 \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}. \] (13)

Logarithmic Loss does not have upper bound and exists in the \([0, \infty]\). Logarithmic Loss nearer to 0 indicates higher accuracy, whereas if Logarithmic Loss is away from 0 then it indicates lower accuracy.

IV. RESULTS AND DISCUSSION

![Plot of training and testing errors as a function of training epochs for 8-16-16-1 network.](image)

**FIG. 3:** Plot of training and testing errors as a function of training epochs for 8-16-16-1 network.

A fully-connected neural network architecture is implemented and trained to discriminate between “healthy” and “non-healthy” Lagrangians for a classical theory with one degree of freedom. A number of different architectures, regarding the depth and the width of the network, were tested and the most promising was selected, namely a structure with two hidden layers of 16 neurons each. The optimal number of epochs to be used for training the network in order to minimize training error on the one hand while also avoiding over-fitting is found by comparing training and validation errors. Over-fitting occurs when we observe an increase in the testing error while the training error is consistently decreasing, [21, p. 202]. However, in our case the testing error seems to be decreasing over the epochs resulting in a better “behaviour” of the network, as can be seen in Fig. 3. Moreover, we also apply the metrics defined in Section III at different stages of the training procedure, as can be seen in Table II.

V. CONCLUSIONS

A neural network architecture was implemented, trained and tested in order to decide if a given Lagrangian will result equations of motion with higher order derivatives, without explicitly performing the analytical calculations. Validation of the trained network using the explicit standard procedure proved that for the toy model under study, the efficient discrimination of healthy and non-healthy Lagrangians was indeed implemented.
By suitably labeling the training data-sets, one can employ different criteria, resulting a trained network that could decide for more complex cases. There are various applications for this kind of approach, ranging from gravitational theories to solid state physics. In all cases, the search for a Lagrangian possessing some pre-defined properties (i.e symmetries) could be substantially simplified in the context of our approach. There is a possible limitation for generalized use of our approach, that is the exact form of the map between the Lagrangian space and the $n$-dimensional real space need to be defined for different classes of Lagrangians. Exploring the different ways to “translate” a Lagrangian to multidimensional real space in an effort for a general description is deemed very fruitful. The aforementioned direction could also lead to new results regarding data-preproccesing techniques.

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