Title

Subtitle

by

Mikkel Metzsch Jensen

THESIS

for the degree of

MASTER OF SCIENCE

Faculty of Mathematics and Natural Sciences
University of Oslo

Spring 2023

Title

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Mikkel Metzsch Jensen

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http://www.duo.uio.no/

Printed: Reprosentralen, University of Oslo

Abstract

Abstract.

Acknowledgments

Acknowledgments.

Contents

List of symbols?

Maybe add list of symbols and where they are used like Trømborg.

Chapter 1

Introduction

1.1 Motivation

1.1.1 Friction

Friction is a fundamental force that takes part in almost all interactions with physical matter. Even though the everyday person might not be familiar with the term "friction" we would undoubtedly notice its disappearing. Without friction, it would not be possible to walk across a flat surface, lean against the wall or secure an object by the use of nails or screws [p. 5] [1]. Similarly, we expect a moving object to eventually come to a stop if not supplied with new energy, and we know intuitively that sliding down a snow covered hill is much more exciting than its grassy counterpart. It is probably safe to say that the concept of friction is well integrated in our everyday life to such an extent that most people take it for granted. However, the efforts to control friction dates back to the early civilization (3500 B.C.) with the use of the wheel and lubricants to reduce friction in translational motion [2].

Friction is a part of the wider field tribology derived from the Greek word *Tribos* meaning rubbing and includes the science of friction, wear and lubrication [2]. The most important motivation to study tribology is ultimately to gain full control of friction and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages regarding energy effeciency. It has been reported that that monetary value of tribological problems has significant potential for economic and environmental improvements [3]:

> "On global scale, these savings would amount to 1.4% of the GDP annually and 8.7% of the total energy consumption in the long term." [4].

On the other side, the reduction of friction is not the only sensible application for tribological studies. Increasing friction might be of interest in the development of grasping robots or perhaps breaking system (get some sourced examples maybe), and ideally being able to turn friction up or down would be a groundbreaking step forward (to much?).

In the recent years an increasing amount of interest has gone into the understanding of the microscopic origin of friction, due to the increased possibilities in surface preperation and the development of nanoscale experimental methods such as the Friction Force Mircoscopy [5]. Nano-friction is also of great concern for the field of nano-machining where the frictional properties between the tool and the workpiece dictates machining charascteristics [3].

[6]

1.1.2 Thesis

In recent papers by Hanakata et al. [7](2018), [6](2020) numerical investigations has showcased that the mehcanical properties of a graphene sheet, yield stress and yield strain, can be altered through the introduction of so-called kirigami inspired cuts into the sheet. By the use of machine learning through accelerated search [7] and inverse design [6], they are able to extract cut pattern proposals which optimizes the mechanical properties in certain ways, e.g. stretchability or resistance to yield. This kind of study shows how numerical modelling and machine learning can extremely usefull for the designing of metamaterials, i.e. materials with properties not found in naturally occurring materials. Hanakate et al. assert the complexity of the mehcanical properties of the kirigami cut sheet to the out of plane buckling accouring when the sheet is stretched.

Since it is generally accepted that the surface roughness is of great importance for fritional properties it can be hypothesized that the cut and stretch procedure can be exploited for the design of fricitonal metamaterials as well. If successfull, the link between stretch and friction properties might also rise to a metamaterial with tunable friction properties after the point of manufacturing. That is, a material which fricitonal properties will change during stretch and relaxtion. For such a material, coupling the normal load and stretch of the sheet through a nanomachine design would allow for an altered friction coefficient which in theory might take negative values in certain ranges of normal load. To the best of our knowledge kirigami has not yet been implemented to alter the frictional properties on a nanoscale. However, in a recent paper by Liefferink et al. [8](2021) it is reported that macroscale kirigami can be used to dynamically control the macroscale roughness of a surface by stretching which can be used to change the frictional coeffcient by more than one order of magnitude.

Something about machine learning and inverse design.

1.2 Approach

Explain my specific approach in more detail one this is settled in completely.

1.3 Objective of the study

1. Design a MD simulation to evaluate the frictional properties of the grapehene sheet under different variations of cut patterns, stretching and loading, among other physical variables.
2. Find suitable kirigami patterns which exhibit out of plane buckling under tensile load.
3. Create a procedure for generating variaiton of the selected kirigami patterns along with random walk based cut patterns in order to create a dataset for ML training.
4. Train a neural network to replace the MD simulation completely.
5. (Variation 1) Do an accelerated search using the ML network for exotic frictional properties such as low and friction coeffcients and a strong coupling between stretch and friction.
6. (Variation 2) Make a GAN network using the forward network in order to extract cut configuration proposals for above frictional properties.
7. Make a nanomachine or artifical numerical setup which couples normal load and stretch with the intention of making a proof of concept for negative friction coefficients.

1.4 Contributions

What did I actually achieve

1.5 Thesis structure

How is the thesis structured.

Part I

Background Theory

Small introtext to motivate this chapter. What am I going to go over here.

1.6 Fourier Transform (light)

Find out where to put this if nessecary.

Fourier transform is a technique where we transform a function $f(t)$ of time to a function $F(k)$ of frequency. The Forward Fourier Transform is done as

$$F(k) = \int_{-\infty}^{\infty} f(t)e^{-2\pi ikx}dx$$

For any complex function $F(k)$ we can decompose it into magnitude $A(k)$ and phase $\phi(k)$

$$F(k) = A(k)e^{i\phi(k)}$$

Hence when performing a Forward Fourier transform on a time series we can determine the amplitude and phase as a function of freqeuncy as

$$A(k) = |F(k)|^2, \qquad \phi(k) = \Im \ln F(k)$$

Chapter 2

Machine Learning (ML)

- Feed forward fully connected
- CNN
- GAN (encoder + decoder)
- Genetic algorithm
- Using machine learning for inverse designs partly eliminate the black box problem. When a design is produced we can test it, and if it works we not rely on machine learning connections to verify it's relevance.
- However, using explanaitons techniques such as maybe t-SNE, Deep dream, LRP, Shapley values and linearizations, we can try to understand why the AI chose as it did. This can lead to an increased understanding of each design feature. Again this is not dependent on the complex network of the network as this can be tested and veriied independently of the network.

2.1 Feed forward network / Neural networks

2.2 CNN for image recognition

2.3 GAN (encoder + deoder)

2.4 Inverse desing using machine learning

2.5 Prediction explanation

2.5.1 Shapley

2.5.2 Lineariations

2.5.3 LRP

2.5.4 t-SNE

Chapter 3

Accelerated Search

3.1 Markov-Chain Accelerated Genetic Algorithms

3.1.1 Talk about traditional method also?

3.1.2 Implementing for 1D chromosone (following article closely)

We have the binary population matrix $A(t)$ at time (generation) t consisting of N rows denoting chromosones and with L columns denoting the so-called locus (fixed position on a chromosome where a particular gene or genetic marker is located, wiki). We sort the matrix rowwise by the fitness of each chromosono evaluated by a fitness function f such that $f_i(t) \leq f_k(t)$ for $i \geq k$. We assume that there are a transistion probability between the current state $A(t)$ and the next state $A(t+1)$. We consider this transistion probability only to take into account mutation process (mutation only updating scheme). During each generation chromosones are sorted from most to least fitted. The chromosone at the i-th fitted place is assigned a row mutation probability $a_i(t)$ by some monotonic increasing function. This is taken to be

$$a_i(t) = \begin{cases} (i-1)/N', & i-1 < N' \\ 1, & \text{else} \end{cases}$$

for some limit N' (refer to first part of article talking about this). We use $N' = N/2$. We also defines the survival probability $s_i = 1 - a_i$. In thus wau a_i and s_i decide together whether to mutate to the other state (flip binary) or to remain in the current state. We use s_i as the statistical weight for the i-th chromosone given it a weight $w_i = s_i$.
Now the column mutation. For each locus j we define the count of 0's and 1's as $C_0(j)$ and $C_1(j)$ resepctively. These are normalized as

$$n_0(j,t) = \frac{C_0(j)}{C_0(j) + C_1(j)}, \quad n_1(j,t) = \frac{C_1(j)}{C_0(j) + C_1(j)}.$$

These are gathered into the vector $\mathbf{n}(j,t) = (n_0(j,t), n_1(j,t))$ which characterizes the state distribution of j-th locus. In order to direct the current population to a preferred state for locus j we look at the highest weight of row i for locus j taking the value 0 and 1 respectively.

$$C'_0(j) = \max\{W_i | A_{ij} = 0;\ i = 1, \cdots, N\}$$
$$C'_1(j) = \max\{W_i | A_{ij} = 1;\ i = 1, \cdots, N\}$$

which is normalized again

$$n_0(j,t+1) = \frac{C'_0(j)}{C'_0(j) + C'_1(j)}, \quad n_1(j,t+1) = \frac{C'_1(j)}{C'_0(j) + C'_1(j)}.$$

The vector $\mathbf{n}(j,t+1) = (n_0(j,t+1), n_1(j,t+1))$ then provides a direction for the population to evolve against. This characterizes the target state distribution of the locus j among all the chromosones in the next generation.

We have

$$\begin{bmatrix} n_0(j,t+1) \\ n_1(j,t+1) \end{bmatrix} = \begin{bmatrix} P_{00}(j,t) & P_{10}(j,t) \\ P_{01}(j,t) & P_{11}(j,t) \end{bmatrix} \begin{bmatrix} n_0(j,t) \\ n_1(j,t) \end{bmatrix}$$

Since the probability must sum to one for the rows in the P-matrix we have

$$P_{00}(j,t) = 1 - P_{01}(j,t), \quad P_{11}(j,t) = 1 - P_{10}(j,t)$$

These conditions allow us to solve for the transition probability $P_{10}(j,t)$ in terms of the single variable $P_{00}j,t$.

$$\begin{aligned} P_{10}(j,t) &= \frac{n_0(j,t+1) - P_{00}(j,t)n_0(j,t)}{n_1(j,t)} \\ P_{01}(j,t) &= 1 - P_{00}(j,t) \\ P_{11}(j,t) &= 1 - P_{10}(j,t) \end{aligned}$$

We just need to know $P_{00}(j,t)$. We start from $P_{00}(j,t=0) = 0.5$ and then choose $P_{00}(j,t) = n_0(j,t)$

Part II

Simulations

Appendices

Appendix A

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