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PREDICTING OF ELASTIC AND THERMAL PROPERTIES OF METALLIC GLASSES USING GAUSSIAN PROCESS REGRESSION

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in front of the jury members

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LAKHDAR CHAIA.

Dedication

Firstly, thank God for his blessings, I dedicate this work to The most precious people in my life, my mom and dad, thank you All the support you gave me. To my dear brother, to my dear sisters And to my aunt and uncle and to all my family, to my dear friend and all my closest friends

LAKHDAR CHAIA.

Abstract

In this study, we used Gaussian process regression (GPR) to predict the elastic moduli and glass transition temperature of metallic glasses based on their atomic composition. The results show that GPR is an effective method for predicting these properties, with high accuracy and low error compared to experimental data. We also analyze the contributions of individual elements to the properties of metallic glasses, providing insight into their underlying physical mechanisms. This study demonstrates the potential of GPR for predicting the properties of complex materials, and highlights the importance of understanding the relationships between composition and properties in metallic glasses.

keywords: Glass, Gaussian process regression (GPR) , Young's modulus (E) , glass transition temperature (Tg) . Machine Learning .

Résumé

Dans cette étude, nous avons utilisé la Régression par Processus Gaussien (RPG) pour prédire les modules élastiques et la dilatation thermique coefficients des verres métalliques en fonction de leur composition atomique. Les résultats montrent que GPR est une méthode efficace pour prédire ces propriétés, avec une grande précision et une faible erreur par rapport aux données expérimentales. Nous avons également analysé les contributions des éléments individuels aux propriétés des verres métalliques, donnant un aperçu de leurs mécanismes physiques. Cette étude démontre le potentiel du GPR pour prédire la propriétés des matériaux complexes, et souligne l'importance de comprendre les relations entre composition et propriétés dans les verres métalliques.

Mots-clés: Verre, régression du processus gaussien (GPR) , module de Young (E) , verre température de transition (Tg) . Apprentissage automatique

ملخص

في هذه الدراسة ، قمنا باستخدام انحدار العملية الغاوصية GPR للتنبؤ بمعاملات المرونة ودرجة التحول الزجاجي للزجاج المعدني على أساس تركيبه الذري. تظهر النتائج أنّ GPR هي طريقة فعالة للتنبؤ بهذه الخصائص بدقة عالية وخطأ منخفض مقارنة بالبيانات التجريبية. قمنا أيضًا بتحليل مساهمات العناصر الفردية في خصائص الزجاج المعدني، مما وفر نظرة ثاقبة على آلياتها الفيزيائية. بشكل عام ، توضح هذه الدراسة إمكانات GPR للتنبؤ خصائص المواد المعقدة و تسلط الضوء على أهمية الفهم العلاقات بين التركيب والخصائص في الزجاج المعدني.

الكلمات المفتاحية : زجاج ، انحدار العملية الغاوصية (GPR) ، معامل يونغ (E) ، زجاج درجة حرارة الانتقال (Tg) . التعلّم الالي .

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General Introduction

1 Introduction

Glass is one of the important materials that are used in many daily applications, as it is used in the manufacture of insulating glass for buildings, cars, electronic devices, medical instruments, and many other applications. Glass has its own distinctive properties such as its transparency, hardness, strength, and resistance to wear and corrosion.

The glass transition temperature and Young's modulus are important information about glass, as they reflect the mechanical properties of the material and are used in the design of structures and devices that use glass. In order to obtain this information, various methods are used, including the GPR Gauss regression method.

Using the GPR Gauss regression method to determine the Young's modulus and glass transition temperature is the latest, most accurate, rapid and efficient measurement method, which can be used in many industrial and scientific applications. It is also considered a safe and easy-to-use method, as it does not require any destructive interventions in the material to be measured.

In addition, the use of the GPR Gauss regression method is characterized by the ability to perform measurements in real time, allowing users to obtain the necessary data quickly and with high accuracy. Thanks to these features, the GPR Gaussian Regression method can be used in many industrial and scientific applications, such as the manufacture of glass, plastics, metals, electronic materials, medical and others.

In general, GPR is used in the glass industry to determine the Young's modulus and glass transition temperature, as this information helps in glass design, quality inspection, and corrosion and fracture resistance testing. By using the GPR gauss regression method, industrialists and engineers can obtain the necessary data quickly and accurately, helping them to make important decisions about the design of structures and devices that use glass. Thus, the GPR gradient method is an important tool in the glass and other

materials industry, contributing to improving product quality and reducing costs and production time.

2 Thesis scope

In this note, we have studied the effectiveness of the GPR (Gaussian regression method) in measuring Young's modulus and the glass transition temperature, using multiple analytical and applied methods. This research aims to understand the capabilities of the GPR Gaussian regression method in predicting Young's modulus and glass transition temperature, and to determine the accuracy and reliability of this method in measurement. This study will be implemented by conducting practical experiments on different samples of glass using the Gaussian regression method (GPR), and analyzing the data extracted from these experiments using multiple analytical tools, including descriptive statistics, statistical analysis, and quantitative analysis of the data. Different models of glass will also be used in this study.This is to determine the extent to which different glass properties affect the ability of the GPR Gaussian Regression method to measure Young's modulus and glass transition temperature.

In general, this research aims to improve our understanding of the GPR method and its capabilities in measuring Young's modulus and glass transition temperature, and to apply these capabilities in many industrial and scientific applications. This research will also help improve the quality of glass products, develop new device designs and structures that use glass, and can contribute to improving efficiency and reducing costs in production and design processes. Thus, the scope of this note includes an in-depth study of the capabilities of the GPR Gauss regression method in predicting Young's modulus and glass transition temperature, and applying this method to improve our understanding of the properties of glass and to develop its applications in industry and science.

3 Thesis structure

In addition to this general introduction, this thesis is organized as followed:

Chapter 1: We begin with a brief overview of glass and the glass transition temperature, then we discuss the elastic coefficients and explain how to define them.

Chapter 2: In this chapter we will introduce a concept about machine learning and mention some of its techniques and introduce the machine learning method GPR Gaussian process regression that we used to predict Young's modulus and glass transition temperature from glasses combinations.

Chapter 3: We will present the results obtained from the technique used to predict the properties of Young's modulus and the glass transition temperature and we found a relationship between them.

A general conclusion summarizing all of our findings is provided at the end of this manuscript.

Chapter 1

Theory of elasticity

1 Introduction

In this chapter, we will introduce a short basic concepts about glass as well as briefly address the theory of elasticity in glass and experimental methods for determining its elastic coefficients.

2 The Glassy State

2.1 Definition of glass

Glass is annealed and amorphous without long-term arrangement although it is short-term.It is characterized by the phenomenon of glass transitions, obtained by rapid cooling of a supercooled liquid [1]. The glass state is characterized by the presence of a vitreous transition and is a characteristic transformation observed when cooling, when moving from a supercooled liquid phase to a glass phase or, conversely, when heating the glass to a supercooled liquid [2].

2.2 The vitreous state

This case is characterized by the occurrence of the phenomenon of glass transitions, in which the transition from the viscous liquid phase to the glass phase. When we rapidly and continuously cool a viscous viscous liquid, It shrinks in volume with a decrease in temperature until it becomes less than the melting temperature .the lower the temperature, the higher the viscosity ratio and the liquid begins to solidify until it turns into a crystal. By continuing the cooling process and decreasing the temperature, the volume

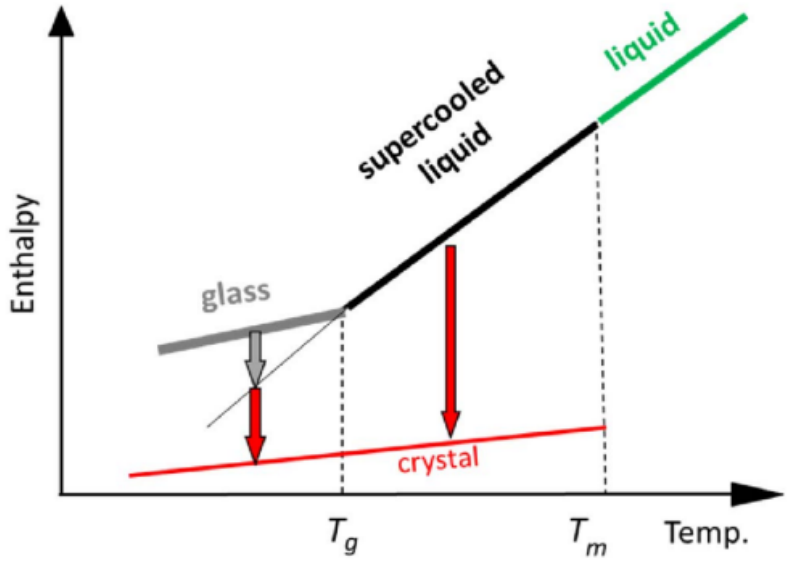

Figure 1.1: the glass transition phenomenon[4]

is stabilized, and then the temperature is called the glass transition temperature [3]. In equilibrium, thermodynamically stable liquids (L) exist only above the melting point or temperature of the liquid, Tm.They never crystallize. Supercooled liquids exist between Tm and the glass transition temperature (Tg). They eventually crystallize after a certain time. Glasses exist below the glass transition temperature, (Tg). They are thermodynamically unstable and spontaneously relax toward the supercooled liquid state at any nonzero temperature. Glass transition occurs at (Tg) (figure 1.1) [4].

3 Theory of elasticity

3.1 The characterization of elastic properties of solids

The mechanics of solids, regarded as continuous media, forms the content of the theory of elasticity. The macroscopic behavior of a solid is described by a continuum field theory, the theory of elasticity, which describes the way a solid deforms when external stresses are applied . Under the action of applied stress, solid body exhibits shape and volume changes to some extent, and every point in the solid body is in general displaced. Let the position vector before the deformation be r and after the deformation has a value r' with component xi. The displacement of this point due to deformation then given by the displacement vector $u = r - r^{'}$ or $u_i = x_i^{'} - x_i$. If u_{ij} (x_1, x_2, x_3) is the jth component of the displacement at point (x_1, x_2, x_3), the strain tensor for small deformations is [5].

$$u_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial u_j} + \frac{\partial u_j}{\partial u_i}) \tag{1.1}$$

When a deformation happens, the body ceases to be in its original state of equilibrium, and the forces, which are called internal stresses, therefore arise which tend to return the body to its equilibrium state. If the deformation of the body is fairly small, it returns to its original undeformed state when the external forces cease to act. Such deformations are elastic. For large deformations, the removal of the external forces does not result in the fully recovery of the deformation. Such deformations are plastic . There are different types of moduli, where the type of modulus depends on the type of deformation that the material is subjected to, such as elongation, bending, and others. All coefficients are represented by finding the stress-strain ratio within the limits of elasticity [5].
Stress is a quantity that describes the magnitude of forces that cause deformation. Stress is generally defined as force per unit area. And stress types of them [6].

- **Tensile stress:** Produced by a change in length , when forces pull on an object and cause its elongation, like the stretching of an elastic band.
- **Compressive stress:** Affect body size, when forces cause a compression of an object.
- **Shear stress (tangential stress):** It results in a change in shape, when the forces of deformation affect the surface of the body.

the relation between strain and stress does not need to be linear. Only when stress is sufficiently low is the deformation it causes in direct proportion to the stress value. The proportionality constant in this relation is called the elastic modulus. In the linear limit of low stress values, the general relation between stress and strain is
(Stress = (elastic modulus) $\times$ strain).
As we can see from dimensional analysis of this relation, the elastic modulus has the same physical unit as stress because strain is dimensionless.
We can also see from Equation that when an object is characterized by a large value of elastic modulus, the effect of stress is small. On the other hand, a small elastic modulus means that stress produces large strain and noticeable deformation. For example, a stress on a rubber band produces larger strain (deformation) than the same stress on a steel

band of the same dimensions because the elastic modulus for rubber is two orders of magnitude smaller than the elastic modulus for steel.

The elastic modulus for tensile stress is called Young's modulus; that for the bulk stress is called the bulk modulus; and that for shear stress is called the shear modulus. Note that the relation between stress and strain is an observed relation, measured in the laboratory [6].

3.2 Elastic moduli

Glass is a flexible solid, which means that when subjected to mechanical stress, it reflects completely.this theory is defined by the details to the response of materials to the stresses applied to them,as it uses defferent coefficients known as elastic coefficients: E young's modulus, K physical modulus, G tranverse modulus, L longitudinal modulus, in addition to poisson's ratio ν [7].

The elastic moduli give a macroscopic view of the hardness of materials and reflect an idea of both the nature of atomic bonds and cohesion [7].

3.2.1 Longitudinal Modulus

The longitudinal modulus L expresses the elongation of the sample under the influence of longitudinal stress, expansion occurs in a direction perpendicular to the transverse contraction elongation [7].

$$L = \rho v_L^2 \tag{1.2}$$

Where:

v_L is longitudinal sound velocity

3.2.2 Somatic Modulus

The physical coefficient describes the response of the body's strain to the hydrostatic pressure,which works to change the size without changing the shape and applies stress on all sides, and this leads to a pressure that determines the physical coefficient K and its expression is given [7].

$$K = \rho(v_L^2 - \frac{4}{3}v_s^2) \tag{1.3}$$

Where:

v_L is longitudinal sound velocity

v_s is transverse sound velocity

3.2.3 Shear modulus:

The shear modulus is related to the response of the body's strain to the shear stress, which works to the shape without changing the size, and the shear stress leads to the shear process,the corresponding modulus G carries many names,namely shear modulus,transverse modulus and torsion modulus , and is expressed [7].

$$G = \rho v_s^2 \tag{1.4}$$

Where:

v_s is transverse sound velocity

3.2.4 Young's Modulus:

Young's modulus know as tensile modulus is measure of the stiffress of an isotropic material. It is defined as the ratio of unixial stress over unixial strain in an elastic system.this can be determined empirically from the stress strain curve created during tensile or compression tests performed on the material.incorrectly, young's modulus is called the modulus of elasticity because young's modulus E is the most famous elastic constant, which is most commonly used in engineering design [7].

$$E = \rho v_s^2 (\frac{3v_L^2 - 4v_s^2}{v_L^2 - v_s^2}) \tag{1.5}$$

Where:

v_L is longitudinal sound velocity

v_s is transverse sound velocity

3.2.5 Poisson ratio:

Named after simeon poisson ,it is an important physical property used in the analysis of elasticityof materials,when a material is compressed in one direction, it ususlly tendsto expand in the other two directions of perpendicular to the direction of compression.this phenomenon is called the poisson effect, and it is a ratio between trasverse shrinkage and relative elongation and is given by the expression [7].

$$\nu = \frac{v_L^2 - 2v_s^2}{2(v_L^2 - v_s^2)} \tag{1.6}$$

Where:

v_L is longitudinal sound velocity

v_s is transverse sound velocity

3.3 Experimental methods for determining elastic moduli of glasses:

The elastic moduli of a matter are determined by its interatomic forces, the structure and its vibrational properties. And hence the values of the elastic constants K, G, and E and Poisson's ratio ν can be experimentally measured by many methods such as mechanical deformation or ultrasonic-wave propagation. For liquids, instantaneous elastic constants can be obtained from velocity measurements of high-frequency sound waves in order to avoid contributions of fast structural relaxations. In solids, basically, the methods for determining the elastic moduli are divided into static and dynamic methods.

The static and dynamic methods can be regarded as isothermal and adiabatic measuring conditions, respectively. The basic theory for static method is to measure the stress–strain curve in the elastic deformation limit, and then calculate the elastic moduli based on the curves. While the experimental conditions such as loading as well as the loading rate significantly affect the measuring accuracy of the elastic moduli. The static method is also difficult to be applied to brittle materials such as glassy materials. The dynamic methods have relative high accuracy. According to the applied frequency range, the dynamic methods are classified as: acoustic method (the frequency is below 104 Hz) and ultrasonic method (the frequency is between 104 and 108 Hz). The dynamic methods are widely applied to study the elastic properties and determine the elastic moduli of glasses and glass-forming liquids. Therefore, in the following we focus on the introduction of one of the dynamic methods -the ultrasonic method and the related theory(figure 1.2) [8].

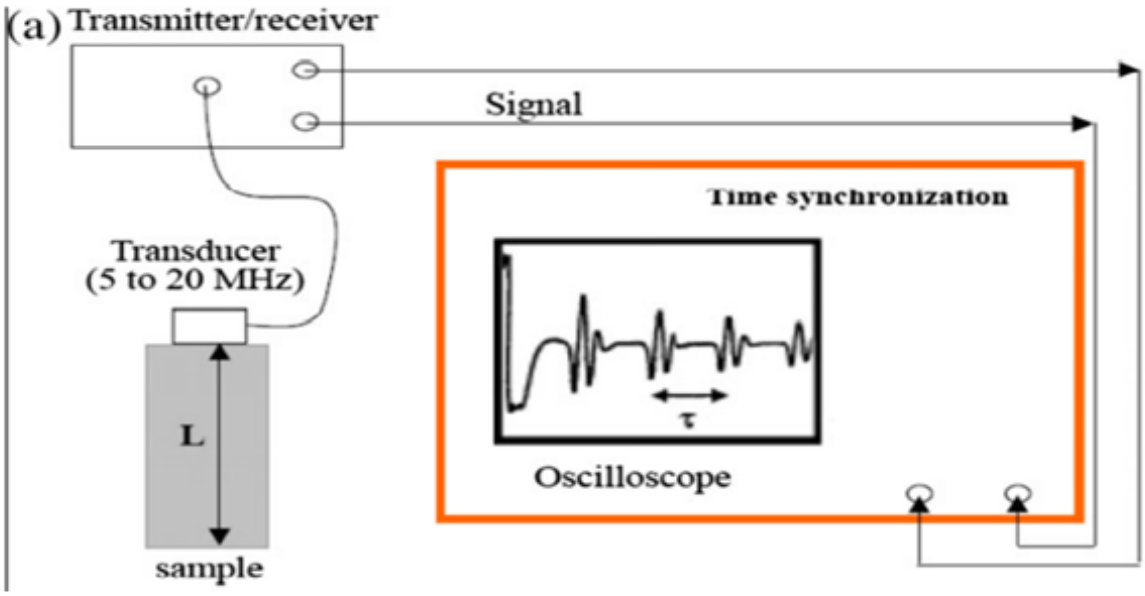

Figure 1.2: The schematic illustrations for ultrasonic method.[8]

3.4 Ultrasonic methods:

3.4.1 theory for ultrasonic measurements:

The propagation velocity of the ultrasonic waves such as longitudinal and shear waves depends on the nature of the materials. However, in a given material, the propagation velocity of the ultrasonic wave is independent of its frequency and the dimension of the material. In isotropic and homogeneous solids such as glassy materials, the one-dimensional acoustic wave equations are expressed as [5].

(Longitudinal mode or compressional wave)

$$\frac{\partial^2 u}{\partial t^2} = \frac{L\partial^2 u}{\rho \partial x^2} \tag{1.7}$$

(Shear mode or transverse mode)

$$\frac{\partial^2 u}{\partial t^2} = \frac{G\partial^2 u}{\rho \partial x^2} \tag{1.8}$$

where u is displacement, L is longitudinal modulus. From above equations, one obtains:

$$G = \rho v_s^2 \tag{1.9}$$

$$L = \rho v_L^2 \tag{1.10}$$

where v_L and v_s are longitudinal and transverse sound velocities, respectively. It can be approximately generalized that the v_s is half of the v_l in homogenous metallic materials, that is $v_l = 2v_s$. the E, K, and m of the isotropic solids such as glasses can be given in terms of v_l , v_s and density as :

$$K = \rho(v_L^2 - \frac{4}{3}v_s^2) \tag{1.11}$$

$$\nu = \frac{v_L^2 - 2v_s^2}{2(v_L^2 - v_s^2)} \tag{1.12}$$

$$E = \rho v_s^2(\frac{3v_L^2 - 4v_s^2}{v_L^2 - v_s^2}) \tag{1.13}$$

Therefore, ultrasonic velocity measurement and density measurement enable easy access to elastic coefficients.

3.4.2 The information provided from ultrasonic study:

Comparing with other elastic moduli measuremental methods, the ultrasonic measurements can conveniently obtain the longitudinal and shear acoustic velocities in the glassy materials. From the technological perspective, knowledge of the elastic constants is necessary to design structural components. From the scientific perspective, the magnitude of the elastic constants provides information about the strength of the interatomic forces and nature of the glasses. Since acoustic property is particularly sensitive to the microstructure as well as its change, the studies of the acoustic and elastic properties of glasses can provide important information about their structural and vibrational characteristics which are quite difficult for other methods to accessible [5].

4 conclusion

In this chapter we have explained the theory of elasticity and we have also shown the elastic coefficients, which are the longitudinal and Somatic , shear, Young's modulus and Poisson's ratio, and we mentioned experimental methods for determining these coefficients, and among these methods we explained the ultrasound method.

Chapter 2

Machine learning

1 Introduction

Machine learning gives computers the ability to learn without being explicitly programmed for the task at hand. The learning happens when data is combined with mathematical models [9].

In recent decades, the world has experienced a real explosion in the volume of data which is the main reason that made scientists use data to infer and obtain information about many unexplained phenomena therefore a smart data analysis leads to a significant scientific progress, one of the domains that deals with data is machine learning.

Machine learning is a sub-domain of intelligence artificial focuses on the development of models capable of representing certain characteristics, learn and detect some statistical pattern from data in order to accomplish various tasks, the term intelligence stands for the ability of these models to generalize, i.e. to extract information from the studied data during an updating process called training, and use these information to automatically infer another information from new data [10].

There are many predictive techniques in machine learning, herein we will use supervised regression namely Gaussian process regression (GPR).

2 Unsupervised learning

Unsupervised Learning (UL) is an elusive branch of Machine Learning (ML), including problems such as clustering and manifold learning, which seeks to identify structure among unlabeled data.

UL is notoriously hard to evaluate and inherently indefinable(Figure 2.1). Unsupervised learning is where you only have input data (X) and no corresponding output variables. The term "unsupervised learning" is generically associated with the idea of using a collection of observation$X_1..., X_n$ sampled from a distribution $p(X)$to describe properties of $p(X)$ [11].

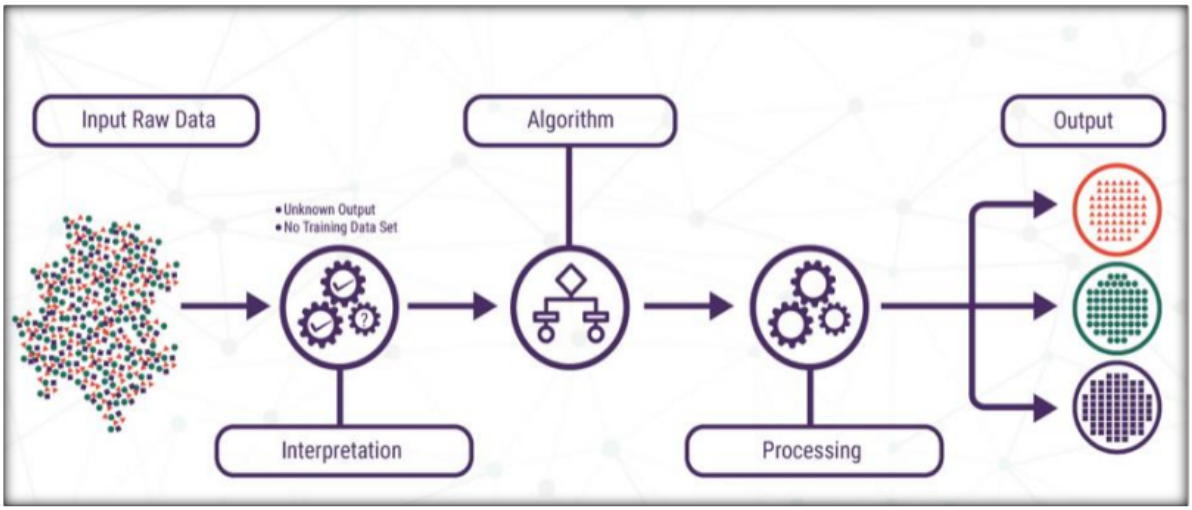

Figure 2.1: unsupervised.[11]

3 Supervised learning

Supervised learning refers to the problem where the data is on the form $\{x_i, y_i\}_{i=1}^n$ where $x_i$denotes inputs and y_i denotes outputs. In other words, in supervised learning we have labeled data in the sense that each data point has an inputx_i and an output y_i which explicitly explains "what we see in the data"

Depending on whether the output of the problem is quantitative or qualitative, we can classify supervised learning into either regression or classification(figure 2.2). Regression means the output is quantitative, and classification means the output is qualitative [9]. This means that whether a problem is about regression or classification depends only on its output.

But in our study we will focus on regression only.

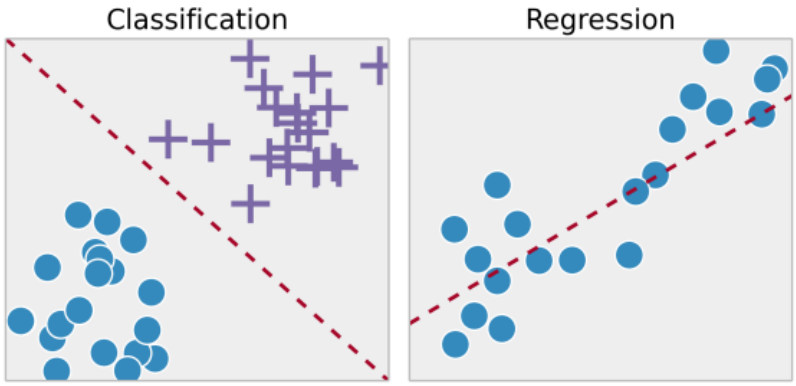

Figure 2.2: Difference between classification and regression [12]

3.1 Regression

Regression is to map an input data to a numerical value. In another words for an input $X_i \in R^d$that represents d dimensional features vector and a continues output space $y \subset R$, the learning algorithm is asked to produce a function f: $R^d \rightarrow R^n$ that maps any given input X_i to a corresponding value $y \in Y$. Examples Neural Networks, Support Vector Regression, Linear Regression, Polynomial Regression . . .[10].

3.1.1 Linear regression

Linear regression is one of the methods of multivariate analysis that deals with quantitative data. It is a way of investigating data from observations, or experiments, where The main goal is to search for a linear link between the quantum Y variable and One or more X variables are also quantity(Figure 2.3)[13].

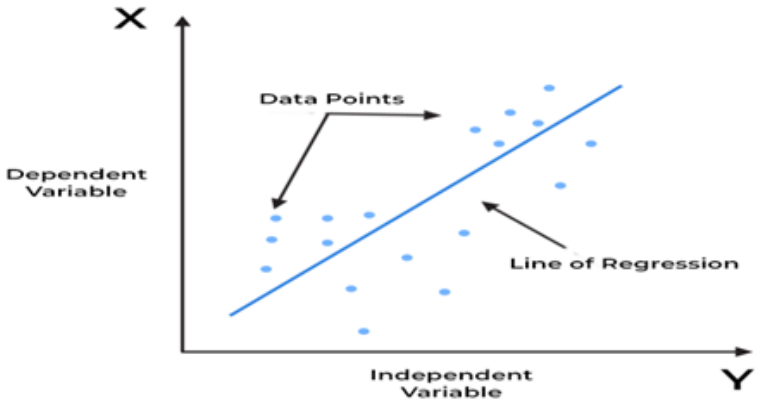

Figure 2.3: Line for a Linear Regression Model.

The simple linear regression model for n observations can be written as:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \tag{2.1}$$

The designation simple indicates that there is only one predictor variable x, and linear means that the model is linear β_0 and β_1. The intercept β_0 and the slope β_1. Are unknown constants, they are both called regression coefficients; ϵ_i'sare random errors. To estimateβ_0 and β_1. We use the method of least squares, it consists of calculating the difference between the observations y_i and the regression line and minimize the following expression(figure 2.4)[14].

$$\sum_{i=1}^{n}(y_i - \beta_0 + \beta_1 x_i)^2 \tag{2.2}$$

And the solution is:

$$\beta_1 = \frac{\sum_{i=1}^{n} x_i y_i + \frac{1}{n}\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n}(\sum_{i=1}^{m} x_i)^2} \tag{2.3}$$

$$\beta_0 = y - \beta_1 x \tag{2.4}$$

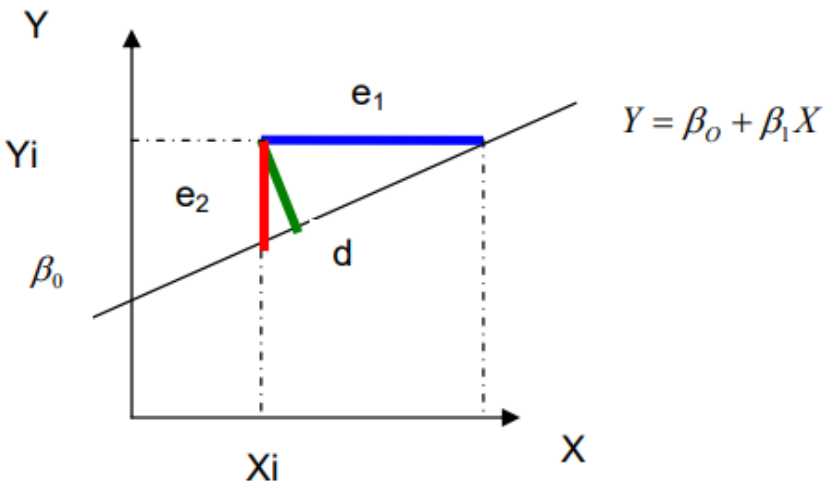

Figure 2.4: Three possible projections of the point (X_i, Y_i) [13]

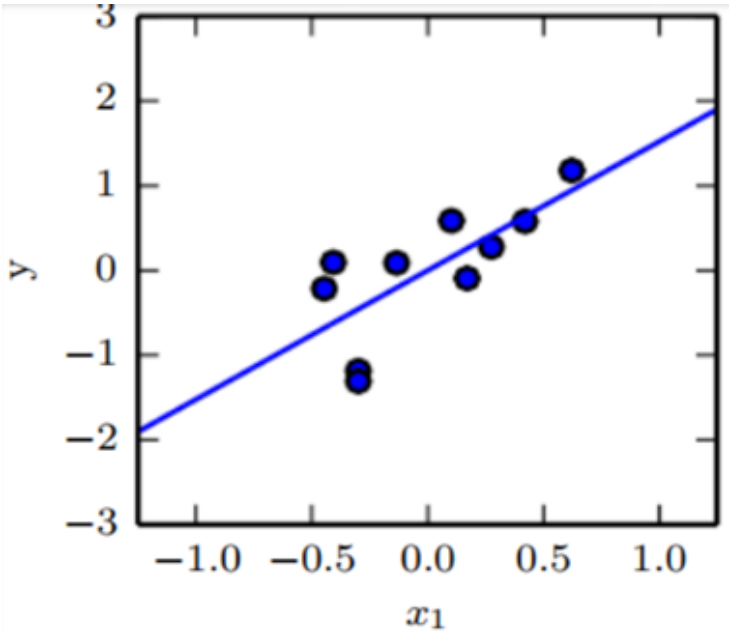

Figure 2.5: A linear regression problem, with a training set consisting of ten data points [14].

3.1.2 Nonlinear regression

The basic idea of nonlinear regression is the same as that of linear regression, namely to relate a response Y to a vector of predictor variables $X = (x_1, ..., x_k)^T$ (see Linear models). Nonlinear regression is characterized by the fact that the prediction equation depends nonlinearly on one or more unknown parameters. nonlinear regression usually arises when there are physical reasons for believing that the relationship between the response and the predictors follows a particular functional form. A nonlinear regression model has the form:

$$Y_i = f(X_i, \theta) + \epsilon_i, i = 1, .., n$$

where the Y_i responses, f is known function of the covariate vector $X_i = (x_{i1}, ...x_{ik})^T$ and the parameter vector $\theta = (\theta_1, ...\theta_p)^p$, and ϵ_i are random errors. The ϵ_i are usually assumed to be uncorrelated with mean zero and constant variance.

The unknown parameter vector θ in the nonlinear regression model is estimated from the data by minimizing a suitable goodness-of-fit expression with respect to θ. The most popular criterion is the sum of squared residuals

$$\sum_{i=1}^{n} [y_i - f(X_i, \theta)]^2 \tag{2.5}$$

and estimation based on this criterion is known as nonlinear least squares [15].

4 Gaussian processes

The Gaussian processes model is a probabilistic supervised machine learning framework that has been widely used for regression and classification tasks [16].The Gaussian process is a set of continuous random variables with limited dimensions, each of which is subject to a normal distribution, and all distributions are normal, The Gaussian process is one of the most important machine learning techniques [17].A Gaussian processes model describes a probability distribution over possible functions that fit a set of points. Because we have the probability distribution over all possible functions, we can calculate the means as the function, and the variances to indicate how confident the predictions are (Figure 2.6) [16].
We have the most important main points:
The function (posteriors) updates with new observations.
A Gaussian process model is a probability distribution over possible functions, and any finite samples of functions are jointly Gaussian distributed.
The mean function calculated by the posterior distribution of possible functions is the function used for regression predictions.
Probability density function is:

$$P_X(x) = \frac{1}{\sqrt{2\pi\sigma}} exp(-\frac{(x-\mu)^2}{2\sigma^2}) \tag{2.6}$$

X=Random variables.

x= the real argument.

σ=Variance.

μ=The independent mean

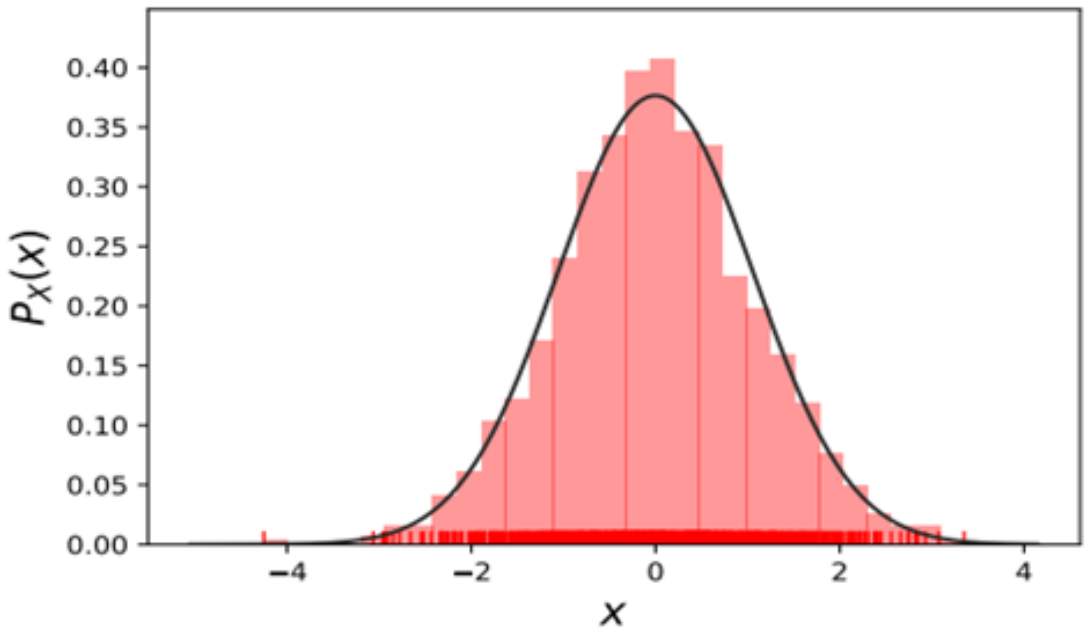

Figure 2.6: Plotting the probability density function in terms of the entereddata points

5 Gaussian processes regression

GPR is one of the nonparametric kernel-based learning algorithms developed from the Bayesian linear regression model. The kernel function is a crucial component of GPR, because it represents the assumptions on the object (e.g., systematic prediction error) that we wish to learn. Specifically, the kernel function defines the closeness and similarity among the samples, under the assumption that 'close' input data will probably result in 'close' output data Therefore, kernel function determines GPR's performance in handling systematic prediction error.

The squared exponential (SE) function is the most widely-used kernel function in GPR (Figure 2.7) [18].

The Gaussian process regression model is a non-parametric model, which means that it does not assume a specific form for the studied function, but the form of the relationship between the inputs and the objectives is completely determined by the data that may include an unlimited number of functions, and the basic function that produces the data is unknown, but predictions are generated Through a group of functions that are subject to a Gaussian distribution in the function space, the Gaussian process regression model is one of the most recent prediction methods[17].

The Gaussian process regression model is:

$$y_i = f(x_i) + \epsilon_i \ ; \ i = 1, ..., n \ ; \ \epsilon_i \sim N(0, \sigma^2) \tag{2.7}$$

We have a Gaussian process regression function:

$$f(x) = GP(\mu(x), K(x, x^{'})) \tag{2.8}$$

$$\begin{bmatrix} f_1(x) \\ : \\ f_n(x) \end{bmatrix} \sim N(\begin{bmatrix} \mu_1(x) \\ : \\ \mu_n(x) \end{bmatrix} , \begin{bmatrix} k_1(x, x^{'}) \\ : \\ k_n(x, x^{'}) \end{bmatrix}) \tag{2.9}$$

Where:

$\mu(x)$ Represents the mean function and $K(x, x^{'})$ kernel function and (σ^2)represents random noise variance.

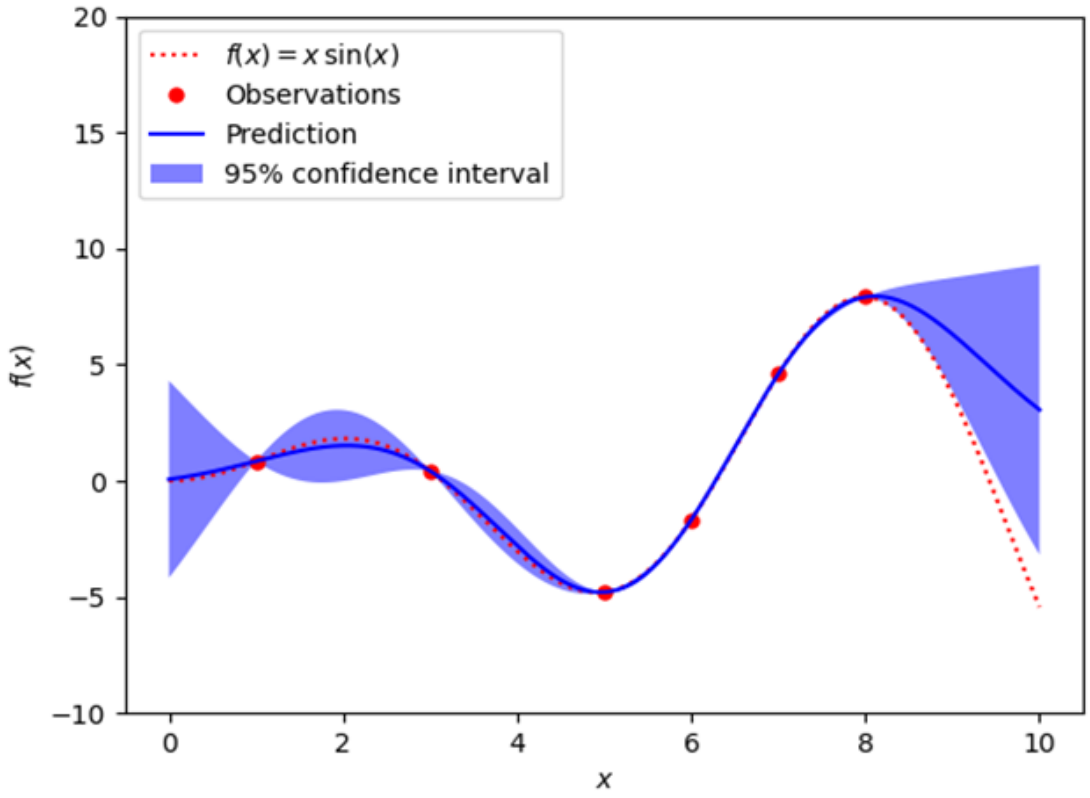

Figure 2.7: Gaussian process regression

6 Kernel Functions

The value of the kernel function $k(z, z^{'})$ is an indicator of the interaction of two states$(z, z^{'})$. Thus, an essential part of GPR is the selection of the kernel function and the estimation of its free parameters $\phi_1, \phi_2, \ldots \phi_{n\phi}$, called hyperparameters[19].

6.0.1 linear kernel

The equation for the linear kernel is given by

$$k(z, z^{'}) = z^T z^{'} \tag{2.10}$$

The linear kernel is a dot-product kernel and thus, non-stationary. The kernel can be obtained from Bayesian linear regression. The linear kernel is often used in combination with the constant kernel $k(z, z^{'}) = \phi_1^2$ to include a bias [19].

6.0.2 Polynomial Kernel

The equation for the polynomial kernel is given by

$$k(z, z^{'}) = (z^T z^{'} + \phi_1^2) \ ; \ p \in N \tag{2.11}$$

The polynomial kernel has an additional parameter, $p \in N$, that determines the degree of the polynomial. Since a dot product is contained, the kernel is also non-stationary. The prior variance grows rapidly for $\|z\| \succ 1$ such that the usage for some regression problems is limited. It depends on a single hyperparameter $\phi_1 \in R \succ 0$ [19].

6.0.3 RBF kernels

The equation for radial basis function kernel is given by

$$k(z, z^{'}) = \phi_1^2(-\frac{\left\|z - z^{'}\right\|^2}{2\phi_1^2}) \tag{2.12}$$

Probably the most widely used kernel function for GPR is radial basis function kernel. The hyperparameter $\phi_1$describes the signal variance which determines the average distance of the data-generating function from its mean. The lengthscale ϕ_2 defines how far it is needed to move along a particular axis in input space for the function values to become

uncorrelated. Formally, the lengthscale determines the number of expected upcrossings of the level zero in a unit interval by a zero-meanGP [19]

6.0.4 Rational Quadratic Kernel

The equation for the rational quadratic kernel is given by

$$k(z, z^{'}) = \phi_1^2(1 + \frac{\left\|z - z^{'}\right\|^2}{2p\phi_2^2}) \tag{2.13}$$

This kernel is equivalent to summing over infinitely many squared exponential kernels with different lengthscales. Hence, GP priors with this kernel are expected to see functions which vary smoothly across many lengthscales. The parameter p determines the relative weighting of large-scale and small-scale variations [19]

$$k(x_1, x_2) = exp(-\frac{\|x_1 - x_2\|^2}{2\sigma^2}) \tag{2.14}$$

Where

σ Is the variance and our hyperparameter.

$\|x_1 - x_2\|$ Is the Distance between two points x_1 and x_2.

7 Hyperparameters Optimization

Most machine learning algorithms have hyperparameters, settings that we can use to control the algorithm's behavior [20]. Hyperparameters optimization is essential. Here we will use the most widely used kernel,RBF, as an example to explain the hyperparameters optimization. The general RBF function is given by.

$$k(x_i, x_j) = \sigma_f^2 exp(-\frac{1}{2l}(x_i - x_j)^T(x_i - x_j)) \tag{2.15}$$

Where σ_f and l are hyperparameters. The vertical scaleσ_f describes how much vertically the function can span. The horizontal scale l indicates how quickly the correlation relationship between two points drops as their distance increases. The effect of l was shown in (Figure2.8). A higher l provided a smoother function and a smaller l gave a wigglier function [16].

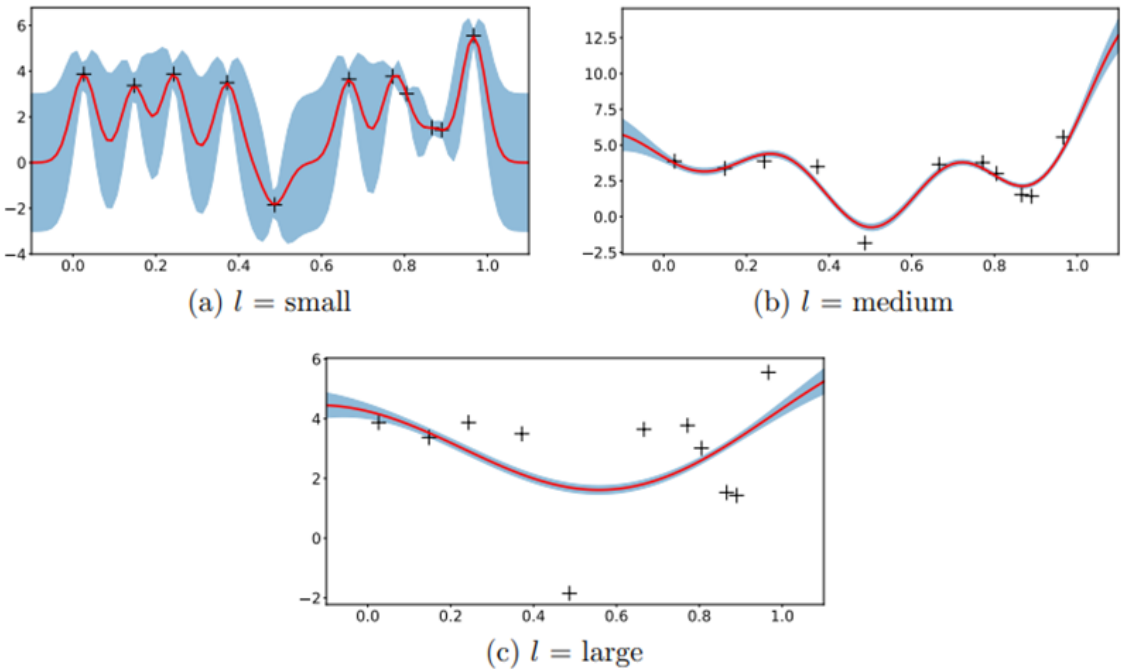

Figure 2.8: The function smoothness affected by the horizontal scale l of Hyperparameters.

The optimal hyperparameters θ^* are determined by the log marginal likelihood as.

$$\theta^* = argmalogxp(y|x,\theta) \tag{2.16}$$

Thus, considering hyperparameters, a more general equation of predictions at the new testing points is.

$$\overline{f_*}|X, y, X_*, \theta \sim N(\overline{f_*}, cov(f_*)) \tag{2.17}$$

Note that after learning/tuning the hyperparameters, the predictive variance $cov(f_*)$ depends on not only the inputs X and X_* but also the outputsy [16].

8 Training process

The central challenge in machine learning is that we must perform well on new, previously unseen inputs, not just those on which our model was trained. The ability to perform well on previously unobserved inputs is called generalization. Typically, when training a machine learning model, we have access to a training set, we can compute some error measure on the training set called the training error, and we reduce this training error [14].

For example in a linear model we train the model by minimizing the following error

$$\frac{1}{m^{(train)}}\left\|x^{(train)}\omega - y^{(train)}\right\|_2^2 \tag{2.18}$$

- **Underfitting:** Is when a machine learning model can not properly learn from the training data (have low accuracy). Some of the reasons why underfitting happens in neural networks is to have a small model or using a linear model with none linear dataset (features in the dataset are complex). Another reason is the noisy data (containing wrong labels) (Figure 2.9) [10].

- **Over-fitting:** is when a machine learning model gives a high prediction accuracy on the training data, but the prediction accuracy gets low if the model tested on previously unseen data (a data that was not present during the training),another term for describing overfitting is "high generalization error". Overfitting occurs when the model gets closely fit to the training data, this is because the training data is not all the possibilities of input data. A good model should have a good accuracy on the training data and the other. In other word, (it should be able to generalize) (Figure 2.9)[10].

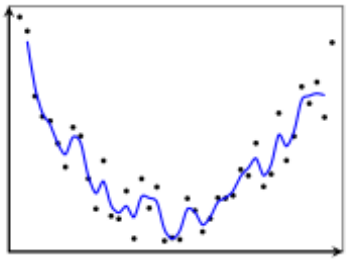

Figure 3.4: Overfitting

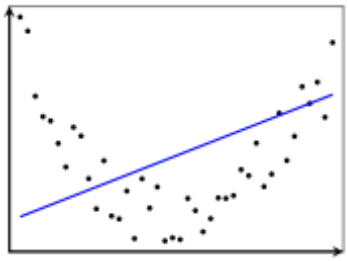

Figure 3.5: Underfitting

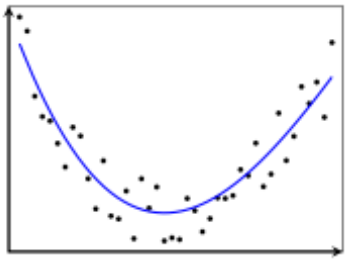

Figure 3.6: Robust Fit

Figure 2.9: The difference between overfitting, underfitting [10]

Chapter 3

Results and discussion

1 Introduction

In this chapter we will begin by presenting the data set and pre-data that we embarked on next, we will present GPR model that we created to predict the Young's modulus and the glass transition temperature (E, Tg), finally we will discuss the obtained result .

1.1 Method:

We used data from articale of Bulat N. Galimzyanov, Maria A. Doronina , Anatolii V. Mokshin (Machine learning-based prediction of elastic properties of amorphous metal alloys)[21].
In our work, we will focus on predicting Young's modulus and the glass transition temperature using Gaussian processes regression.

1.2 Data analysis:

In this particular study, the Young's modulus of amorphous metal alloys with various compositions and mechanical properties is determined using machine learning techniques based on Gaussian process regression (GPR). The calculation relies on a dataset comprising experimental information gathered from metal alloys containing Al, Au, Ca, Co, Cu, Fe, La, Hf, Mg, Ni, Pd, Pt, Re, Sr, Ti, W, Zr,and rare earth elements [21]. To train the GPR model, specific physical characteristics are selected as input parameters.These characteristics include the total molar mass (M) of the alloy components, the number of components (n), the yield stress (σ_y), and the glass transition temperature (T_g). By

feeding these parameters into the GPR, the model can predict the Young's modulus of the amorphous metal alloy under investigation.

d	materials_name	M	n	sigma_y	Tg	E
1	Al35La33Gd17Ni10Co5	9083.08	5	1.05	560	62.0
2	Al35La30Ce20Ni15	8794.24	4	1.16	542	66.0
3	Al35La33Er17Co15	9861.00	4	0.82	586	54.0
4	Al40La35Y10Ni15	7710.41	4	1.31	586	71.0
5	(Al0.84Y0.09Ni0.05Co0.02)95Sc5	3528.81	5	1.51	560	79.0

Figure 3.1: Dataset head

we examined the correlation between the Young's modulus (E) and several key parameters in amorphous metal alloys,namely the total molar mass (M), the number of components (n), the yield stress (σ_y), and the glass transition temperature (Tg).

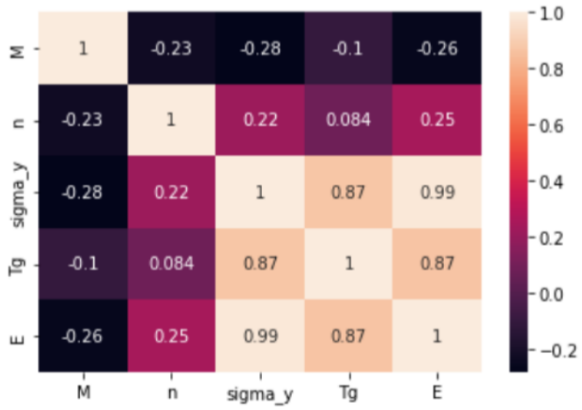

Figure 3.2: Correlation matrix

Our analysis revealed interesting relationships between these variables. We found a moderate negative correlation between the total molar mass and the Young's modulus, suggesting that higher molar mass is associated with lower stiffness or rigidity in the material. Conversely, the number of components showed a moderate positive correlation with the Young's modulus, indicating that an increase in the number of components leads to higher stiffness. Furthermore, we observed a strong positive correlation between the yield stress and the Young's modulus, indicating that materials with higher yield stress exhibit greater stiffness. Similarly, the glass transition temperature showed a strong

positive correlation with the Young's modulus, suggesting that materials with higher glass transition temperatures tend to have increased stiffness.

2 Gaussian process regression

GPR is a non-parametric kernel-based model that aims to build a probability distribution of a set of non-parametric functions to describe the relationship between the inputs and targets following the Bayesian inference paradigm.Gaussian process (GP) is a set of normally distributed random variables $f(x_i)$ which are defined by prior mean function $m(x)$ and covariance function (kernel function) $k(x, x^{'})$, thus the GP is denoted as:

$$f(x) \sim GP(m(x), K(x, x^{'})) \tag{3.1}$$

In which $m(x)$ represents the expected value of $f(x)$ and it is generally set to be zero. The kernel function measures the confidence level of $m(x)$. Furthermore, the regression response y_i can be calculated using the following probability distribution:

$$p(y_i|f(x_i), x_i) \sim N(y_i|h(x_i)^T\beta + f(x_i), \sigma^2) \tag{3.2}$$

where $h(x_i)$ is a non-linear basis function that transforms the vector feature from R^d to a new feature vector in R^p,β is $p \times 1$ vector of basis function coefficients. GPR was also conducted using Sklearn package, with the combination of three kernel functions, RBF (Eq. (2.12)), rational quadratic (Eq. (3.13)) to smooth the regression fit, and white noise kernel to reduce overfitting :

$$k(x^{'}, x)_{RQ} = \sigma^2(1 + \frac{(x - x^{'})^2}{2\alpha l})^{-\alpha} \tag{3.3}$$

where σ^2 is the total variance, l is the length scale and α is the scale mixture.[22]

3 Model evaluation

The performance of ML models was evaluated using leave one out cross validation ($LOOCV$), this cross-validation procedure is a special case of k-fold cross-validation where the number of the testing instance is equal to the number of the training data, thus the models have been repeatedly fitted using $n - 1$ of the total number of samples (n) and tested for the

remaining single item testing set, the chosen cross-validation method is very useful in the case of small dataset since the computation cost will be high for largerdatasets, moreover, it provides unbiased measures and enables the learning algorithms to better learn data representation.The coefficient of determination R^2 and root mean squared error ($RMSE$) were used as metrics to quantify the models' fitness and accuracy, which can be defined as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{'} - y_i)^2}{\sum_{i=1}^{n}(y_i^{'} - \hat{y}_i)^2} \tag{3.4}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i^{'} - \hat{y}_i)^2} \tag{3.5}$$

where N is the number of samples, $y_i^{'}$, $\hat{y}_i$ and y_i are the model predicted value, actual value, and an average of the actual values respectively. Further, R^2 is a non-negative metric variate from 0 to 1 and it measures the model robustness in fitting the real data,the closer its value to 1 the better the model, whereas the accuracy of the model is good when the $RMSE$ tends to 0 [22].

4 Result and discussion:

Based on the results obtained, our study shows that the model has a strong predictive capability for predicting the glass transition temperature and Young's modulus of the material.The R-squared values of 0.93 and 0.98 indicate that a high proportion of the variation in the output variables can be explained by the input variables. Additionally,the root mean squared error (RMSE) values of 28.67 and 4.83 suggest that the average difference between the predicted and actual values is relatively low.

RMSE = Root mean squared error

R2 score = coefficient of determination

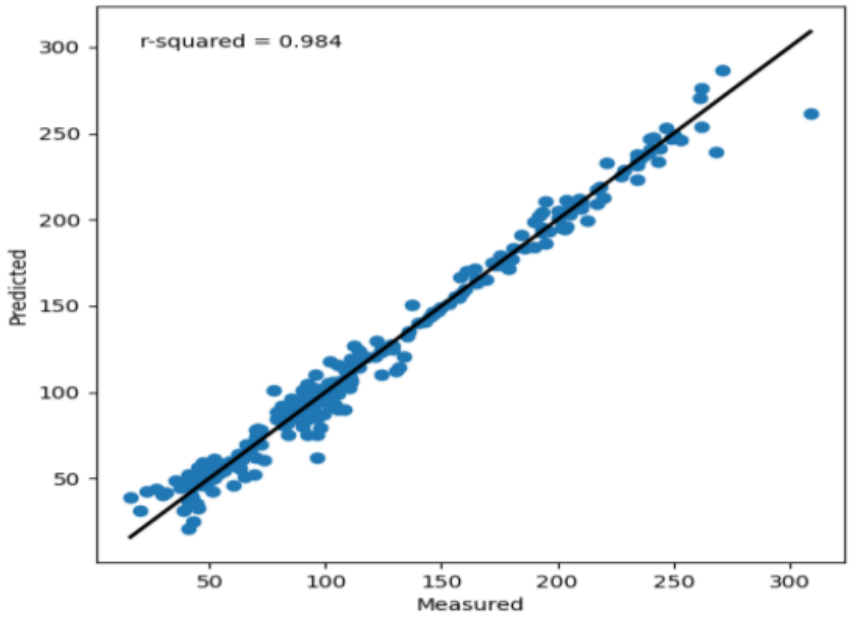

Figure 3.3: Predicted Young modulus of metallic glasses compared to the measured values.

	R2 score	RMSE
Glass transition température	0.93	28.67
Young modulus	0.98	4.83

Table 3.1: Prediction performance in term of R^2 score and RMSE (Root mean squared error)

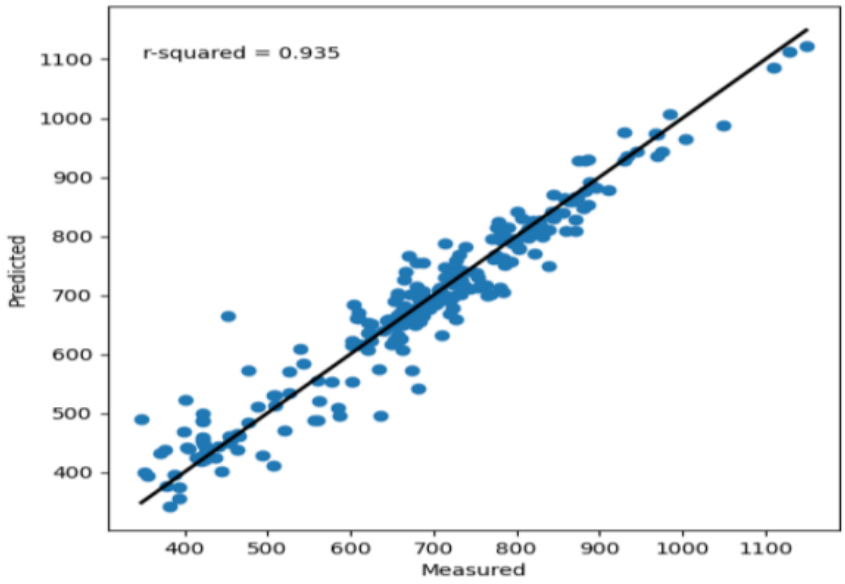

Figure 3.4: Predicted glasses transition temperature of metallic glasses compared to the measured values.

5 Conclusion

In this work, we investigated the predictive performance of machine learning Algorithm, GPR, for Young's modulus and glass transition temperature Tg, using different mechanical combinations and properties. For this, the calculation is based on a data set that includes experimental information collected from metal alloys containing Al, Au, Ca, Co, Cu, Fe,La, Hf, Mg, Ni, Pd, Pt, Re, Sr, Ti, W, Zr, and rare earth elements.

We also concluded in this work that. there is a strong positive correlation between Young's modulus and the glass transition temperature, as this correlation indicates that materials with a higher glass transition temperature tend to increase the hardness. There is a hardness positive relationship between yield stress and Young's modulus, which indicates that the materials with higher yield stress show greater toughness.

Chapter 4

General Conclusion

Glass is one of the important materials that are used in many daily applications, as we find that glass is an amorphous body, and we also found that different types of glass lead to a difference in composition, and glass has its distinctive characteristics such as its transparency, hardness, strength, and resistance to corrosion and corrosion.

The glass transition temperature and Young's modulus are important information about Glass, because it reflects the mechanical properties of the material. We also examined the relationship between Young's modulus and several key parameters in amorphous alloys, namely total molar mass, number of components, yield pressure, and glass transition temperature. We here found the direct relationship between the number of components and Young's modulus, which is that the higher the number of components, the greater the hardness.And we noticed a strong positive relationship between yield stress and Young's modulus, which shows that materials with higher yield stress show greater hardness, and the results also showed that the glass transition temperature and Young's modulus have a positive correlation strength, which indicates that materials with higher glass transition temperatures tend to increase the hardness.

In this study, we explored the use of a machine learning model to predict two important material properties: the glass transition temperature and Young's modulus. Our results show that the model has a strong predictive capability, with high R-squared values and relatively low RMSE values for both properties. Specifically, we obtained an R-squared value of 0.93 and an RMSE value of 28.67 for the glass transition temperature, and an R-squared value of 0.98 and an RMSE value of 4.83 for Young's modulus. These results suggest that the model has the potential to be a valuable tool for predicting material properties, with implications for a wide range of industries and applications.However,

it is important to note that the performance of the model may vary depending on the specific context and requirements of the problem at hand. Further research is needed to evaluate the model's performance in different settings and to explore its limitations.

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