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Machine Learning for MEMS Structure Design and Pulse Signal Analysis

By

Ruiqi Guo

A dissertation submitted in partial satisfaction of the

requirements for the degree of

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in

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in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

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Abstract

Machine Learning for MEMS Structure Design and Pulse Signal Analysis
by

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Doctor of Philosophy in Mechanical Engineering

University of California, Berkeley

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The rapid progress in computation power has led to drastic advances in the field of machine learning technologies to carry out data-driven predictions without explicitly programmed instructions. Different from the deterministic algorithm that heavily depends on the prior knowledge and human expertise, the self-evolving machine learning approaches have the potential to greatly reduce the human labor for superior performances. This work focuses on two goals: (1) data-driven MEMS structural designs with machine learning techniques for next generation sensing systems; (2) the combination of advanced sensing technologies and machine learning techniques inspired by the Traditional Chinese Pulse Diagnosis for mobile health applications.

Accelerating MEMS design processes by machine learning from pixelated binary images have been developed using binary pixelated 2D images to represent MEMS device structure, including disk-shaped resonators and piezoelectric energy harvesters. Numerical simulation results are used to train the deep neural network (DNN) to accurately predict the target physical properties, such as resonant frequency, quality factor, and output voltage. After the adequate training process, the obtained machine learning (ML) analyzers can precisely predict the physical properties from images with more than 95% accuracy. Compared to the traditional numerical simulation approaches, the ML analyzers can achieve 4.6×10^3 , 2.6×10^4 and 3×10^4 times faster computation speed for frequency, quality factor and output voltage calculation respectively.

The wrist pulse diagnosis is based on computational feature extraction and selection, as well as machine learning techniques. In this study, conformal ultra-flexible piezoelectret sensor (with $\sim 112 \mu m$ thickness) are attached to volunteers for the data acquisition. The signal was then preprocessed, extracting the identical features via the wavelet-based computational methods, filtering out redundant features with statistical hypothesis and the suitable statistical learning algorithms are selected for the classification tasks. It has been proved that the proposed system can correctly identify every user ($\sim 99\%$ F1 score on each tested category) simply based on wrist pulses.

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Chapter 1: Introduction

1.1 Background and Motivation

Over the past decades, machine learning (ML) has been an important innovation with prodigious adaptations and successes in industrial applications¹. The key aspect of ML is to improve itself automatically by uncovering the critical relationship between raw inputs and final outputs from the given dataset, instead of programming algorithms based on mathematical formulas or physical/chemical theories. The self-updating nature of the ML techniques can greatly help with the science and engineering problems that are data-intensive or hard to solve with human expertise. As such, the ML techniques have been adopted in a broad range of interdisciplinary researches, such as robotics², health informatics³, protein engineering⁴, statistical physics⁵, computational chemistry⁶, and material discoveries⁷. On the one hand, advanced and miniaturized sensing systems have supported the data acquisition processes in the modern society. The advent of “big data era” has provided unprecedentedly rich information for the development of ML algorithms⁸. In order to better transform collected data to actionable intelligence, this work aims at addressing two major challenges: (1) structural design of sensing devices to provide high quality data with optimal performances; and (2) the proper preprocessing and analysis of the sensing signals for intelligent systems.

In the modern sensing systems, the Microelectromechanical System (MEMS) technologies have played important roles. MEMS sensors exhibit excellent capability in miniaturization due to their small dimension, low power consumption, superior performance, and batch fabrication⁹. The proper structural designs of MEMS devices are vital for achieving desired sensing functions. However, the often-complex MEMS geometries make it hard to predict the performances with human intuitions or analytical methods. As such, numerical computation tools like finite element analysis (FEA) have been commonly used in the design iteration process^{10–17}. In general, candidate structures are modeled and the variables of interest (force, frequency, displacement, etc.) are calculated by solving many differential equations. While FEA simulations have greatly improved the design efficiency in the MEMS field and provided an economic solution to predict experimental outcomes, the computation cost is still very high since the FEA computation and model building can take a substantial amount of time. As such, it is desirable to reduce the human involvement, increase the computational speed, and visit the design space that is impossible to explore by human intuitions.

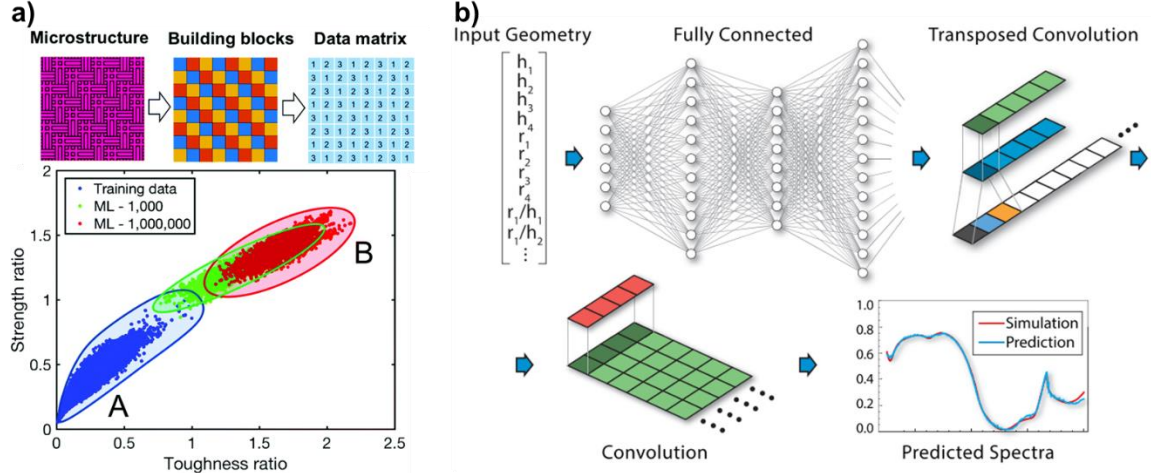


Figure 1.1: The examples of ML surrogate model to predict the structural properties. **(a)** Predicting the strength and toughness of composites from building block configurations¹⁸. **(b)** Predicting the transmittance spectra of optic meta-surfaces from input geometric parameters¹⁹.

We believe the answer lies at the intersection of the modern ML technologies and the computational mechanics. The basic idea behind the ML concept is to teach a computer program with labeled example data to optimize a certain performance criterion²⁰. For example, the criterion for the age prediction task is to correctly identify the ages of users from the facial images. As such, the training samples of this regression task would be the image form data labeled with the age values of people. Despite various types of different target ML applications, they can all be encoded to vectors for the mathematical calculations. If we define data inputs as structure configurations or parameters, data outputs as the values of target properties, and the performance criterion to minimize the difference between properties predicted by ML and numerical simulations, we can train an ML surrogate model to predict the structural properties. The ML-surrogate models have resulted in several orders of magnitude faster computation speed than those of pure numerical simulations, such as predicting the strength and toughness of composites (Fig. 1.1a) or the transmittance spectra (Fig. 1.1b) of optic meta-surfaces. Interestingly, MEMS structures are usually defined by lithography processes using photomasks, which are also binary 2D images (Fig. 1.2). Therefore, one major mission of this work is to discover the feasibility of accelerating the design and optimization of MEMS structures by using ML methods.

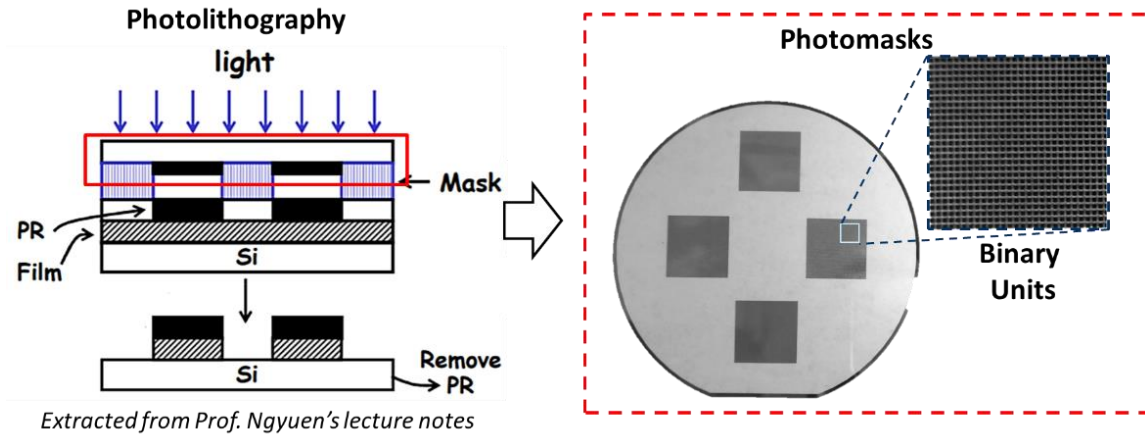


Figure 1.2 The schematics of photolithography process ²¹ and photomask samples, showing that the MEMS structures can be expressed as binary 2D images.

Digital signals have been collected continuously via the data sampling operation and are almost available in every part of the modern life. Among various types of digital signals, the biological signal is information-rich and complex. Traditionally, biological signals are processed by physicians and the extensive workload for data analysis becomes challenging with high levels of expertise ²². In recent years, the wide adoption of wearable and personalized health monitoring devices have acquired tremendous biological signals through the mobile network. From the monetary perspective, the wearable device market is forecasted to grow rapidly in the coming years, with a more than 20% annual growth rate and reaching the market value of 150 billion EUR by 2028 ²³. The growth has attracted both industry and academic interest to further invest in the wearable health field and one promising engineering solution is to seamlessly integrate advanced wearable sensors with the autonomous data analysis systems (Fig. 1.3). Researchers are improving the wearable health applications at both the sensor hardware and software level, where the advanced signal acquisition hardwares are becoming sensitive, light-weight and flexible and the embedded data analysis softwares are becoming precise, intelligent and fast responding.

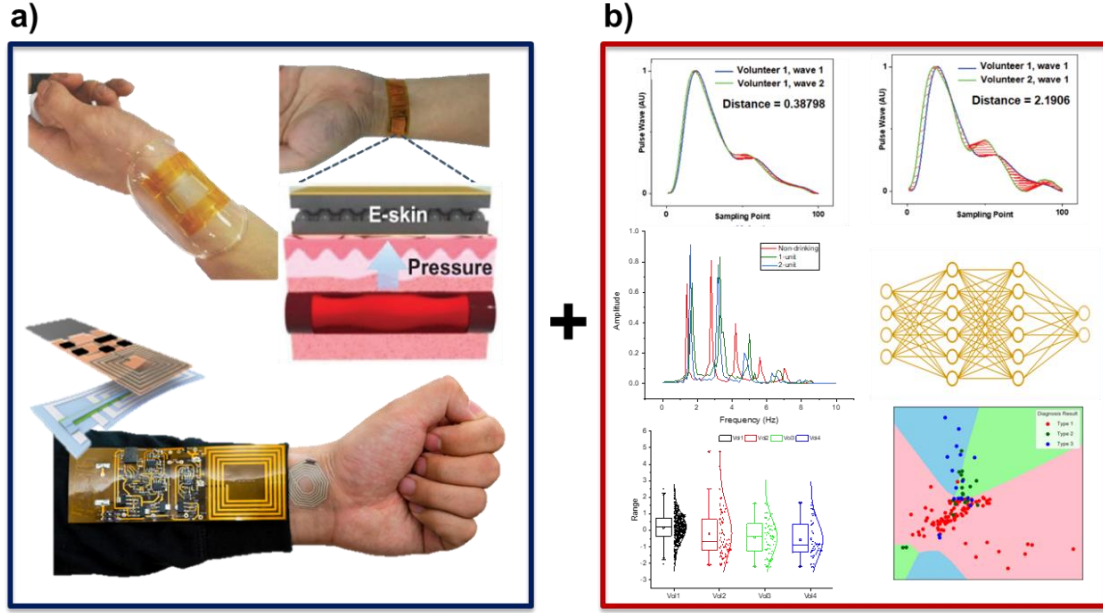


Figure 1.3: The schematic of the next-generation smart wearable system seamlessly integrating (a) advanced wearable sensors^{24–26} with (b) autonomous data analysis systems²⁷.

Among various wearable devices, the wrist-based smart devices take up the majority of the market²⁸. For example, pulse acquisition is one prevalent function integrated in the wrist mounted devices. It is non-invasive to reflect various types of the human health conditions suitable for continuous health monitoring. Specifically, Traditional Chinese Medicine (TCM) doctors can take the wrist pulse with finger touch and qualitatively describe the pulse patterns into 28 basic types in terms of their depth, rate, regularity, width, length, smoothness, stiffness and strength²⁹ (Fig. 1.4 a). However, the difference between some of the basic types are not sharp in their descriptions³⁰ and the definitions of pulse types are subjective³¹, which increases the difficulty of accurate diagnosis. Inspired by the TCM approaches, this work emulates the finger touch of TCM doctors with the flexible electret sensors to extract wavelet pulse features through the modern computational pulse analysis techniques (Fig. 1.4 b). In this way, the biological features of human pulses can be described quantitatively. After the feature selecting process, the ML algorithms can be trained to predict the health status. In this work, the human wrist pulse diagnosis is used as a study case to investigate the proper signal acquisition and analysis approaches for the intelligent wearable systems.

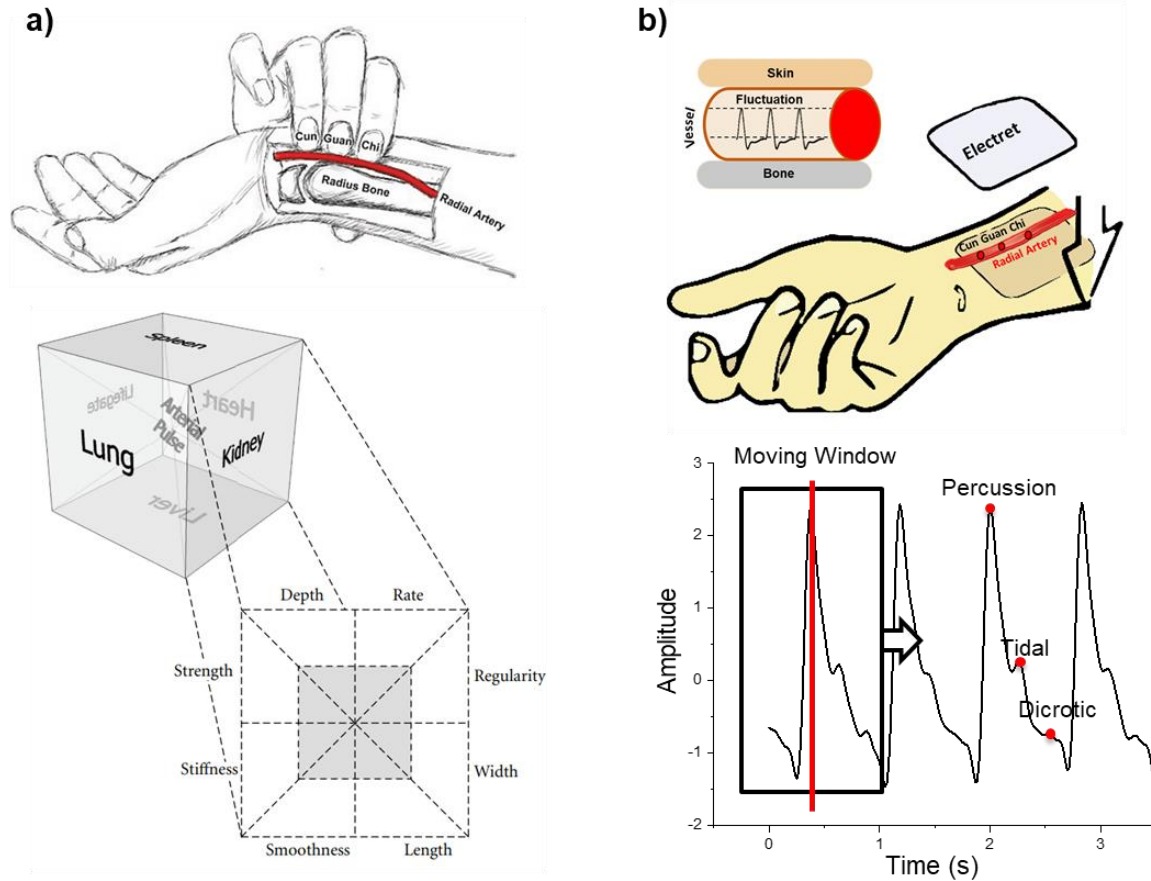


Figure 1.4: The comparison between TCM pulse taking approaches and proposed pulse acquisition and feature extraction. **(a)** TCM wrist pulse taking with fingers³² and qualitative feature extraction²⁹. **(b)** Proposed pulse acquisition with flexible sensor and computational feature extraction.

1.2 Dissertation Outline

Fig. 1.5 illustrates the key contributions of this thesis focuses on the adoption of machine learning techniques for two types of applications: (1) the data-driven MEMS device structural design, and (2) the intelligent pulse acquisition and diagnosis system. Chapter 2 reports the use of machine learning to accelerate MEMS design processes. As shown in Fig. 1.5a, the circular-shaped disk resonator and MEMS energy harvester have been used as examples to demonstrate the capability of the proposed method. Candidate designs are represented by pixelated binary 2D images. Instead of computational tools like FEA, the neural network is trained (Fig. 1.5b, left) to quickly obtain the key physical properties for each candidate design. Chapter 3 demonstrates the pulse signal diagnosis based on piezoelectret sensors and the intelligent signal analysis system (Fig. 1.5c). This chapter describes the sensor design, signal preprocessing, comprehensive feature extraction, statistic-hypothesis-based feature selection, and the machine learning modeling. The proposed system can tell the user identity from different wrist pulse signatures of

volunteers (Fig. 1.b, right). Chapter 4 summarizes the work done in this thesis and provides suggestions for future development.

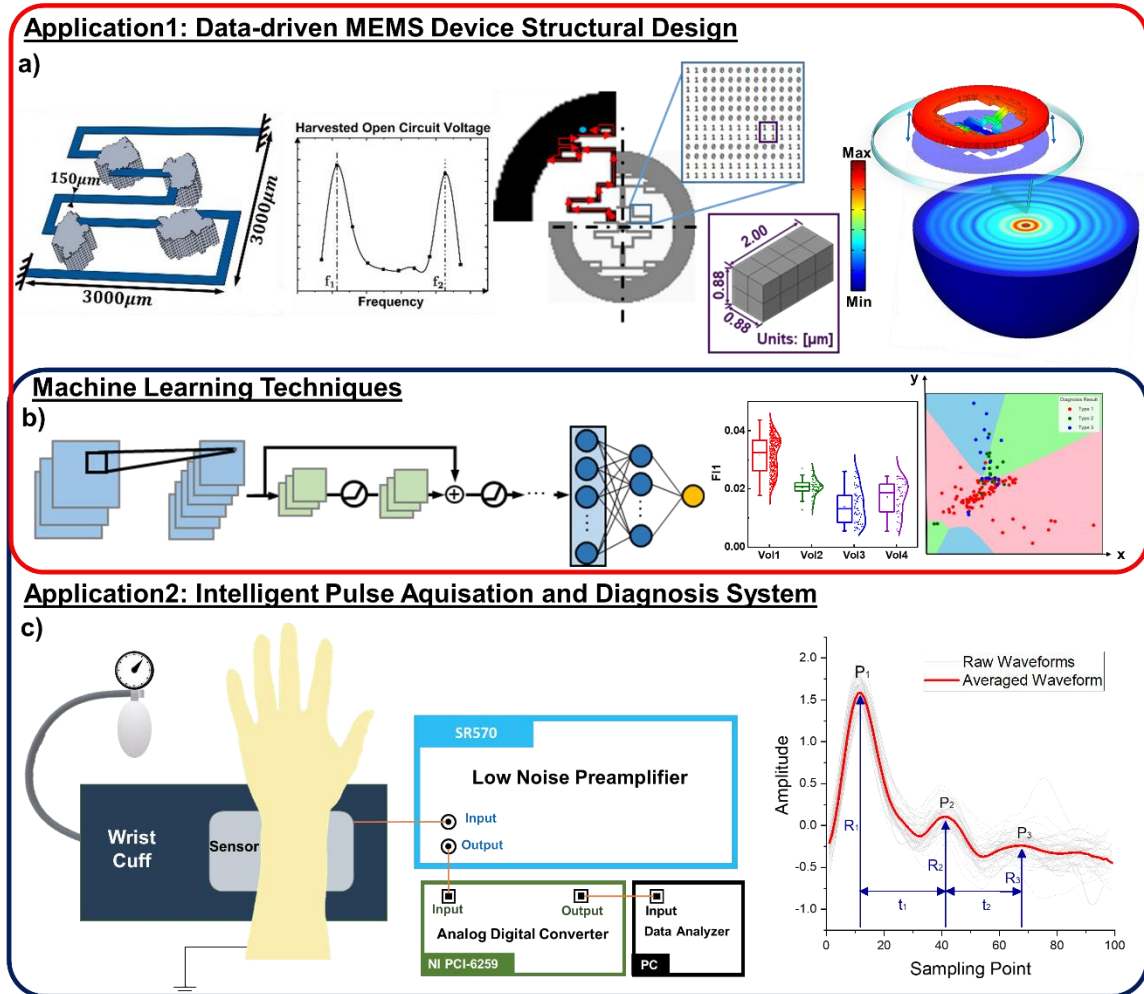


Figure 1.5: Illustration of major dissertation contributions: (a) data driven MEMS device structural design, (b) machine learning techniques, and (c) intelligent pulse acquisition and diagnosis system. Where the machine learning techniques played an important role in both (a) and (b) applications.

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Chapter 2: Accelerating MEMS Design Process through Machine Learning from Pixelated Binary Images

2.1 Literature Review and Motivation

Modern ML technologies combined with advances in mechanics can assist the optimal structural designs in MEMS. In previous works, ML techniques have been successfully implemented to analyze device signals¹⁻³ and to design device structures⁴⁻⁷. While these works have led to pioneering results for the data-driven design of MEMS, they generally require a high level of prior knowledges. In these works, the basic design topology is parameterized according to physical intuitions, and the detailed structural parameters are optimized by ML algorithms. In this study, the scheme of data-driven non-parameterized design is introduced as an important alternative to construct target structures voxel by voxel from the scratch without constraints in given topologies⁸⁻¹⁴. Specifically, after a few design variables are provided, such as the overall size and material properties, an astronomical number of design combinations can be created. Historically, this approach could be computationally expensive by using traditional ML schemes, which generate innumerable datasets and result in complexities during analyses. The Deep Learning (DL) technique used in this section provides a good solution to effectively learn the hidden patterns from the large number of datasets. This DL approach builds predictive models with multiple levels of simple but nonlinear modules that transform the representations at the lower level to a slightly higher level. With enough number of layers, the very complex hidden patterns can be picked up by the model¹⁵. Here, an automated system framework is developed for the experience-free, non-parameterized MEMS device design based on DL models. Two common MEMS devices have been chosen for case studies: the disk-shaped resonators and energy harvesters, to demonstrate the capabilities of the proposed approach.

2.2 Deep Learning for the Non-parameterized MEMS Disk-shaped Resonator Structural Design

2.2.1 Introduction

MEMS resonator has been intensively studied in the past decades for a wide range applications, such as the timing references, filters in wireless communication system, and sensing elements in various devices¹⁶. As a vibrating structure, the performance of the MEMS resonator is characterized by two important parameters: resonant modes/frequencies and quality(Q)-factors. Theoretically, a continuous system has infinite resonant modes with specific corresponding mode shapes but only a limited number of them would have practical usages, such as flexural mode¹⁷, bulk mode¹⁸ and wine-glass mode¹⁹. For many applications, a critical design goal is to reduce the energy loss of given modes as a high Q-factor system can significantly improve its sensitivity, resolution, and accuracy²⁰. The geometric configuration of the resonant structure can profoundly influence both the resonant frequencies and energy losses²¹⁻²³ but it is very difficult and time-

consuming to design complex MEMS structures with human intuitions. In this regard, this work aims to illustrate the application of machine learning schemes to reduce human involvements with increased capabilities in computational power to explore a wide-range design space that is previously unexplored and not possible to be investigated by pure human insights.

The proposed scheme is tested on the specific disk-shaped MEMS resonator configurations, which are represented with binary pixelated images. The addressed physical properties of interests are the resonant frequencies and the Q_{anchor} - the anchor loss as it is one of the major contributors to Q factor^{18,24,25}. Given that the finite Element Analysis (FEA) based methods have been widely adopted to precisely predict the MEMS/NEMS performances^{26–30}, the physical properties of disk-shaped resonator configurations are labeled with FEA results. As demonstrated in Fig. 2.1, the proposed method seamlessly bridges the design pattern generation and performance evaluation, then accelerated through DL techniques. After trained with tens of thousands of samples, the DL model would accurately predict both two parameters as validated by FEA simulations and resulted in a considerable reduction of computation cost. It is expected that the proposed method could contribute to the design automation of a broader range of MEMS devices.

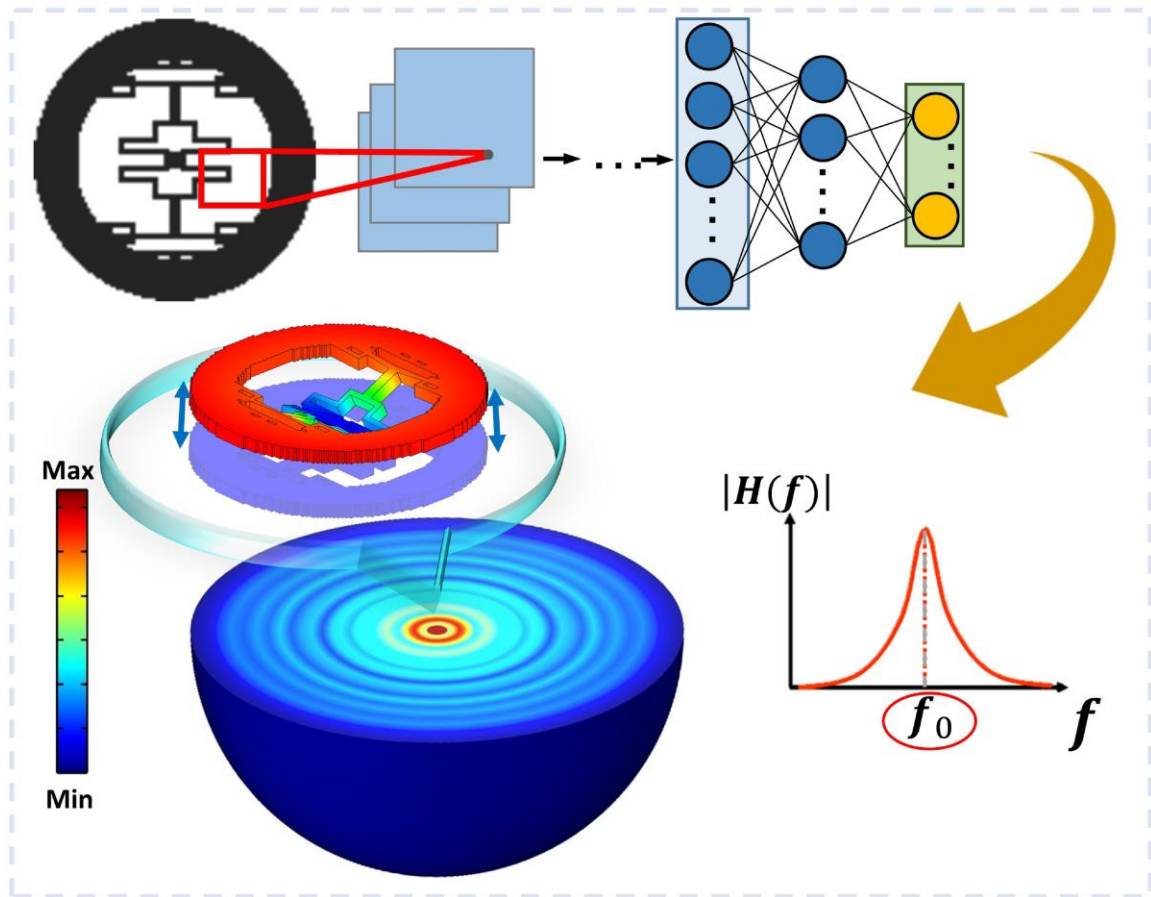


Figure 2.1: Schematic for the DL assisted disk-shaped resonator structural design. Featuring the DNN, modal frequency and the Q_{anchor} prediction.

2.2.2 System Architecture

The major components of the proposed system are illustrated in Fig. 2.2a, including the training process and the testing process. In the training process, a structure generator creates binary images representing the resonator structures, while the physical properties (f and Q_{anchor}) of the corresponding geometries are labeled with results from FEA. The DL model is trained by abundant labeled samples (referred to as “training samples”) in many epochs in order to form a DL Calculator with good accuracy. In the testing process, the structure generator passes new samples (referred to as “testing samples”) to the DL Calculator, and the DL Calculator predicts the physical properties of these samples that have never appeared in the training process. After enough training, the DL calculator would be able to accurately analyze the physics of candidate designs and help select the good designs without the need of additional numerical simulations.

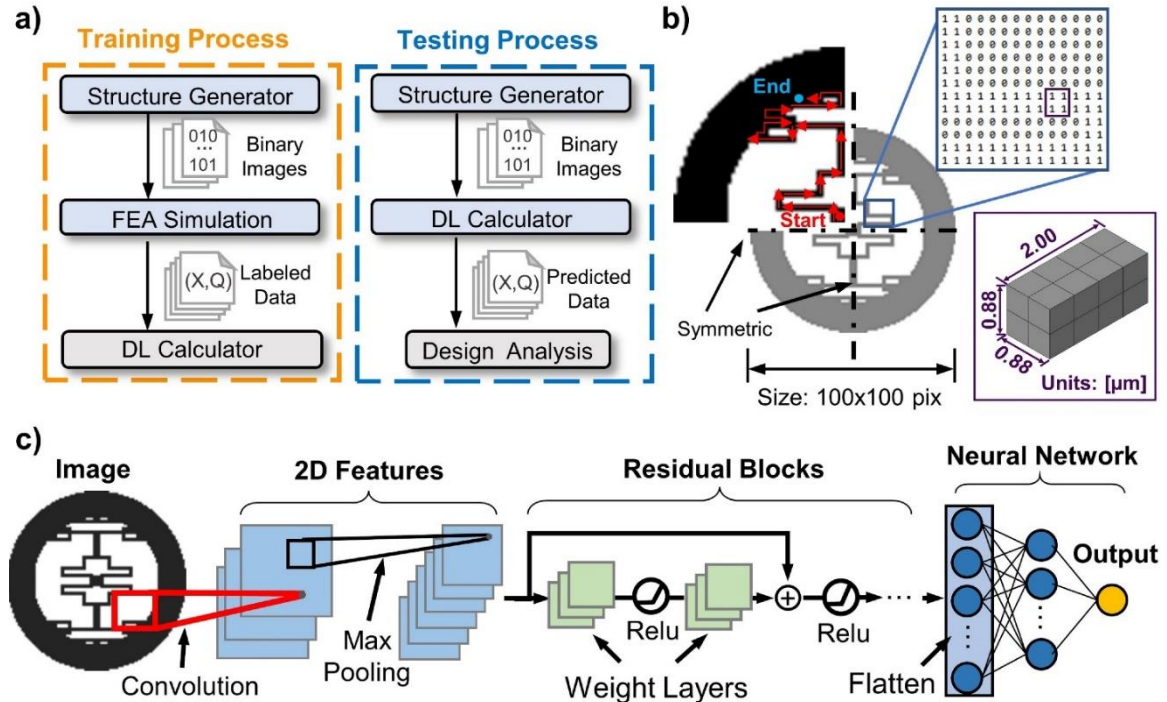


Figure 2.2: System components of the DL assisted non-parameterized MEMS design. (a) The major components for the proposed system architecture, which includes the training process and the testing process. (b) An example disk resonator pattern generated from the Brownian motion, followed by folding along the two axes of symmetry. The pattern is represented as a 100×100 pixel matrix, where 0 is a void element and 1 is a solid element. Inset: representative finite element mesh for a 2×2 solid region. (c) The structure of the Deep Residual Neural Network model used in this work, featuring input image, 2D features, residual blocks, the neural network, and the output target.

In this work, the resonators are made of polysilicon with density $\rho=2.3\times10^3\text{kg/m}^3$, Young's modulus $E=150\text{ Gpa}$, and Poisson's ratio $\nu=0.29$. For each disk resonator configuration, the diameters of the inner and the outer ring, the diameter of central anchor stem, and the thicknesses of the disk layer and the anchor stem are fixed parameters, as shown in Fig. 2.3. An example disk resonator pattern is given in Fig.2.2b by a 100×100 binary matrix, where 0 represents a void element and 1 represents a solid element. For the structural layer, each voxel is $0.44\text{ }\mu\text{m}$ in width and length, $0.5\text{ }\mu\text{m}$ in depth. This binary representation of the geometries is the key to achieve non-parameterized design. The agent is defined as a $2\times2\times4$ solid elements region that can move randomly stepwise along the four cardinal directions within one quadrant of the design domain. The trajectory of the Brownian-like motion for the agent always begins from the start point near the center anchor stem and stop at the endpoint near the inner annulus of the resonator. As another geometric constraint, the total covered area by the trajectory can be assigned as a programmable value. By folding the trajectories along the two axes of symmetry, the agent connects the anchor stem and the outer annulus of the resonator. As such, the non-parameterized and pixelated geometric configurations of the resonator are formulated. The physical property of the resonator structures are predicted with the Deep Residual Neural Network (ResNet) model³¹ shown in Fig. 2.2c, which features the input image, 2D features, residual blocks, the neural network, and the output target. The ResNet architecture in this work is customized from the reported ResNet50 model within the PyTorch³² package to suit the need of this study.

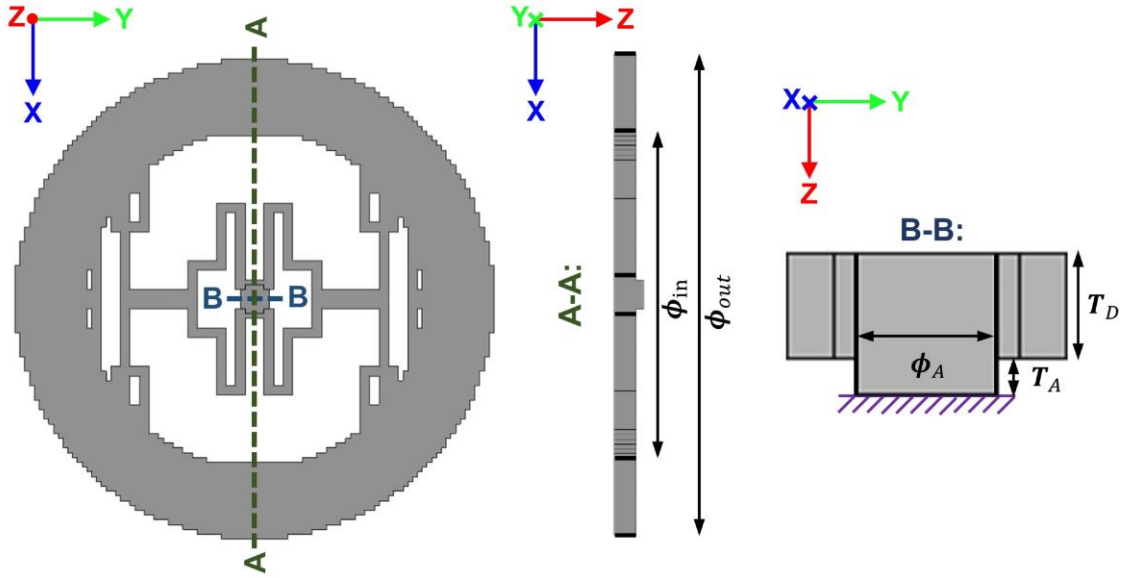


Figure 2.3: The top, and two representative cross-sectional views of an example resonator pattern. Dimensions: the outer ring diameter $\phi_{out}=44\mu\text{m}$, inner ring diameter $\phi_{in}=30.8\mu\text{m}$, stem anchor diameter $\phi_A=2.64\mu\text{m}$. The thickness of the disk $T_D=2\mu\text{m}$, and the height of the anchor $T_A=0.7\mu\text{m}$.

2.2.3 Modal Frequency and Anchor Loss Simulation

In this study, FEA is conducted extensively to generate results that are considered as the “ground truth” in the training and validation processes. Two types of FEA are performed, namely 1) natural frequency analysis for identifying the vibrational mode of interest, and 2) complex frequency analysis for extracting Q-factors. The natural frequency analysis yields the ideal, undamped frequency (real eigenvalue), the mode shape, and the effective mass corresponding to each vibrational mode. For a certain mode i , the vibration motion of the resonator can be projected into six directions (j), namely translation along X, Y, or Z axis ($j = \text{XT, YT, or ZT}$) and rotation about X, Y, or Z axis ($j = \text{XR, YR, or ZR}$). The effective mass from FEA outputs m^{eff} is a two-dimensional tensor, with one component m_{ij}^{eff} describing the amount of mass in the system participating in motions along a certain direction j in a vibration mode i . Using this critical tensor m^{eff} , a vibrational mode i can then be identified automatically by comparing the relative values of each component m_{ij}^{eff} in this row, instead of through tedious human visual inspections of the mode shapes. In this manner, the corresponding vibrational modes at calculated natural frequencies can be distinctly identified and labeled, which significantly reduces the time and labor consumptions during the data (training or testing) preparation process, when dealing with thousands of samples. As an example, Figures 2.4a-d show the mode shapes (upper row) and the distribution of effective mass components (lower row) corresponding to the first four vibrational modes of one resonator. The four modes are torsional mode about X axis ($i=1$), torsional mode about Y axis ($i=2$), in-plane spinning mode ($i=3$), and out-of-plane flexural mode ($i=4$), respectively. The radar charts show the ranking of the six directional effective mass components in this mode, from the highest (ranking=1, outermost) to lowest (ranking=6, innermost). As expected, the corresponding rotational components ($m_{1\text{XR}}^{\text{eff}}$, $m_{2\text{YR}}^{\text{eff}}$, $m_{3\text{ZR}}^{\text{eff}}$) are ranked first in the two torsional modes and the spinning mode, while the Z-direction translation ($m_{4\text{ZT}}^{\text{eff}}$) is the highest in the flexural mode. Utilizing this information, we can conveniently distinguish the mode of interest (the “flexural mode”, $i=4$) from all the modes computed by FEA, and obtain its corresponding natural frequency ω_{flex} .

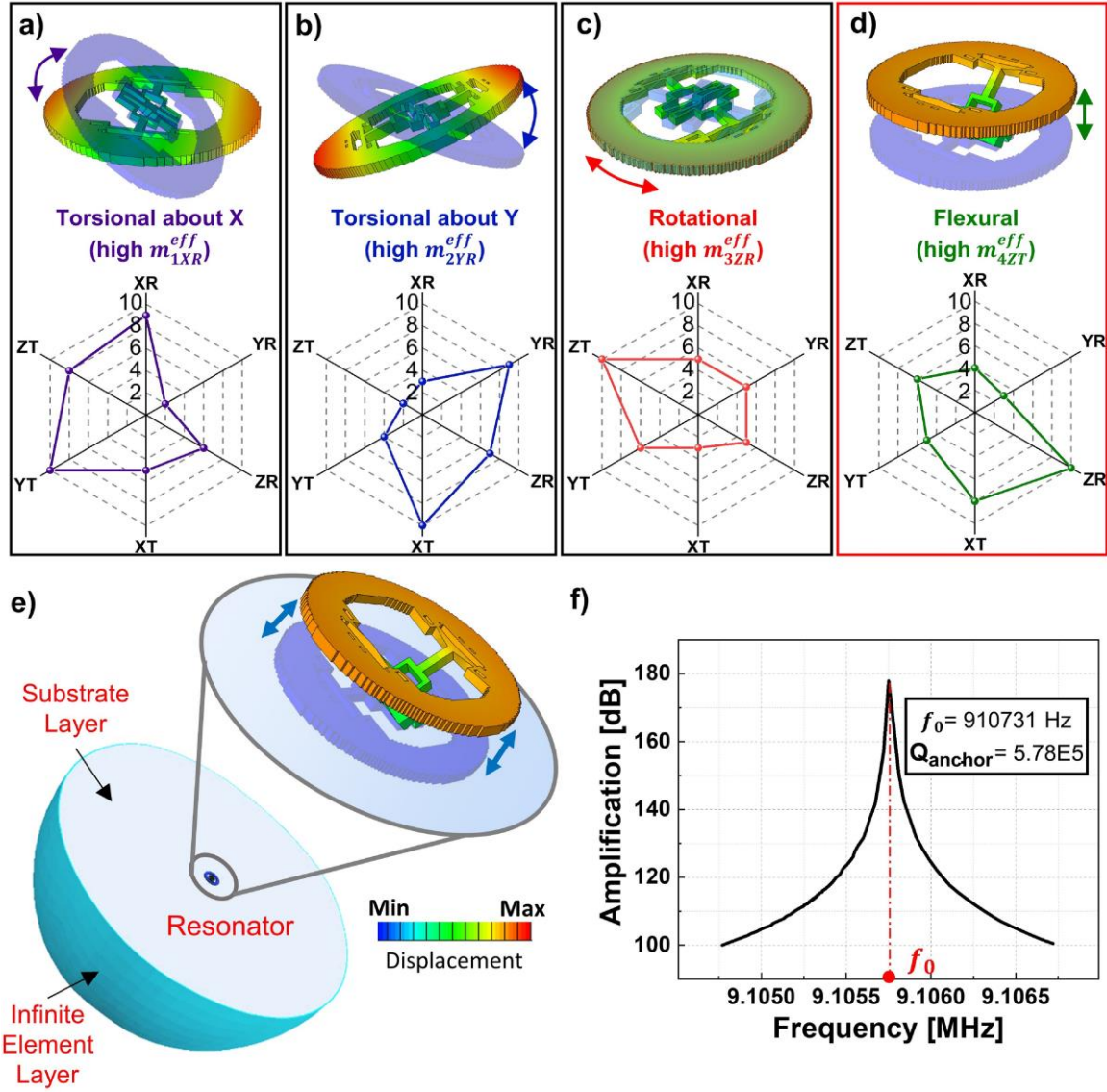


Figure 2.4: Computational methods for mode frequency identification and Q_{anchor} calculation. **(a-d)** The mode shapes (top row) and ranking distribution of directional effective mass components (bottom row) of the disk resonator in its first four modes. The rankings are ascending with the given m_{ij}^{eff} among the 10 earliest appearing modes. **(e)** The schematic of the finite element simulation to estimate the Q_{anchor} , using the infinite element method. Different colors on the resonator structures in a-e represent normalized out-of-plane displacement magnitudes in the mode shapes. **(f)** The frequency-amplitude response of the sample resonator structure.

The computed natural frequency for the flexural mode, ω_{flex} , is then used in the subsequent complex frequency analysis studies, where $0.98 \cdot \omega_{\text{flex}}$ and $1.02 \cdot \omega_{\text{flex}}$ define the lower and upper bound for frequency searching. The $\pm 2\%$ range accounts for the difference in value between damped and undamped natural frequency. As shown in Fig. 2.4e, the bottom surface of the resonator's anchor is attached to a sufficiently large hemispherical substrate (radius = 0.5 mm, 22.7 times larger than that of the resonator structure) in the complex

frequency analysis. The substrate is enclosed by a layer of infinite elements for absorbing the transmitting elastic waves without reflection. With this FEA setup, we can calculate the complex-valued frequency for the flexural mode, ω_{flex}^C , and obtain the Q-factor due to anchor loss, $Q_{\text{anchor}} = \frac{\text{Real}[\omega_{\text{flex}}^C]}{2\text{Imag}[\omega_{\text{flex}}^C]}$, to label each sample. Fig. 2.4f illustrates the frequency response of the representative resonator structure shown in Figs. 2.4a-e, featuring the peak at the damped natural frequency and the corresponding Q_{anchor} value. For the resonator structure in Figs. 2.4a-e, this complex frequency analysis step yields the damped natural frequency and Q_{anchor} as 910,731 Hz and 5.78E5, respectively. These values are consistent with the frequency response shown in Fig. 2f obtained from a steady-state dynamics study.

2.2.4 Dataset description and DL Calculator Interpretation

The region between the anchor stem at the center and the outer annulus structure introduces a vast design space. To provide a sufficient number of training samples, 29,984 unduplicated resonator patterns are created. One of the patterns is shown in Fig. 3a as an example, in which the ratio of void elements versus the total pixel numbers in the design space is defined as “porosity” and labeled to the pattern. To provide a balanced representation of the design space with the dataset, equal numbers of samples are generated around 15 levels of porosity values, which are evenly spaced from 0.2 to 0.9, with 0.05 as the interval. The computation cost for generating each pattern is as low as 1.2 seconds on average thus the proposed pattern configuration generation method is high throughput. Fig. 3b illustrates the relationship between the resonant frequency, porosity and the Q_{anchor} value of samples. As can be observed from the dataset, the dominating trend is that the energy loss increases and the Q_{anchor} value decreases as the resonating frequency increases, which is typical for MEMS resonators^{33–35} and reveals the difficulty in achieving high Q_{anchor} and high frequency simultaneously. All obtained $f \cdot Q_{\text{anchor}}$ products are of the same order of magnitudes, with an average value of $(2.2 \pm 1.0) \times 10^{11}$. The correlations among porosity, frequency and Q-factor are plotted in Figs. 2.5b-d. While as an overall trend, the resonant frequency and Q-factor increases and decreases respectively with increasing porosity, the wide spreads of data (almost ten times different) in these graphs suggest that we cannot oversimplify the dependency of resonator properties on geometric details to one on a single parameter, such as porosity. Therefore, we need to utilize DL to comprehensively learn the geometric details from pixelated images and find more hidden patterns in order to accurately predict these physical properties.

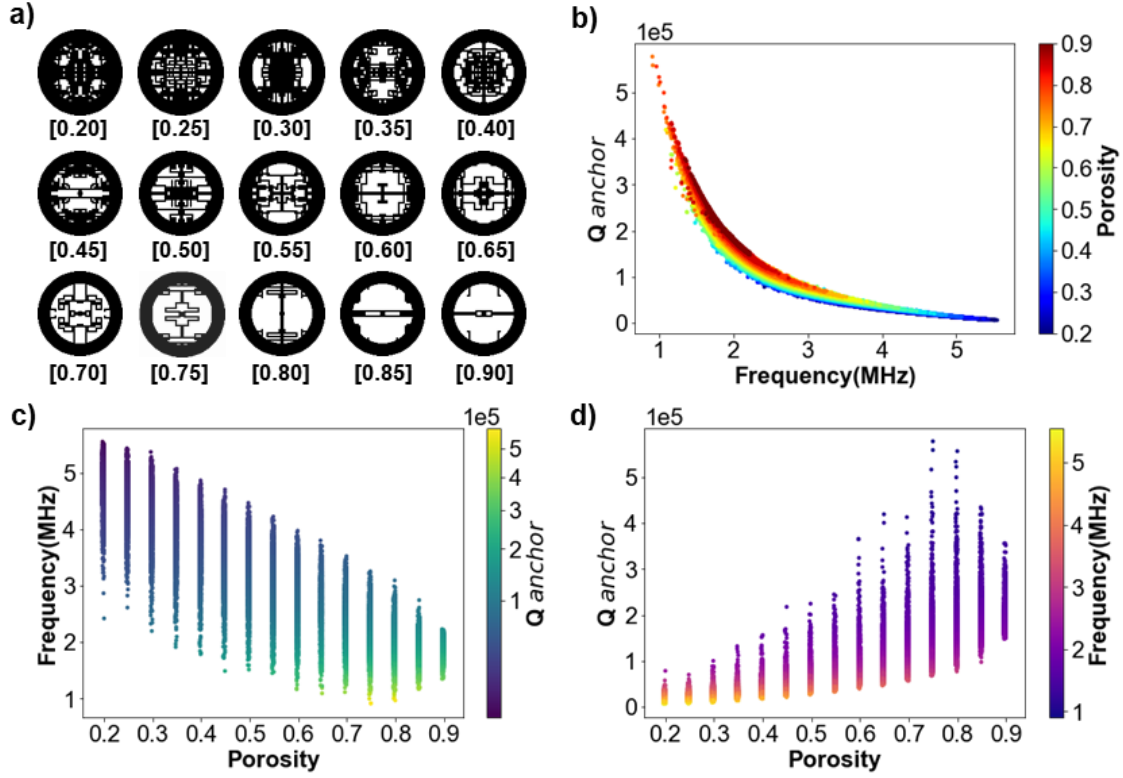


Figure 2.5: Sample configurations and visualized dataset **(a)** Examples of generated resonator patterns with different porosity values. **(b)** Frequency vs porosity plot for 29,984 samples. Color denotes the Q_{anchor} value of each sample. **(c)** Frequency vs porosity plot, where more high-frequency samples are at low porosity and more low-frequency samples are at high porosity. Color denotes the Q_{anchor} Value of each sample. **(d)** Q_{anchor} value vs porosity, where more high Q_{anchor} samples are at high porosity and more low Q_{anchor} samples are at low porosity. Color denotes the Frequency of each sample.

In the data preparation process, ~90% of the dataset (26,985 samples, all with FEA results) are labeled and used as the training set, and the remaining ~10% (2,999 samples) as the testing set. The two DL models for frequency and Q-factor predictions are trained separately using the training set and validated by the testing set. After the training process, both DL models are explained with the t-distributed stochastic neighbor embedding (t-SNE) method, which visualizes the high-dimensional vectors by assigning each data point a location in a two-dimensional map³⁶. If the vectors share similar features, their corresponding locations are close to each other in the low dimensional map. As each resonator pattern image is inputted into each DL calculator and the last layer hidden neuron values are calculated, a high dimensional vector with the size of 2048 is obtained. For the predictions of the DL calculator on the testing set, the corresponding high dimensional vectors are grouped together and visualized through t-SNE in Fig. 2.6 for training (Figs. 2.6a-d) and testing set (Figs. 2.6e-h) respectively. Data points are colored by the original frequency labels (Figs. 2.6a, e), the original porosity labels (Figs. 2.6b, d, f, h) and Q_{anchor} labels (Figs. 2.6c, g). It can be observed that the frequency and Q-factor values of testing samples are smoothly changed from one end of the shape to the other end, indicating

effective training of the DL networks, as testing samples with similar physical properties would indeed be neighboring points at the high dimensional space. The same visualization approach is also applied to the training set samples, where the dominating trend matches well with results from the testing set. In addition, we find that data points colorized by porosity values do not yield a smooth transition in color. This finding agrees with the results in Figs. 2.5b-d and further prove that the physical properties of a resonator would depend on the geometric details, not on just the porosity of the structure.

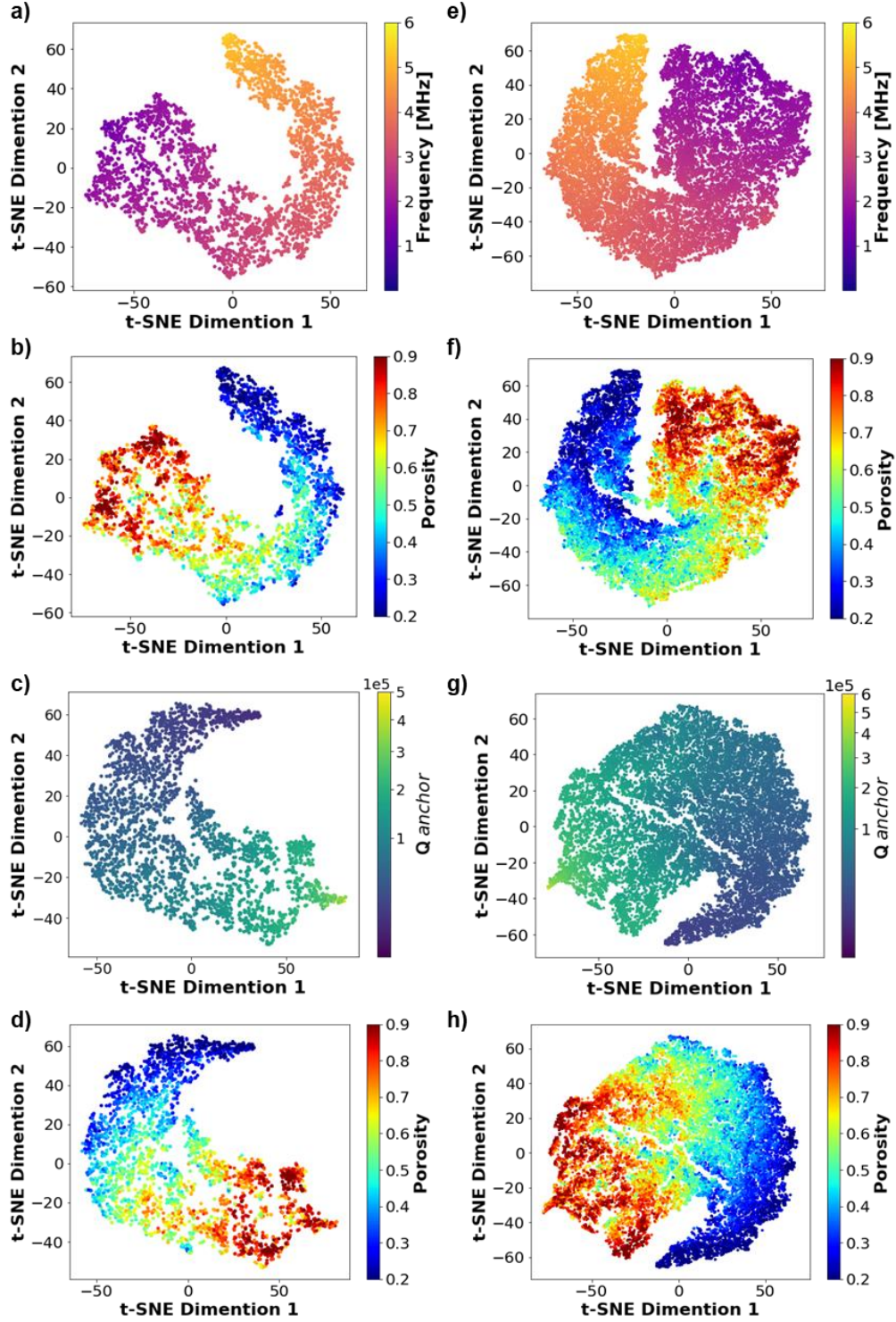


Figure 2.6: Two-dimensional t-SNE analysis of the DL calculators' hidden layer vectors for the (a-d) testing set and (e-h) training set. Data points are colored by (a), (e) the original frequency labels, (b), (d), (f), (h) the original porosity labels and (c), (g) Q_{anchor} labels. (a), (b), (e), (f) are generated via the DL calculator for frequency prediction and (c), (d), (g), (h) are generated via the DL calculator for the Q_{anchor} prediction.

2.2.5 Performance Evaluation of The DL calculator for Regression Accuracy

The regression accuracy of the frequency or Q_{anchor} are evaluated with the following metric for each sample point: $\text{Accuracy} = 1 - \left| \frac{y_i - \hat{y}_i}{y_i} \right|$, where y_i is the actual label value of sample i and $\hat{y}_i$ is the predicted value. Figures 2.7a-b show the comparison between DL predictions and FEA simulations for frequency and Q_{anchor} , respectively. The highest average accuracies of the testing set are $98.8 \pm 1.6 \%$ and $96.8 \pm 3.1 \%$ for the frequency and Q_{anchor} regression, where the whole dataset with 29,984 samples participated in the training and testing process. The model is trained by the stochastic gradient descent optimizer with an initial learning rate of 0.1 and momentum of 0.9. The learning rate is scheduled to multiply 0.1 for every 70 epochs, and the whole training process takes 230 epochs. The learning curves for this experiment in Figs. 2.8a, b show the L1 loss versus training epochs, and both training and testing curves converge in the end.

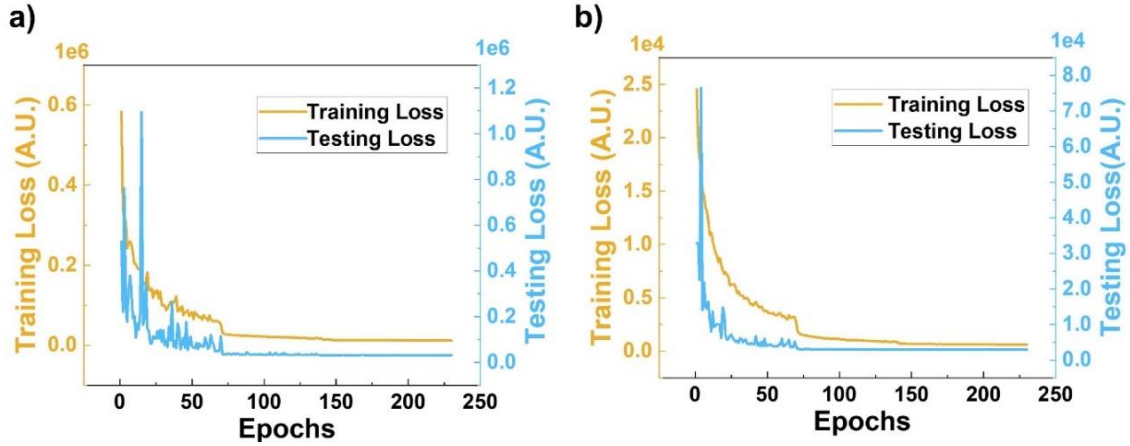


Figure 2.7: The L1 training loss and testing loss during the 230-epoch training process. For (a) the frequency DL calculator, and (b) the Q_{anchor} ML calculator.

Figures 2.8c, d illustrate the sample distribution of data in DL and FEA testing set, for the frequency and Q_{anchor} , respectively. For both cases, the DL and FEA distributions show good alignment. The frequency distribution is basically a right-skewed distribution that with peak density at around 2 MHz and nearly evenly distributed from 2.5 to 4.8 MHz. It is interesting to note that Q_{anchor} also has a right-skewed distribution but it has high kurtosis, which means the majority of geometries provide low Q_{anchor} values. In Figs. 2.7e-f, the regression accuracy is plotted with the number of samples in the dataset for frequency and Q_{anchor} , respectively. The result indicates that with the increasing number of sample numbers, the accuracy increases and the standard deviation decreases. When the sample amount reaches 10,000, the performance enhancement with increasing sample numbers becomes less obvious. Given that for both frequency and Q_{anchor} , the average testing accuracy surpasses 95% with 29,984 samples, we consider at this point, the sample amount is sufficient.

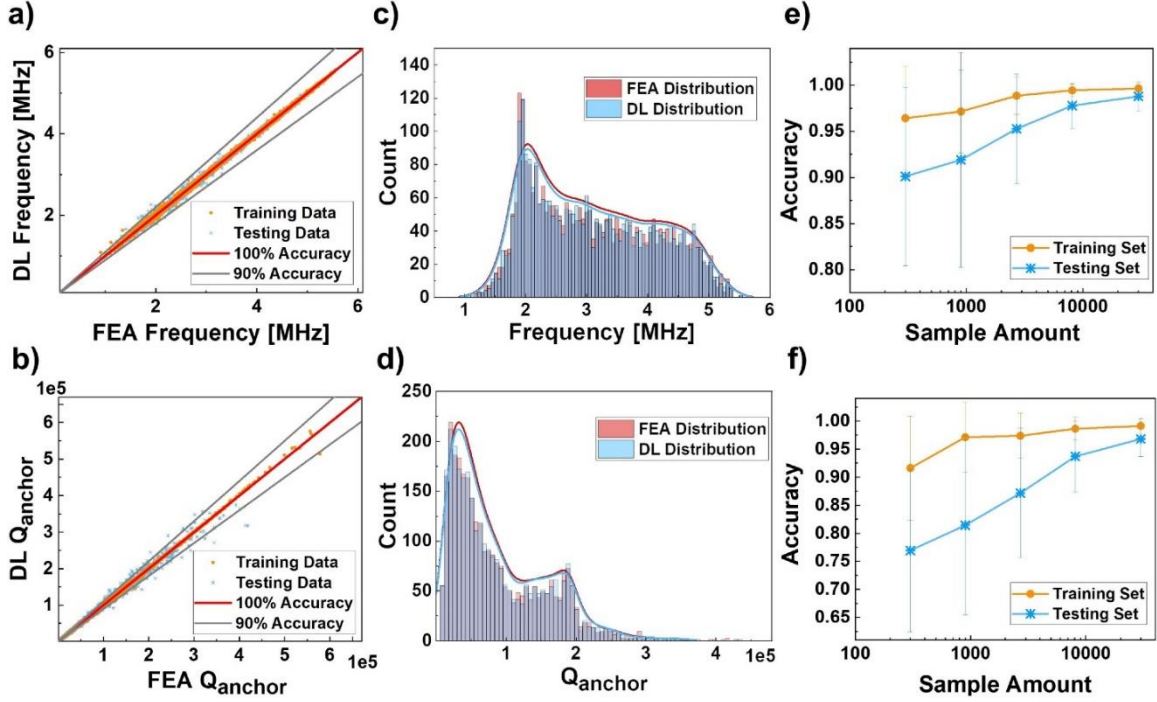


Figure 2.8: The DL regression performance evaluation for resonant frequency (top row) and Q_{anchor} (bottom row) of the DL calculators. **(a), (b)**, The comparison between DL predictions and the FEA simulation for **(a)** frequency and **(b)** Q_{anchor} . **(c), (d)**, The distribution of data in DL and FEA for the testing set in **(c)** frequency and **(d)** Q_{anchor} . **(e), (f)**, Learning accuracy vs number of samples in the dataset for **(e)** frequency and **(f)** Q_{anchor} studies. Error bars denote standard deviations.

2.2.6 Ranking performance and Computation Cost Evaluation of The DL Calculators

Since high Q_{anchor} structures with low energy losses are preferred in resonator designs, the performance of DL calculators for the ranking problem is further evaluated based on Q_{anchor} values. The DL calculators can recognize whether one design is superior to the other, and the evaluation metric is the ranking accuracy (RA), which is expressed as:

$$RA = \frac{\#\{(i,j) | (x_i - x_j)(i-j) > 0, 1 \leq i, j \leq n\}}{n(n-1)/2} \quad (1)$$

where n is the number of selected samples for ranking. The samples are sorted with their FEA rankings and the corresponding DL predicted ranking of samples forms the sequence $X = \langle x_1, x_2, \dots, x_n \rangle$. Each correct predicted pair of unique elements x_i and x_j at the i^{th} and j^{th} position of sequence X should satisfy $(x_i - x_j)(i-j) > 0$. The total number of possible combinations is $n(n-1)/2$. The proportion for the correctly predicted pairs over all of the possible pairs is defined as the ranking accuracy RA, quantifying the performance in the ranking problems. The ranking performance is evaluated based on the results of the testing data set and the overall RA value is 0.9844 as shown in Fig. 2.9a. For the top 10% samples in Fig. 2.9b, the RA value is 0.8983. The specific structures of the top 8 ranked samples are shown in Fig. 2.9c, which is within the top 0.3% the entire dataset and the RA still has

a decent value of 0.8214. The RA value decreases at the high Q_{anchor} range due to the aforementioned right-skewed Q_{anchor} distribution. With a small amount of training samples, the DL prediction is less precise. However, even for the extreme conditions such as the top sample rankings, the predicted position of the No.1 and No.8 patterns match very well with the original sequence. As such, while the exact sequence is off, the method can distinguish the top 0.3% of data from the rest since the two critical boundary values are correct. Besides the overall Q_{anchor} ranking, another important metric is to measure the RA for top designs at the specific frequency of interest. Top 8 Q_{anchor} design samples at 7 equally distributed frequencies checkpoints between 2.0-5.0 MHz are selected for a case study. As illustrated in Fig. 2.10, the highest RA in the checkpoints is 0.9643 at 2.0 MHz, where the frequency is near the maximum count density region as shown in Fig.4c. Therefore, increasing the sample amount would be a promising approach to enhance the ranking performance at other frequencies.

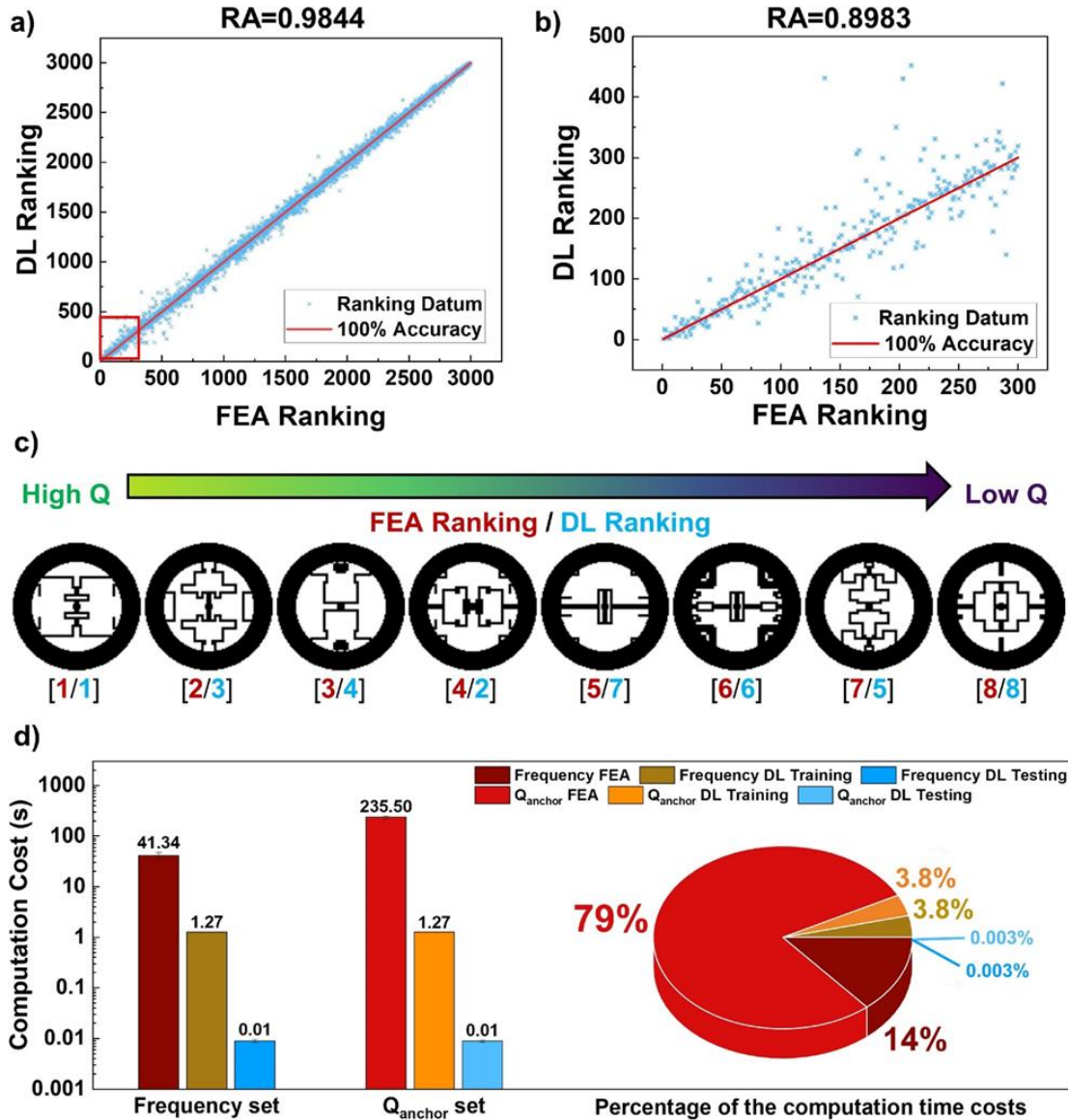


Figure 2.9: Ranking performance and computation cost. **(a)** Comparison of ranking obtained from the DL model and FEA simulation for the entire testing data set. The red box features the top 10% of data in ranking. **(b)** Magnified view of the boxed region in a. **(c)** Patterns of the top eight designs based on high Q_{anchor} values in the testing data set as calculated by the DL model. The numbers in the bottom square brackets are: FEA Ranking/DL Ranking. **(d)** The histogram shows the computation time costs in terms of seconds of the FEA simulation, the DL Training process, and the DL testing process for frequency and Q_{anchor} respectively. The pie chart shows the percentage of the computation time costs by the FEA simulation, DL training, and DL testing processes to analyze the frequency and Q_{anchor} of the MEMS disk resonators for the testing data.

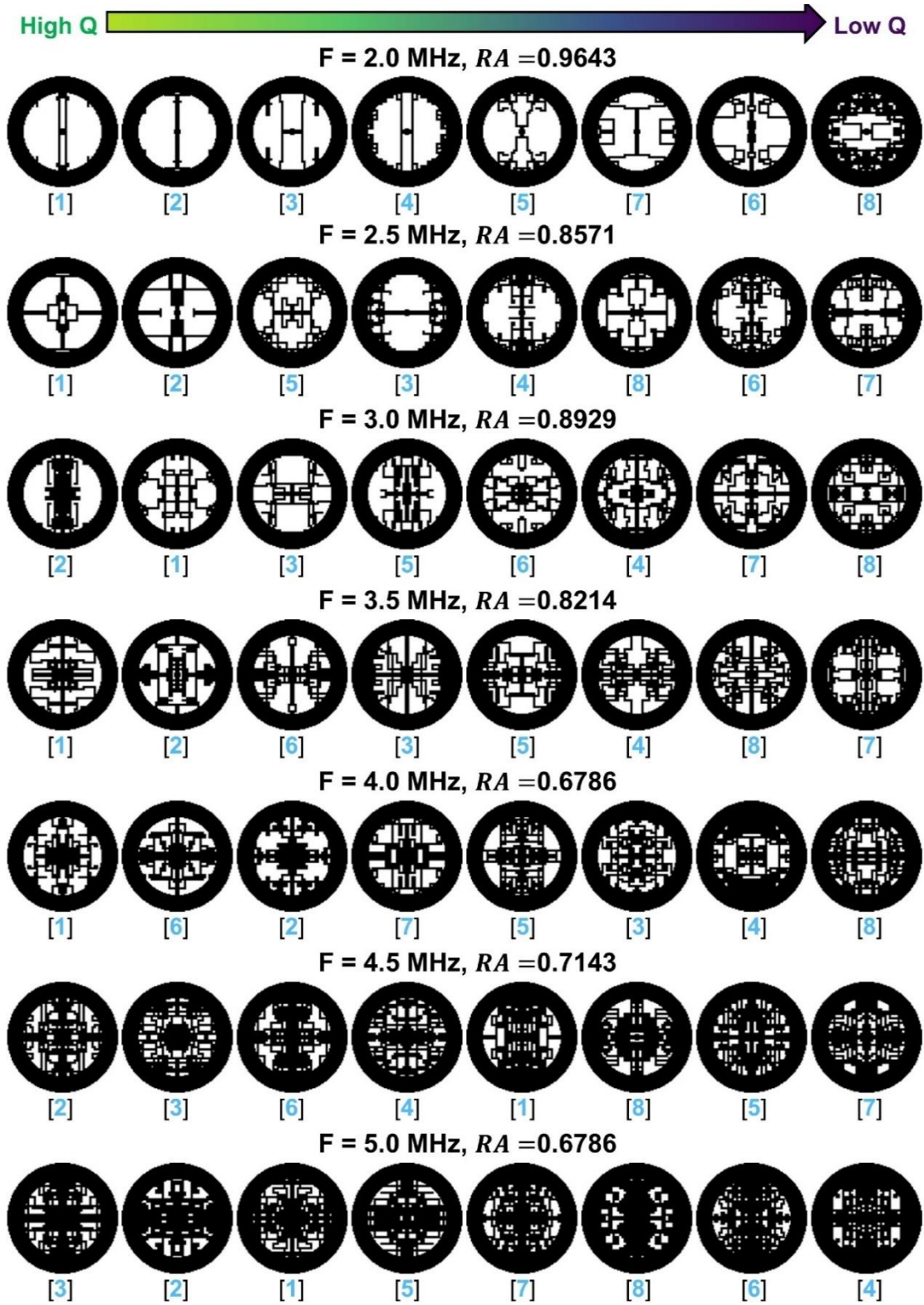


Figure 2.10: Top eight design patterns based on high Q_{anchor} values at specific frequencies, as calculated by the FEA simulation. From left to right, patterns are sequentially demonstrated according to the descending order of Q_{anchor} factors. F is the flexural mode resonating frequency of the design. The RA is the ranking accuracy by comparing the DL

model predicted sequence order and the FEA sequence order. The numbers below the patterns are the relative sequence for rankings, as calculated by the DL model.

In this work, the computation cost of DL calculator is largely reduced by leveraging the Tesla K80 GPU. As illustrated in Fig. 2.9d, the averaged single sample computation cost of the DL calculator is compared against that of the FEA simulation. The FEA simulation will cost 41.3 ± 6.2 seconds and 235.5 ± 14.1 seconds to get results for the resonant frequency and Q_{anchor} , respectively. On the other hand, the training or the testing process of the DL calculator doesn't make a significant difference in the computation cost among different tasks. The training (back propagation) costs are 1.27 ± 0.013 seconds and 1.26 ± 0.008 seconds to get results for the resonant frequency and Q_{anchor} . After the training process is complete, the testing (forward calculation) costs are $8.9 \pm 0.67 \times 10^{-3}$ seconds and $8.9 \pm 0.48 \times 10^{-3}$ seconds to get results for the resonant frequency and Q_{anchor} . These results indicate that DL calculators can execute the forward calculations 4.6×10^3 times faster than those of FEA simulations to obtain resonant frequency results and 2.6×10^4 times faster than those of FEM simulations to obtain Q_{anchor} results. The pie chart summarizes and compares the total computation cost of the FEA simulation, DL training, and DL testing processes for the testing data set. It should be noted here that different from the testing cost and the FEA simulation cost, the total training cost is based on training samples instead of testing samples. The result suggests that FEA simulations (resonant frequency and Q_{anchor}) take as high as 93% of the total computation cost compared to those of 7% from DL calculators. Therefore, with the current data arrangements, 93% of computation cost with FEA can be saved by using the DL calculators for the design analysis.

2.2.7 Summary

In this study, we provide a systematical approach to rapidly predict the vibration frequency and anchor loss of the non-parameterized disk shape resonators. The progress is driven both by the advent of the MEMS/NEMS big data and by the integration of the deep learning techniques. The design big data of the resonator configurations are generated with the high-throughput Brownian motion algorithm and labeled with FEA simulations. The geometric information of the resonator structures is expressed as finite elements and represented by the 2D binary matrices, which serve as the sample inputs of DL model. By training the DL algorithms with a sufficient amount of labeled samples, the algorithm is able to extrapolate the correct relationship between different geometries and the resulting physical properties. Likewise, the ranking information of the unseen geometries for a certain desired physical property (high Q_{anchor}) can also be accurately predicted by DL methods. Compared with the traditional FEA simulation methods, the DL calculator operates order of magnitude faster and can reduce a significant amount of total computation cost.

2.3 Data-driven Freeform MEMS Energy Harvester Design Enabled by Deep Learning

2.3.1 Introduction

As one promising solution to the power distributed electrical devices, MEMS energy harvesters that convert ambient kinetic or elastic energy into electricity have attracted substantial attention from both academia and industry in the past two decades³⁷. Among various approaches to realize mechanical energy harvesters, the piezoelectric mechanism has shown advantages in high power density, ease of implementation, and good compatibility with the micromachining processes^{38,39}. However, piezoelectric energy harvesters (PEHs) need to operate under broad operational frequency bandwidths for high power outputs around their resonant frequencies. To tackle this problem, approaches such as multi-mode harvesters have been widely explored but it is rather difficult to design highly efficient PEHs due to their very complex geometries^{38–40}.

Recently, machine learning for structural designs has made good progresses in interdisciplinary fields such as the MEMS resonator design that has been demonstrated in section 2.2. The basic idea is to encode the structural information into pixelated 2D black-and-white images; assign them with specific properties; and send thousands of the labeled binary files to train in a neural network. This results in the identification of the concerned properties of similar designs to lead to the optimal designs in the design space. In this section, we have further developed an experience free method to generate freeform PEH designs, which are represented by pixelated images at first, and then translated to COMSOL through MATLAB. The first two natural frequencies of the PEH structure, namely f_1, f_2 , and the mean harvested open-circuit output voltage between f_1 and f_2 are calculated by COMSOL. Labeled with these properties, pixelated images are sent to train the neural network framework. PEHs from 200,000 unlabeled freeform designs are analyzed to obtain the optimal geometry. As one example, the optimal designs around the frequency of 165 Hz are identified to have about 12.9% larger operational frequency bandwidth, 3.4% higher output voltage as compared with those of designs based on 5,000 freeform inputs. These results show the great potential for the design of complex PEHs by DL-aided methods and the same methodology could be applied to a wide range of MEMS device designs.

2.3.2 System Architecture

Fig. 2.11 illustrates the proposed system framework, where 100*100 pixelated images are generated through an edge-growing algorithm¹⁰, with some refinements in this work to avoid interspace. Each pixel represents a solid element with size of 30 μ m*30 μ m in Fig. 2.11a. The four black-colored areas represent the four proof masses and each proof mass has a white-color cross inside representing the connection spots. The four connection spots, along with the other two at the corners, are connected by a certain algorithm to form the spring structures.

A final design schematic is shown in the left side of the COMSOL model in Fig. 2.11b. The silicon proof mass has a height of 400 μ m while the connecting beams consist of an

aluminum nitride layer of $0.5\ \mu\text{m}$ and a silicon substrate of $10\ \mu\text{m}$, with a width of $150\ \mu\text{m}$. The connecting spots at the corners are chosen as two fixed boundaries. The bottom electrodes attaching to the five AlN layers are set as ground and the top electrodes are set as five electrically separated terminals to avoid the voltage cancelation effects³⁹. The average output of the five open-circuit voltages from the terminals due to the mechanical deformation of the PEHs is the electrical output of the system, namely harvested open-circuit voltage. As an example, in Fig. 2.11b, the eigenfrequency simulation is first conducted, and the first two natural frequencies f_1 and f_2 are found. Then the device is excited with the acceleration of $0.25\ \text{g}$ under an isotropic damping ratio of 0.02 , at ten frequencies equally spaced between $f_1 - \delta$ and $f_2 + \delta$, where $\delta = (f_1 - f_2)/7$. The harvested open-circuit voltage versus frequency plot is shown in the right side of Figure 1b and the mean harvested open circuit voltage $\bar{V}$ of the 10 data points along with f_1 and f_2 are plotted as illustrated in Fig. 2.11a.

The above modeling & simulation process is common in the COMSOL operations, and the main contribution of this work is the automated process to generate the three labels from a pixelated image through the COMSOL LiveLink with MATLAB. Thousands of freeform pixelated images like Figure 1a are inputted in MATLAB and models are built for the simulations to create the labeled dataset for the Resnet function⁴¹ in Fig. 2.11c. A high-speed analyzer to identify the f_1 , f_2 and $\bar{V}$ values are formed similar to section 2.2, and the process is more than 30,000 times faster than those of the FEM simulation results. Afterward, 200,000 big-data candidates are randomly generated and evaluated by the proposed DL analyzer in Fig. 2.11d and the top 30 candidates working around 165 Hz with the largest frequency bandwidth and highest mean harvested voltage are selected and verified by the FEM to identify superior designs with high performances.

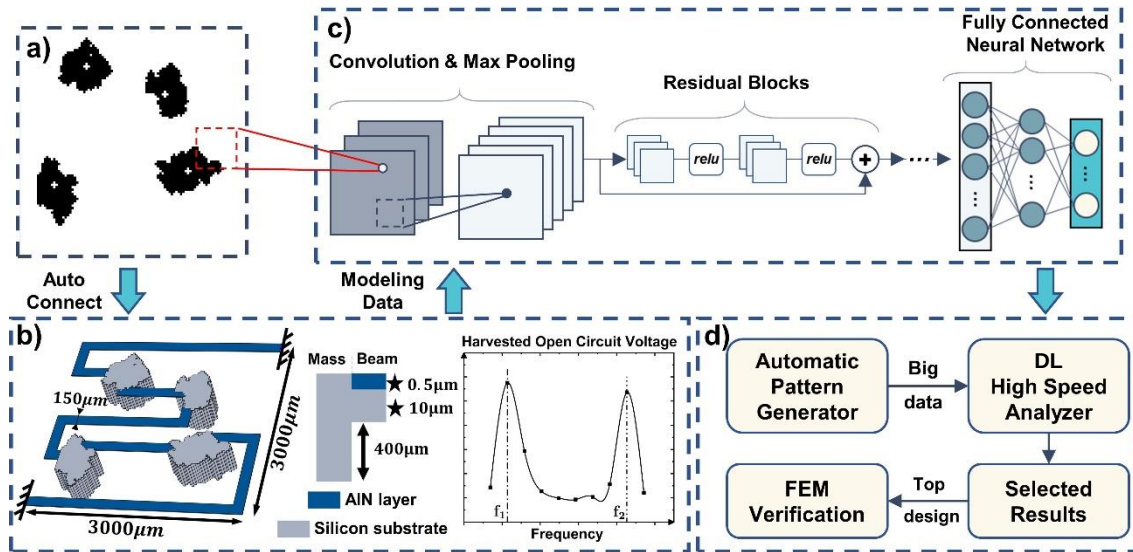


Figure 2.11: (a) Automatically generated energy harvester designs represented by pixelated images. (b) FEM modeling and analysis: grey-color areas represent silicon proof masses and blue-color beams are connecting springs. (c) The schematic diagram for the deep residual neural network. (d) The resulting neural network process flow chart.

2.3.3 Speed, Accuracy and Experiment Matching of the DL Analyzer

The resulting neural network framework is a high speed and high accuracy analyzer when dealing with similar potato-shape designs generated via the edge-growing algorithm. The trained analyzer can figure out the three properties from a pixelated image within around 8 ms per design, while the FEM by COMSOL takes up 3 to 5 minutes each. Fig. 2.12 shows that if sufficient training samples are provided, the proposed scheme can reach remarkable accuracy for testing samples: over 99.2% for f_1 & f_2 and 94.1% for $\bar{V}$, as compared with those of the FEM results.

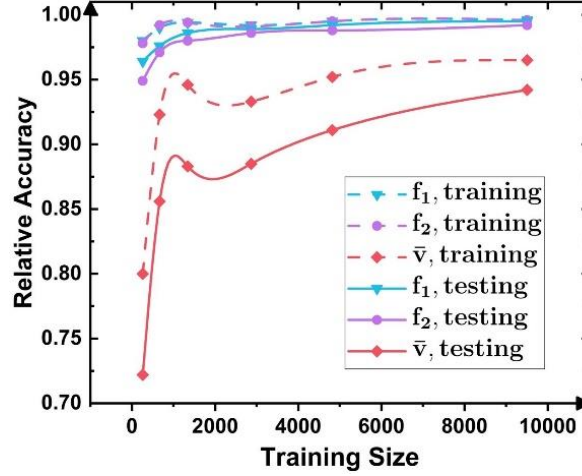


Figure 2.12: The relative training and testing accuracy of the band frequencies and average output voltage versus training data size.

After sufficient training practices, the neural network framework can learn the function between the images and the labels to match the FEM results. However, it is often difficult to match results between FEM and experiments⁴². To validate the proposed DL scheme, MEMS energy harvesters in Ref. 39 have been studied with the parametric properties in Fig. 2.13a. New sets of parameters are randomly generated but deliberately leave out the exact set and encoded into pixelated images. Following the proposed scheme, we translate the images into the COMSOL model, get desired properties in Fig. 2.13b, and develop another DL analyzer to deal with the parametric design in Fig. 2.13a. Table 2.1 compares the DL prediction with the FEM simulation and experimental results. The simulated natural frequencies are very close to the resonant frequencies from experiment data. The relative value of $\bar{V}$ is also in good consistency.

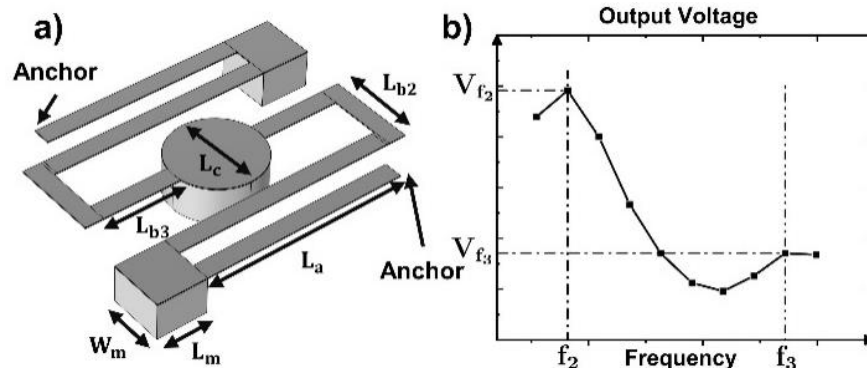


Figure 2.13: (a) Geometry configuration of the fabricated harvester in Ref. 39. **(b)** Output voltage vs frequency predicted by trained DL model.

Table 2.1 Comparison between experimental³⁹, FEM and DL results.

Properties	Experiment Results ³⁹	FEM Results	DL Predictions
f_2 (Hz)	261.8	259.1	258.6
V_{f_2}/V_{f_3}	2.088	2.178	1.931

2.3.4 Exploring the Performance Boundary with Big Data

Fig. 2.14 shows the results of the sample properties distribution from FEM (a and b) and DL candidates (c and d). Here, each point represents a certain design, while $\Delta \mathbf{f} = \mathbf{f}_2 - \mathbf{f}_1$ is the operational bandwidth, and $\bar{f} = (\mathbf{f}_2 + \mathbf{f}_1)/2$ is used as the mean operational frequency. As can be seen from Figs. 2.14a-d, $\bar{f}$ has in the positive correlation with $\Delta \mathbf{f}$ and negative correlation with the volume of the device, while both $\Delta \mathbf{f}$ and $\bar{f}$ as well as $\Delta \mathbf{f}$ and $\bar{V}$ have the negative correlation. These correlations validate the correctness of our DL-based big data design method since they are obvious conclusions.

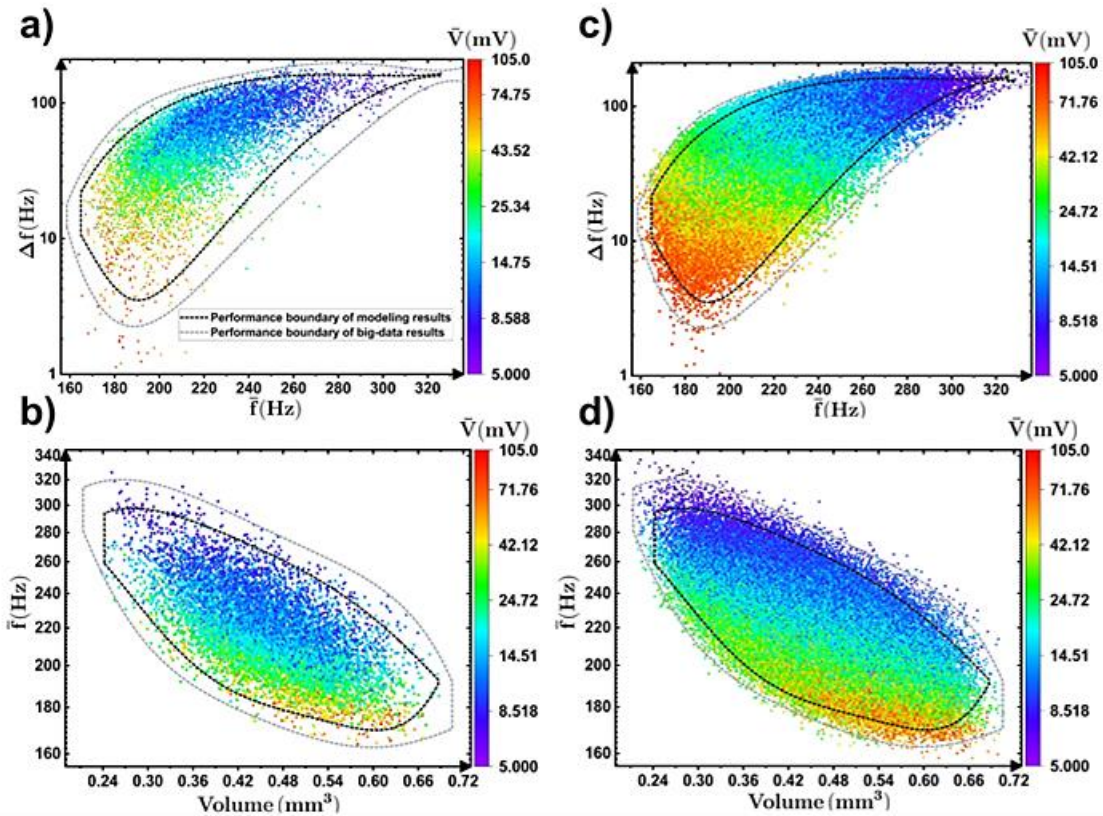


Figure 2.14: (a) Geometry configuration of the fabricated harvester in Ref. 39. **(b)** Output voltage vs frequency predicted by trained DL model.

As can be shown by the performance boundary (the dashed lines) in Fig. 2.14, it is difficult for a broad-operational-bandwidth PEH design to simultaneously have a high $\bar{V}$ and a low $\bar{f}$. However, the performance boundary can be extended by simply generating more designs and evaluating them with our high-speed DL analyzer. Here, designs with $\bar{f}$ in **160~170Hz** with both broad Δf and high $\bar{V}$ are selected for comparison. Figure 2.15a shows that 200,000 ML results can provide a larger population of superior designs than those of the 9,700 FEM results. The best designs are further compared in Fig. 2.15b, where the best ML design shows 12.9% broader operational bandwidth and 3.4% higher harvested voltage than those of FEM results. The properties of superior DL designs have been validated by FEM here.

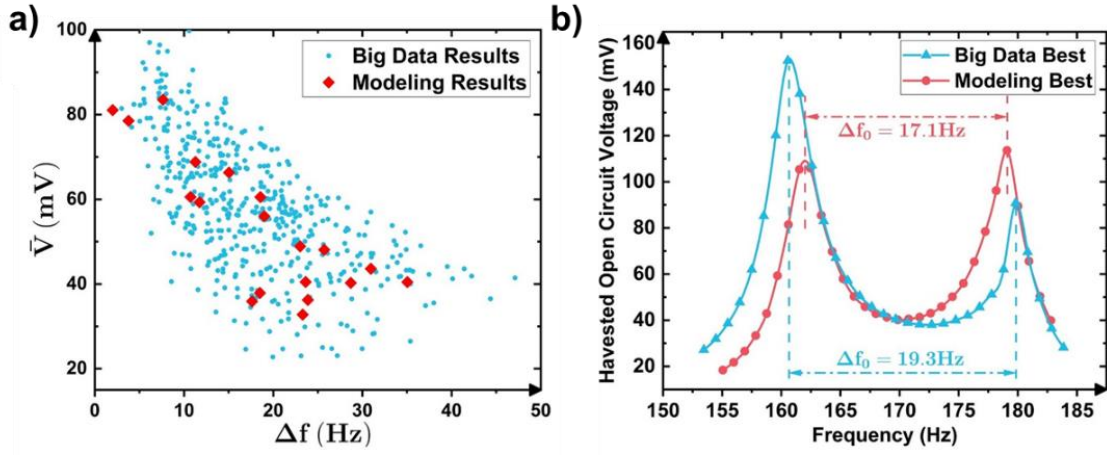


Figure 2.15: Top ranking designs with $\bar{f}$ in 160~170 Hz, **(a)** mean output voltage versus frequency bandwidth for DL (blue dots) and FEM modeling results (red dots), **(b)** the best results of DL (blue) and FEM (red) designs in the voltage vs. frequency plot.

2.3.5 Summary

The study case in this subsection reports on the implementation of the DL scheme for the design of freeform piezoelectric energy harvesters. New algorithms have been developed in this work to generate pixelated images and translate them into multi-layer MEMS models via COMSOL and MATLAB. We further deploy the trained neural network to explore the performance boundaries of PEH designs to achieve superior performances among the variations of complex non-parametric geometries. The proposed DL analyzer not only showed high-throughput screening capabilities for performance prediction, but also successfully identified the optimal design configurations that wasn't included in the initial dataset. These critical features of proposed method indicate the potential for its application in the big-data MEMS design process.

2.4 Conclusions of Chapter 2

In this study, we applied deep learning based surrogate models to calculate the physical properties of MEMS structures effectively and accurately. The geometries of numerous candidate designs were represented by pixelated binary images, which are then labeled by numerical simulation results and used in the training of neural networks. With sufficient training, the networks can learn the hidden patterns in the vast amount of candidate

geometries and calculate the physical properties (including the resonant frequency and quality factor of disk-shaped micro resonators, the resonant frequency bandwidth and output voltage of PEH) quickly and accurately. The networks can also be used to rank thousands of candidate geometries based on a certain quantity of interest, or screen over unlabeled big-data samples in order to guide researchers towards the good designs.

On the other hand, a few challenges and future opportunities exist in the non-parameterized MEMS structure design field. The present method only deals with the geometry information, which is not enough for the simulation of a common MEMS design. The validations of FEM results with experimental data in the absolute values could provide better evidence for the proposed method. Another future endeavor is to combine the DL calculator with a DL designer, such that the calculation results could directly influence the generation strategies of new candidate geometries towards a design goal. We'll also try to incorporate multilayer structural features in MEMS in our neural networks to apply our data-driven approach to even more complex devices.

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Chapter 3: The Pulse Signal Diagnosis Based on Piezoelectret Sensor and Intelligent Signal Diagnosis System

3.1 Introduction

The wrist pulse signal is a convenient and non-invasive parameter for personal health monitoring^{1,2} with rich and critical information to reflect the state of human health³⁻⁴. For thousands of years, the traditional Chinese pulse diagnosis (TCPD) or Traditional Indian Ayurveda pulse diagnosis (TIAPD) has been a central part of the traditional Chinese medicine (TCM) and other related oriental medicine systems⁵⁻¹⁰. As demonstrated in Fig. 3.1 a, TCM practitioners would place three fingers above the radial artery, with the middle position over the end of radius bone. The specific three positions are named Cun, Guan and Chi respectively. The radial artery is close to skin at these positions, which are considered as good palpation positions. TCM practitioners would be able to adaptively manifest the blood flow fluctuation as the pulse is originated from cardiac contraction and relaxation⁸. Other parameters such as the elasticity and thickness of vessel walls, the composition of blood and the conditions of skin will also influence the fluctuations, and these parameters are usually connected with different health conditions¹¹. However, the differences between the basic types are not clearly defined, and the insufficient clinical training of TCM practitioners of inadequate pertinent literatures can lead to the inconsistent diagnosis results¹²⁻¹⁴.

To overcome these issues, artery pulse wave signals have been studied since the 19th century when the sphygmometer (Figure 3.1 b) was modified to provide graphical records¹⁵ to study the force, regularity, and rhythm of arterial pulse in the form of a wave instead of an impact (heartbeat)¹⁶. With today's technological advancements, the concept of mobile health is going to play an important role in the public health. As shown in Fig. 3.1c, by combining the state-of-art wearable devices and the mobile signal analysis, the continuous and real-time monitoring of health conditions has become accessible for individuals. For the next-generation wrist pulse monitoring, the pulse acquisition device is expected to be thinner, flexible and more conformal. The latest artificial intelligence techniques would be a promising technique to process the significant amount of generated data in this emerging field.

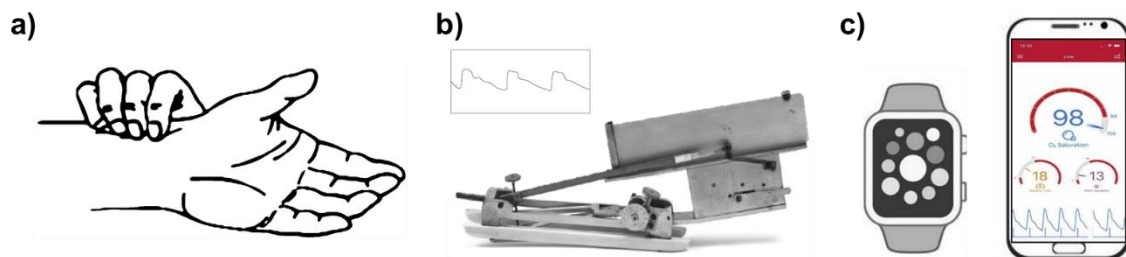


Figure 3.1: The evolution of wrist pulse diagnosis. **(a)** The TCM Pulse taking process¹⁷. **(b)** The sphygmograph to record the pulse wave¹⁵. **(c)** The mobile health with wearable wristbands¹⁸.

Various non-invasive wrist pulse sensing techniques have been reported. In commercial products, there are four types of sensing mechanisms, including the electrocardiographic (Fig. 3.2a), photoplethysmography (Fig. 3.2b), impedance-plethysmography (Fig. 3.2c) and ballistocardiographic measurements (Fig. 3.2d)². The electrocardiographic method measures the action potentials of the cardiac muscle, but the unipolar measurement from a single position is not possible due to its differential nature, such that it is not suitable for the continuous monitoring. The plethysmographic methods measure the blood volume change in the vessel but the plethysmographic methods will have diminished signals with higher applied pressure in pulse taking as shown in Fig. 3.3^{19,20}. Given that applying the conformal pressure has been considered necessary for a better skin contact during measurements^{21–23}, the ballistocardiographic method which measures the displacement or contact force of the local skin is a better analogy to TCPD, and is the preferable approach in this research.

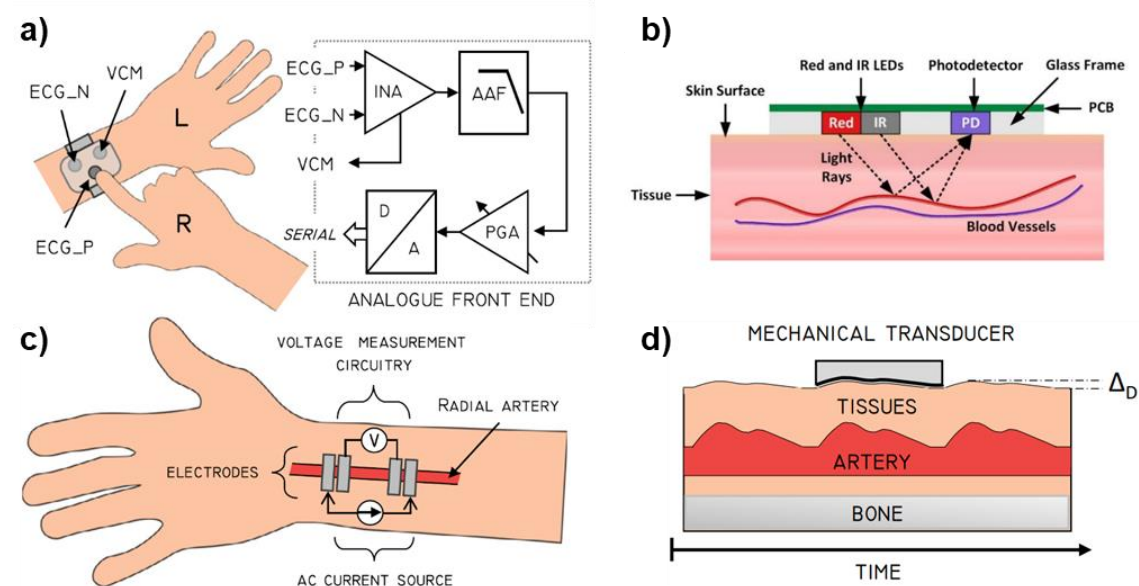


Figure 3.2: The schematics for basic types for non-invasive wrist pulse monitoring^{2,24}. **(a)** The dual-wrist ECG and the analog signal processing. **(b)** The basic components of photoplethysmography method, which is composed of light emitter and the photodetector. **(c)** The impedance plethysmography measurement as the impedance between electrodes varies with the changing blood volume. **(d)** The ballistocardiographic pulse signal acquisition which directly measures the displacement or contact force of the local skin.

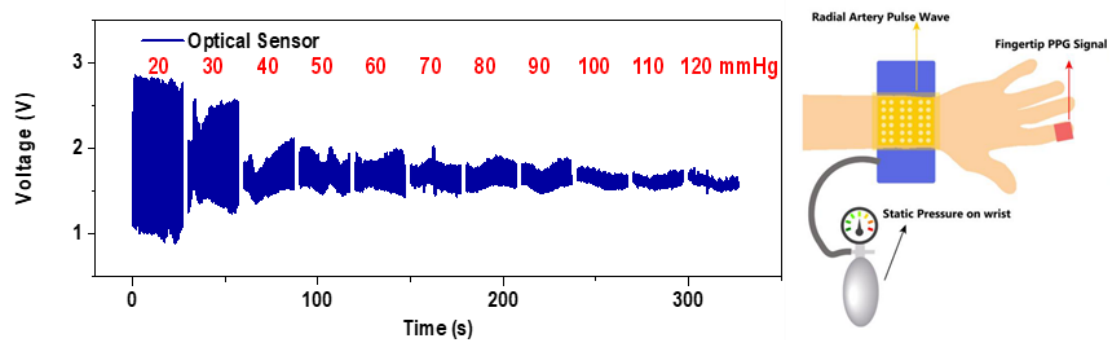


Figure 3.3: Recorded pulse signals of a volunteer by a commercial optical sensor between 20-120 mmHg (left) and the experimental setup for photoplethysmography (PPG) measurements under applied pressure (right)²⁰.

For ballistocardiographic methods, flexible pressure sensors have the good characteristics of high sensitivity, fast response time, low detection limit, outstanding durability, and simple fabrication²⁵. There are three basic types of sensing mechanisms for pressure sensors: including the piezoresistive^{26–33} (Fig. 3.4a), piezocapacitive^{34–41} (Fig. 3.4b), and piezoelectric^{42–49} (Fig. 3.4c) sensors. The piezoresistive effect-based sensors change their resistances due to the changing resistance of conductive fillers inside. The piezocapacitive sensors are based on the principle of parallel plate capacitor, as the capacitance is inversely proportional to the distance between plates. The piezoelectric sensors are based on the movement of the electric dipoles, resulting the potential changes on the electrodes. Among the aforementioned techniques, the piezoelectricity is a self-powered method, and easier to be miniaturized as well as integrated into complex shapes/structures⁵⁰. The piezoelectret material, on the other hand, is a special type of system that exhibits piezoelectricity. As shown in Fig. 3.4d, the piezoelectrets are pieces of dielectric materials, mostly made of polymer films, which have quasi-permanent electric charge, or ‘quasi-dipoles’, distributed on their surfaces or inner air bubbles’ surfaces. The piezoelectrets can perform the piezoelectricity effect while their polymer base can be very thin, flexible, and biocompatible⁵¹. As such, the piezoelectrets are selected as the basic sensing unit for this study.

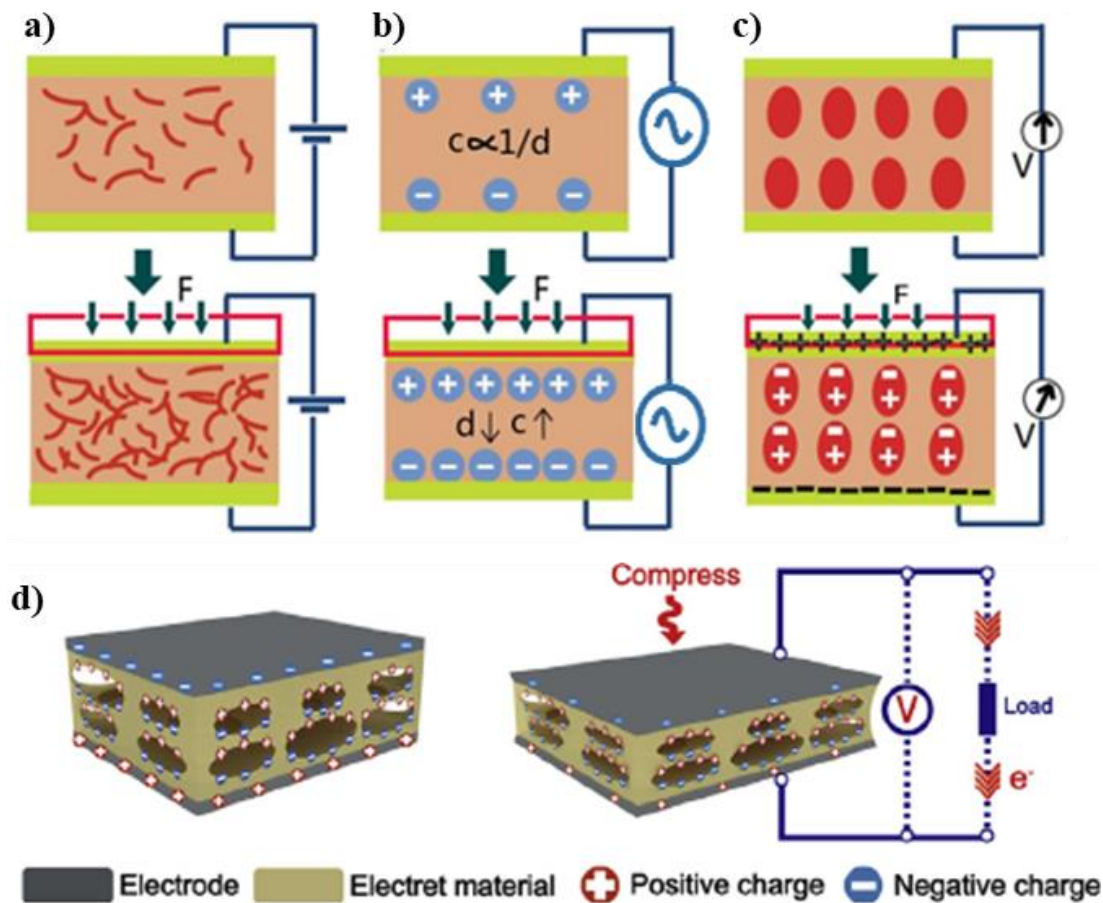


Figure 3.4: Basic types of ballistocardiographic pulse signal acquisition mechanisms^{50,51}. **(a)** The piezoresistive sensor **(b)** the piezocapacitive sensor **(c)** the piezoelectric sensor **(d)** the piezoelectret sensor.

The signal output of the piezoelectrets is of analog type and the quality of sampled signals usually suffers from the inference factors such as measurement noises and body

motions⁵². Therefore, it is important to detect and eliminate these inferences through the modern computational pulse analysis, whose key component includes the data preprocessing, feature extraction and intelligent classification algorithms. Typical pulse data preprocessing solutions to resolve this problem are the curve fitting⁵³, morphology filter⁵⁴, finite impulse response⁵⁵ and wavelet transform⁵². The wavelet-based methods are the most commonly applied techniques^{52,56–59}. The direct analysis of raw pulse data would require a larger amount of computational resources and cause the classification algorithm to overfit and lose generalization capabilities¹¹. As such, a number of pulse feature extraction techniques have been applied to the recognition and classification of pulse waveforms. Usually, the feature extraction techniques can be distinguished by frequency domain methods^{60–63}, time domain methods^{11,64–66}, and nonlinear processing methods^{67–70}. A key task is the classification and diagnosis algorithm to find the effective features and provide the interpretation between the health conditions and features. Machine Learning (ML) algorithms have gained popularity to be trained as classifiers for the diagnostic purpose. Many different classification methods have been adopted, including the nearest neighbor classifier⁷¹, decision trees⁷², Bayesian approaches⁷³, support vector machines⁵⁸, Fuzzy methods⁷⁴ and artificial neural networks⁷⁵. In general, the modern computational pulse analysis could make it possible to objectively analyze the radial artery pulse palpation.

In this work, we first designed and characterized a thin and flexible sandwich structured piezoelectret based on fluorinated ethylene propylene (FEP) for piezoelectric like sensing. Afterward, an artificial intelligent diagnosis system is created with three major steps: pulse acquisition and signal preprocessing, comprehensive feature extraction and statistical hypothesis-based feature selection, and machine learning modeling. A dataset based on the volunteer identification test, which labels pulse data collected from four different volunteers, is used for case study. For user identification, a cross validated testing accuracy or the averaged testing accuracy with 99.5 (± 0.60)% have been achieved through the proposed diagnosis system.

3.2 Sandwich Structured Piezoelectret Sensor

3.2.1 Device Design and Working Mechanism

To emulate the finger touch of TCM doctors and provide accurate pulse readings, a sandwich structured piezoelectret is designed (Fig. 3.5). Two layer of FEP film⁷⁶ with the thickness of $d_{FEP} = 25.4 \mu\text{m}$ are sealed with $d_{air} = 61.0 \mu\text{m}$ using the Acrylic double-sided tape at four edges. During the Corona charging process, the air in between the FEP films is ionized and the electrical dipoles are formed at the film surfaces. The FEP films are electrets with positive charges captured on the upper side and negative charges captured at lower side. After a 30-min Corona charging process at -10 kV, the thin aluminum tapes are deposited as electrodes at the top and bottom of the FEP films.

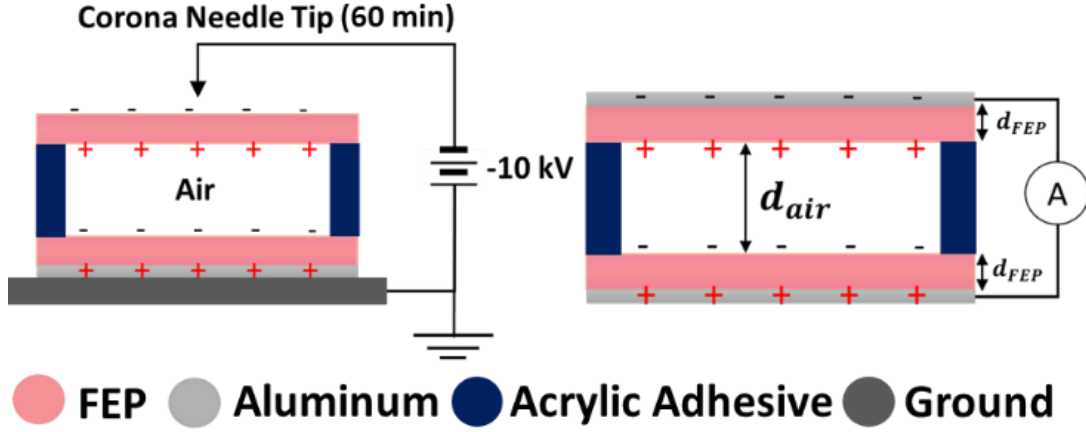


Figure 3.5: Corona discharging (left) and the schematic of sandwich structured piezo electret device (right) where the upper and lower surfaces of FEP films are oppositely charged.

As shown in Fig. 3.6a, the physical model of the sandwich structured piezoelectret sensor can be simplified as three parallel capacitors connected in series and form a circuit with the outer resistance, R . Assuming at a certain quasi-static state, the induced electrical charges are equally distributed on the electrodes and inner FEP film surfaces, with the density of σ_{air} and σ_{FEP} respectively. The direction of electric fields is from the surfaces with positive charges to the negative ones. If we focus on the control volume 1 (CV1) and the control volume 2 (CV2), the Gauss's Law follows:

$$\epsilon_{FEP} \mathbf{E}_{FEP} - \epsilon_{air} \mathbf{E}_{air} = \frac{-\sigma_{FEP}}{\epsilon_0} \quad (1)$$

$$\mathbf{E}_{FEP} = \frac{-\sigma_e}{\epsilon_0 \epsilon_{FEP}} \quad (2)$$

where ϵ_{FEP} and ϵ_{air} are the relative permittivity of the FEP material and air; ϵ_0 is the vacuum permittivity; $\mathbf{E}_{FEP}$ and $\mathbf{E}_{air}$ are the electric field. According to the Kirchhoff's second law under the short-circuit:

$$2d_{FEP} \mathbf{E}_{FEP} + d_{air} \mathbf{E}_{air} = 0 \quad (3)$$

Combine (1)-(3):

$$\sigma_e = \frac{\epsilon_{FEP} \sigma_{FEP} d_{air}}{2\epsilon_{air} d_{FEP} + \epsilon_{FEP} d_{air}} \quad (4)$$

In this regard, at the original state (Fig. 3.6 b, I), the electrical charges on the two electrodes are balanced by the drag and repel force from both electret films, the electrical potential between the two electrodes remains the same at the static state. When an external force is applied to compress the sensor (Fig. 3.6 b, II), the distance between the structures with same type of electrical charges become closer and the repel force increases, which lead to the relocation of electron and a current response can be observed. When the pressure is removed (Fig. 3.6 b, III), the sensor shape recovers back to its original shape due to the elastic deformation, and an opposite current response

can be measured before the electrical potential between the two electrodes reaches a new balance.

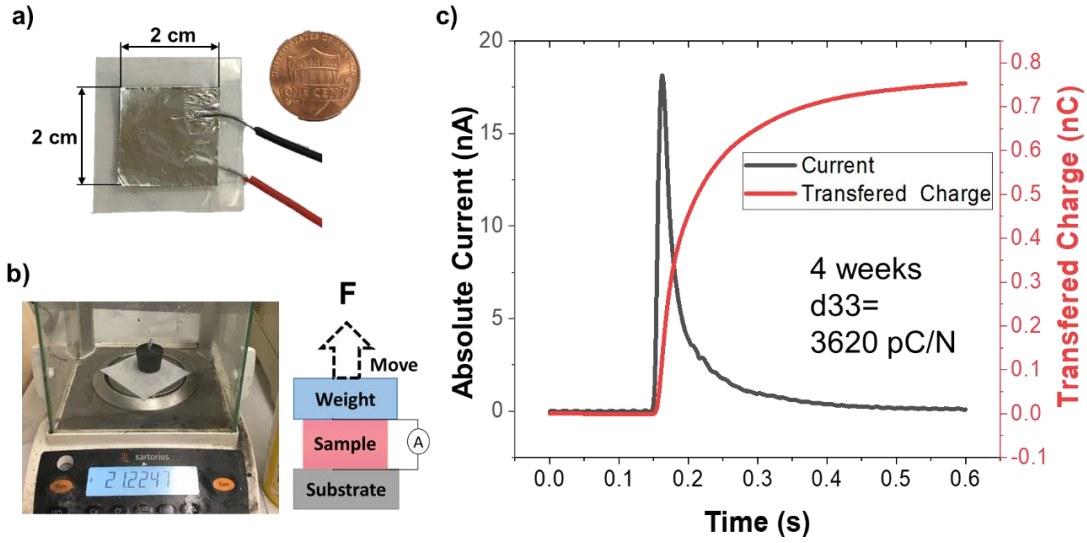


Figure 3.6: (a) Schematics of the simplified device physical model. (b) The current generation process of the piezoelectret when it is at (I) the original state, (II) the compressing state, and (III) the releasing state.

3.2.2 Device Characterizations

To measure the sensitivity of the given sensor system, the equivalent piezoelectric coefficient, d_{33} , of the sensor with a size of 2 cm by 2 cm (Fig. 3.7a) is characterized. The sample is measured by the “weight-moving” method as shown in Fig. 3.7b^{20,77}. Specifically, a known compression force of $F=0.208\text{N}$ is first applied on the device through a given weight, then the weight is removed quickly. Afterward, as shown in Fig. 3.7c, the averaged current response curve is generated by aligning the onsets of 30 manual testing cycles, and the absolute current value is integrated simultaneously to calculate the transferred charge, Q . The quasi-static d_{33} is calculated with the following equation:

$$d_{33} = Q/F \quad (5)$$

Considering the charge decay of FEP electret, the sensor has been placed in the laboratory atmosphere for 4 weeks before the test, the quasi-static d_{33} value of the device is characterized as 3,620 pC/N.

Besides the equivalent piezoelectric coefficient, the stability test is also carried out with a Bose Electroforce 3100 dynamic mechanical analysis (DMA) tester as shown in Fig. 3.8 a. The samples are placed between the cylinder-shaped indenter and force sensor. During the stability test, the square-wave cycling force are applied to the sample with the indenter. The applied force magnitude is 1.75N and the activation frequency is 1 Hz, which is close to the cardiac cycle duration of human pulses. The negative electrode side is placed at the force sensor and grounded, as such, the pressing process will generate a positive current pulse and the releasing process would generate negative current pulse. As shown in Fig. 3.8b, the distance between the maximum current and minimum current of each cycle is recorded as amplitude (AMP). As demonstrated in Fig. 4.8 c, the activation cycle has been repeated 3,360 times and the averaged AMP value is 186.55 ± 4.47 nA.

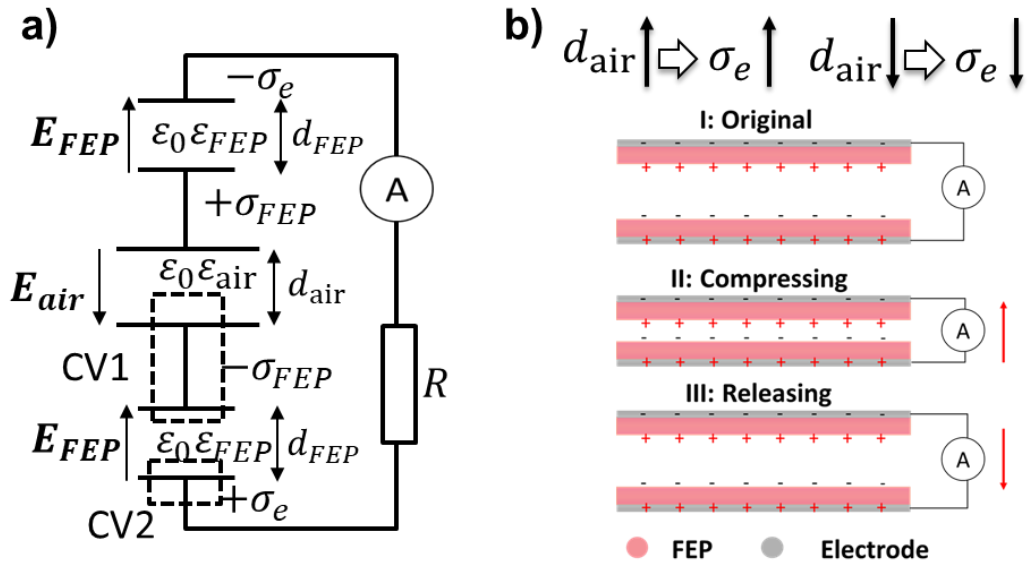


Figure 3.7: The equivalent piezoelectric coefficient test. **(a)** The image of a testing sample with 2 cm by 2 cm effective area. **(b)** The mass of the weight scale and the schematic of the weight-removing process. **(c)** The current response curve and measured piezoelectric coefficient.

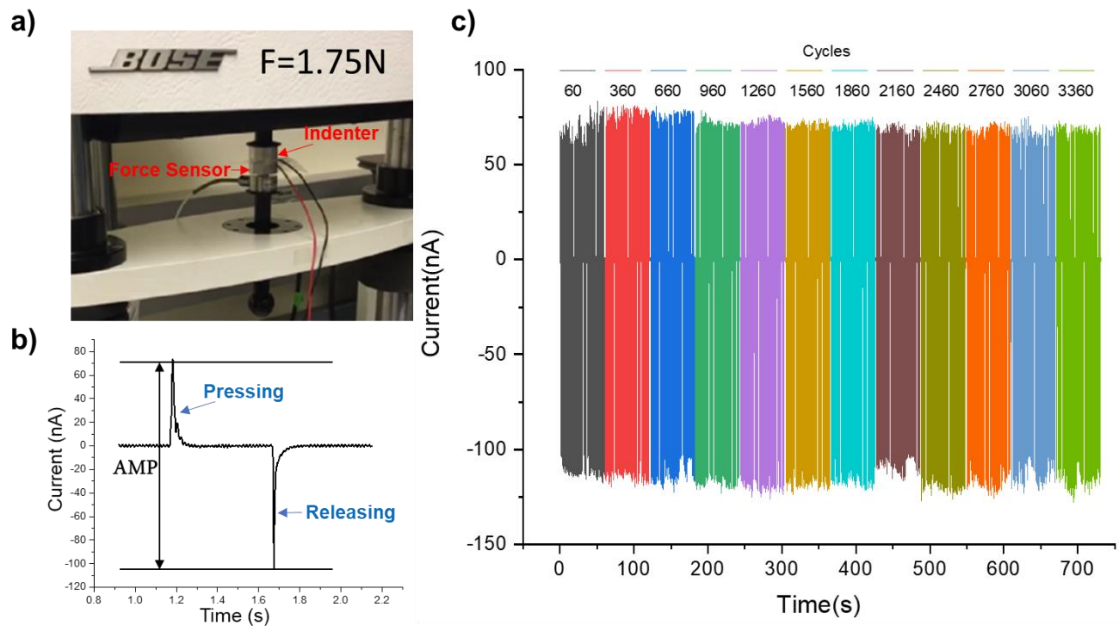


Figure 3.8: The stability test of sensor sample. **(a)** The experiment setup of the Bose Electroforce 3100 dynamic mechanical analysis (DMA) tester. **(b)** The current response of the sensor in each testing cycle. **(c)** The current response of 3,360 cycles with different colors annotating different cycle intervals.

3.3 Intelligent Signal Diagnosis System

3.3.1 System pipeline

The overall system pipeline for the intelligent signal processing system is shown in Fig. 3.9. The original signals are first collected with the wearable device and hardware preprocessing equipment. The signals are then analyzed through software preprocessing techniques, including data normalization and baseline rectification. Given that the total case number of the original database is unbalanced, data balancing has been applied. Afterward, there are two branches in this step: using random under sampling to build the feature extraction dictionary and applying the Synthetic Minority Oversampling Technique (SMOTE)⁷⁸ to train a ML model. Comprehensive feature extraction is the key step after the under sampling process as it would convert the time series signal into 72 kinds of computational features and the identical features are selected using the Time Series Feature Extraction on the basis of Scalable Hypothesis tests (Tsfresh) package⁷⁹. The next step is the variable independence checking to avoid the “Multicollinearity” problem. Redundant features that can be linearly fitted from the others are filtered out by computing the Pearson correlation coefficient values⁸⁰. As such, a certain dictionary that records the identical features are selected for the specific signal analysis task. The final section is the modeling process of ML algorithms to figure out the relationship between selected features and corresponding categories. This section includes the feature selection and standardization by splitting the data to obtain training set and testing set, fitting the ML algorithms with training set, and evaluating the performance with testing set. The final suitable algorithm would be selected according to the evaluation result.

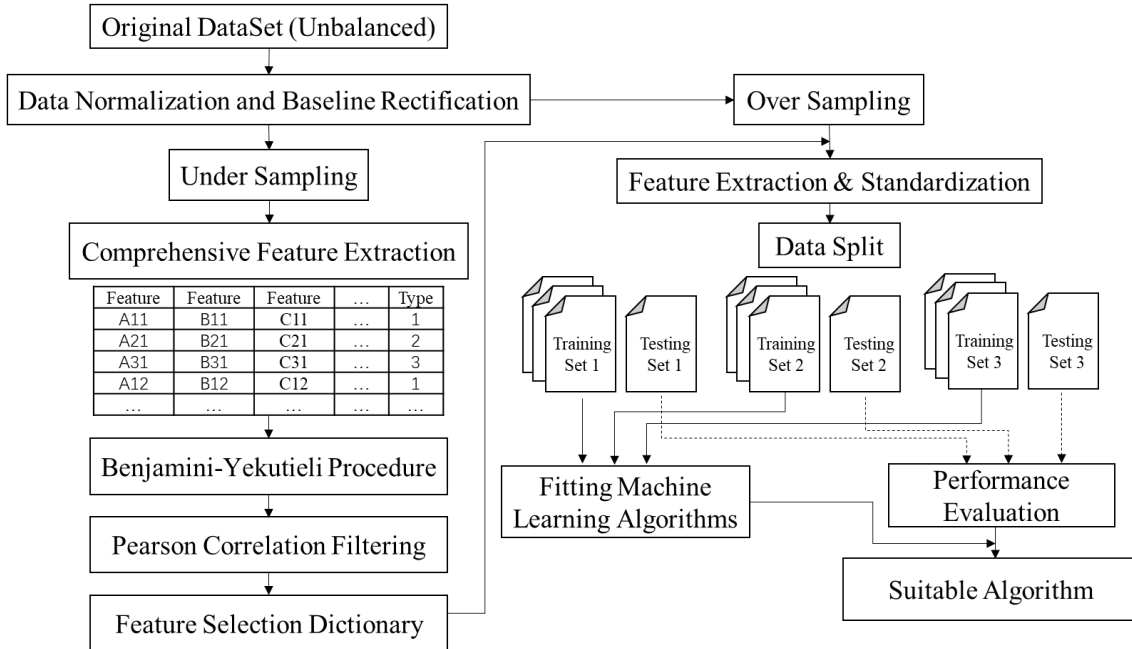
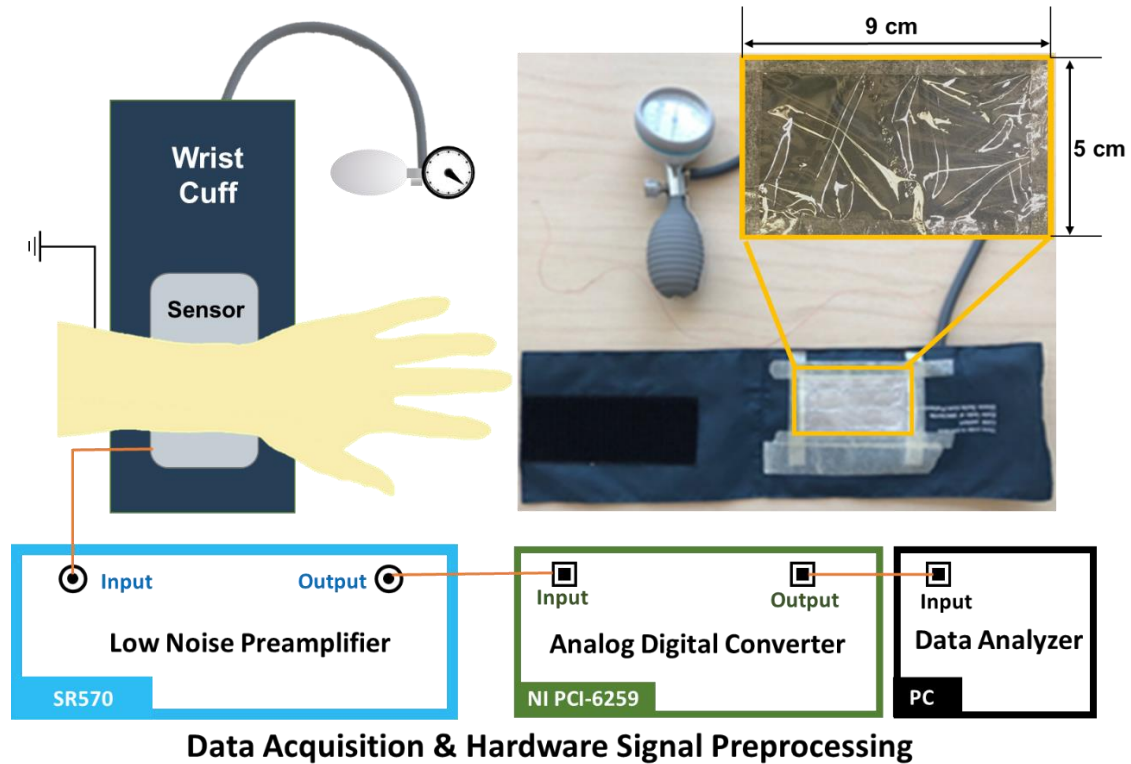


Figure 3.9: The system pipeline for the intelligent pulse signal diagnosis system.

3.3.2 Pulse Acquisition and Signal Preprocessing

The hardware settings of the proposed wrist pulse measurement system are illustrated in Fig. 3.10. The size of the proposed sensor is $5\text{ cm} \times 9\text{ cm}$ which could fully cover the active radial artery area (Cun, Guan, Chi position) on the wrist. To make sure the

conformal skin contact, a medical wrist cuff with aneroid (to measure the applied air pressure) is assembled with the electret sensor. To increase the signal to noise ratio and obtain the appropriate frequency band, prior works^{67,81,82} suggested using low-pass filters to eliminate the high-frequency random noise. Therefore, the raw signal is processed by a preamplifier for signal amplification and a low-pass filter to remove high frequency noises. It has been proved that 99% of the spectral energy distributes within the 10 Hz⁸³, therefore the low-pass filter is set to this value during the experiments. The analog signal is converted to the digital readings through an NI DAQ



system and then passed to the personal computer for data analysis.

Figure 3.10: The device setup for the pulse acquisition, where the sensor is attached to the wrist cuff and the preprocessed with low noise preamplifier, then converted to digital signal and analyzed on PC.

Besides the hardware preprocessing, the recorded pulse signal would first pass through the signal preprocessing algorithm for further data normalization and rectification. This thrust is shared among most data analysis pipelines and is crucial to the success of downstream tasks. One challenge in this process is the “baseline drift” caused by the respiration, body motion and measurement inference^{52,59,84}. To resolve this problem, a Butterworth filter algorithm is adopted using the Biosppy package⁸⁵. The comparison between the normalized original signal, which comes from one 30-second testing cycle of a 23-year-old male volunteer, and its rectified signal is illustrated in Fig. 3.11. When the baseline is aligned, the measurement artifacts would not influence the final pulse diagnosis result.

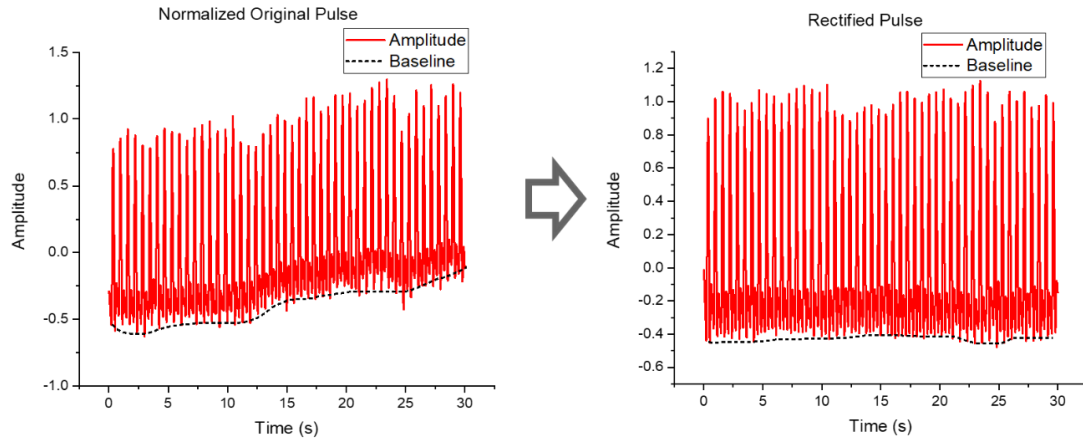


Figure 3.11: The comparison between the normalized original time series signal sample and the rectified signal as the baseline drifts are removed.

3.3.3 Comprehensive Feature Extraction and Statistic Hypothesis Based Feature Selection

As shown in Figs. 3.12 a,b, the pulse features can be extracted on both time and frequency domains. The comprehensive feature extraction scheme includes straightforward methods such as the number and position of peaks which usually represent the averaged pulse cycle of the interested frequency band. It also includes the auto regressive model coefficients, mean approximation of the second derivative on the time domain, the partial autocorrelation at a given lag, the Fourier entropy and the other signal complexity metrics. The full list of extracted time series data features are included in the FRESH⁷⁹ library, and a total amount of 72 calculators and 794 parameter combinations are used in this approach.

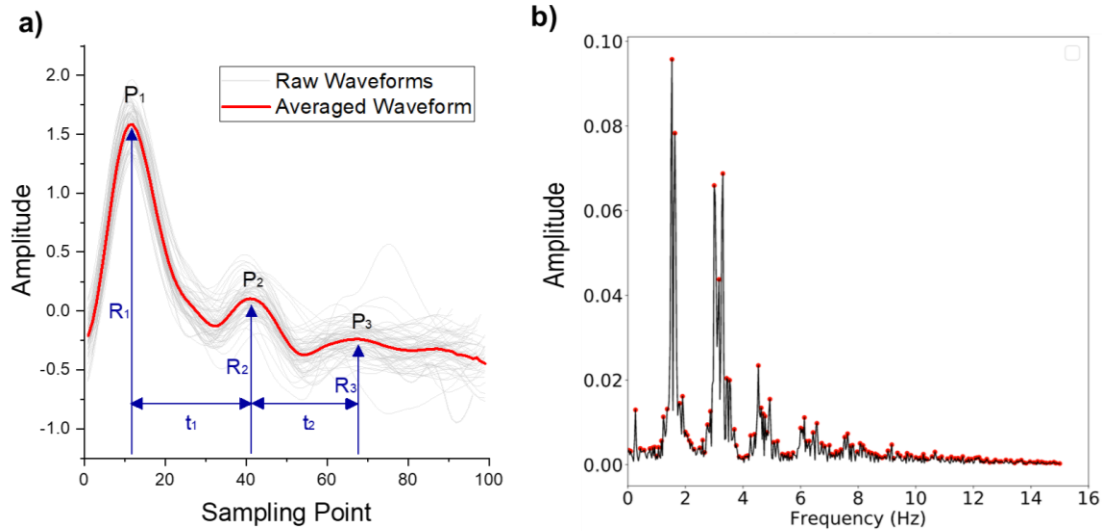


Figure 3.12: Scheme for the feature selection in the time domain and frequency domain. **(a)** Averaged pulse cycle on the time domain, with P₁, P₂, P₃ denote the peak points of the percussion wave, tidal wave and dicrotic wave; R₁, R₂, R₃ denote the amplitudes of P₁, P₂, P₃. The timestamp distance between P₁ and P₂, as well as P₂ and P₃, are t₁ and t₂ respectively. **(b)** The 0-15 Hz frequency domain plot of the pulse signal sample obtained with the Fast Fourier Transform (FFT).

Afterward, the feature selection process is carried out by identifying the statistically significant and independent features. For the significance test, the p-values are calculated and the Benjamini-Yekutieli procedure is performed to select features that can be simultaneously true under different hypothesis tests⁸⁶. For the hypothesis test of a certain feature, ϕ , we need to define the null hypothesis and alternative hypothesis. The null hypothesis, H_0^ϕ , is considered as the default truth which means the feature value, X_ϕ , is irrelevant for predicting the specific group categories of the visited samples. While the alternative hypothesis, H_1^ϕ , states the opposite. The value that judges the hypothesizes is p^ϕ , which is calculated with a certain test statistic method from feature value distributions across the different categories. As an example of a three-class classification problem in Fig. 4.13, a small group variability, p^ϕ , indicates larger variations between the group variability and more likely that the null hypothesis is true. Such that this the feature is filtered out. On the other hand, a smaller p^ϕ implies the alternative is true and the feature is accepted. The threshold T^ϕ for making the decision is usually set to 0.05 to assure 95% of confidence⁸⁷.

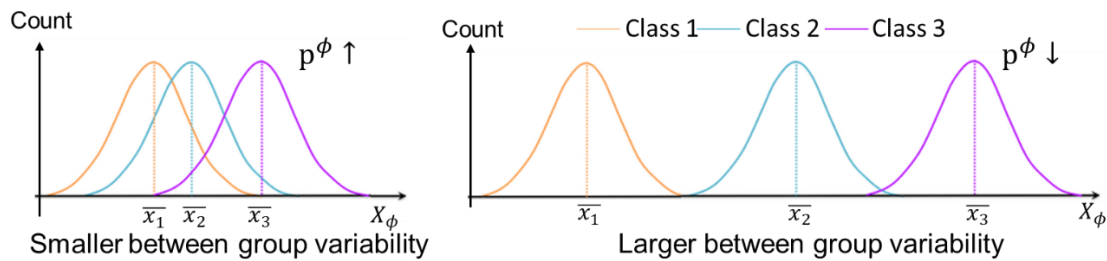


Figure 3.13, The schematic of the feature value X_ϕ distribution with different curve colors indicating different group categories of the samples. The smaller p^ϕ indicates larger variations between the group categories.

In this way, most of the features are correctly selected but there are still some false features that should come from the null hypothesis H_0^ϕ . As such, the False Discovery Rate (FDR) is defined to be the unobserved proportion of False Discoveries (FD) among total rejections under the specific threshold T^ϕ . The FDR control mechanism is demonstrated in Fig. 3.14. As shown in Fig. 3.14 a, by calculating the p^ϕ across the features, a distribution is observed. The warm color region with the uniform distribution is from the null hypothesis H_0^ϕ , while the cold color region with a skew distribution is from the alternative hypothesis H_1^ϕ . The horizontal true boundary is unable to be observed, such that a vertical p-value threshold is set to retain the most relevant features. The FDR control process can further eliminate the warm color region by the p^ϕ correction. As shown in in Fig. 3.14 b, each box represents a feature and recorded with the p^ϕ , which is ranked from small to large. The p^ϕ correction process simply multiplies the original value with the total number of p^ϕ at the horizontal line and divide its own rankings in the line. Afterward, the p^ϕ below the threshold remains below the threshold for the alternative hypothesis but the null hypothesis won't satisfy the requirement.

With the aforementioned feature selection process, the remaining features would be highly related to the final target. To further reduce the computation cost, the feature

indecedy test is conducted and the linearly correlated feature pairs (x,y) can be identified with the Pearson correlation coefficient, r_{xy} , which is expressed as:

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (6)$$

Where n is the total number of samples. For the i^{th} sample, the (x_i, y_i) is the corresponding pair of feature values; $\bar{x}$ is the averaged value of $x_1, x_2, \dots, x_n$; and $\bar{y}$ is the averaged value of $y_1, y_2, \dots, y_n$. The absolute values of the calculated Pearson correlation coefficient that are above 0.7 usually indicate a very strong relationship between the two variables and the values above 0.9 suggests nearly perfect linearity⁸⁸. In this research, we chose a threshold of 0.8 for the redundant feature filtering process for selected features.

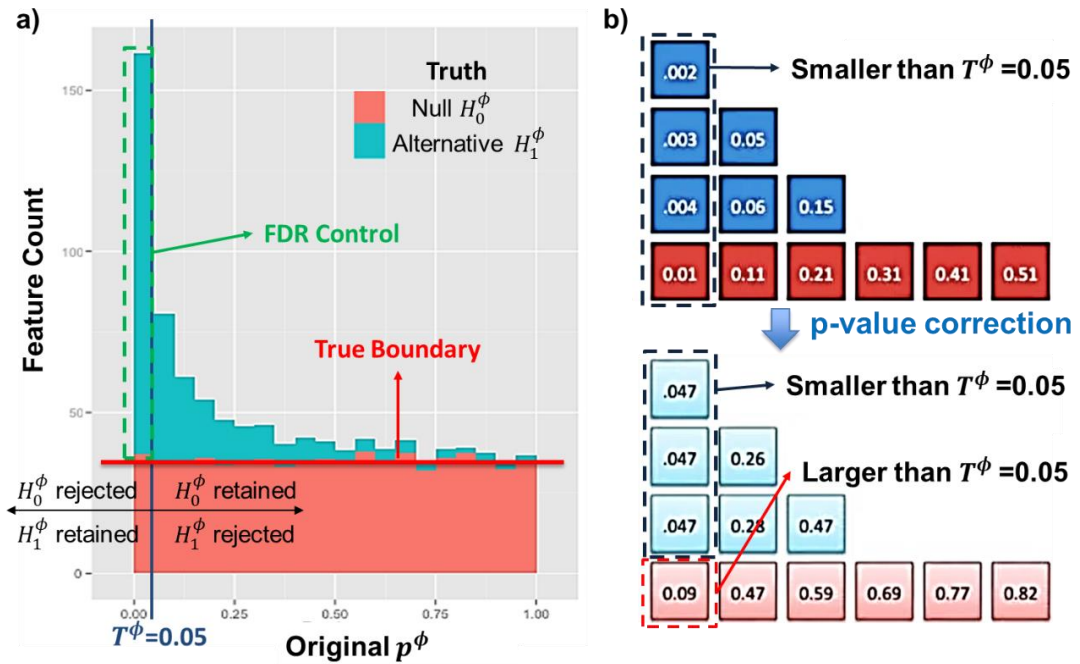


Figure 3.14: The schematics of the FDR control mechanism⁸⁹. **(a)** Distribution of original p^ϕ versus the number of features with the neighboring p^ϕ values. **(b)** The FDR control process by p-value correction.

3.3.4 Machine Learning Modeling

After extracting features from the oversampled pulse signals according to the feature selection process, the feature standardization process (z-score normalization) is conducted, which is a commonly adopted approach in feature scaling⁹⁰. The new feature value x_i' can be expressed as $(x_i - \mu)/\sigma$, where μ is the average value of x samples and σ is the standard deviation. The training data and testing data are split into 10 cross validation groups through the shuffle split iterator at the ratio of 4:1. The training data is fed into the eight basic types of supervised machine learning algorithms^{91,92}, including: Random Forest (RF), XGBoost (XGB), Artificial Neural Network (ANN), k-nearest neighbors (KNN), support vector machine (SVM), logistic regression (LOG) and gaussian naive bayes (GNB). The testing data is then passed to the trained

models and the confusion matrix (Table 3.1) is obtained for performance evaluation. Four metrics are calculated by the following equations:

$$\text{Precision} = \frac{TP}{FP + TP} \quad (7)$$

$$\text{Recall} = \frac{TP}{FN + TP} \quad (8)$$

$$F1 = 2 \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} \quad (9)$$

$$\text{Accuracy} = \frac{TP + TN}{FN + TP + TN + FP} \quad (10)$$

Precision is the number of correct predictions divided by the sum of all results that are predicted as the said class, while recall is the correct predictions divided by the total number of the samples of the predicted class. The F1 score is the harmonic mean of Precision and Recall and can be used to evaluate the prediction performance of each class. Accuracy is the sum of all correctly predicted samples divided by the total sample number, which can be used to evaluate the overall performance of the model. The machine learning models and evaluation matrix are built on the scikit-learn package⁹³.

Table 3.1 Confusion Matrix

		Actual Classification	
		True	False
Prediction Results	True	True Positive (TP)	False Positive (FP)
	False	False Negative (FN)	True Negative (TN)

3.4 Case Study and Result Analysis

For mobile healthcare services, the correct user identification can be very important as the biological patterns vary across different individuals. Manually inputting the user information each time before using the device would require extra effort and introduce human errors. Here, an intelligent system is proposed to automatically recognize the user identity from their unique wrist pulse patterns. During this task, the wrist pulse data from 4 volunteers between 22 and 24 years old, with 3 males and 1 female are collected (Table 3.2). The volunteers are asked to sit down and take the pulse by the designed sensor system, and the pulse signals are recorded at the sampling rate of 60 Hz under 80 mmHg applied pressure and each testing cycle lasts for 30 seconds. The whole database is composed of 413 trails of data over 5 months.

Table 3.2 Collected Data Cases

Volunteer	Gender	Age	Sample Number
1	M	22	387
2	M	24	66
3	M	24	59
4	F	23	46

The pulse signals are labeled by the volunteer codes. The schematic for the final collected time series waveform of the four volunteers is shown in Figs. 3.15 a-d. From

the naked eyes, it can be observed that the wave shapes on the time domain are different among volunteers. For example, the tidal wave is not obvious for volunteer 1 but the dirotic wave is very strong. The R1, R2 and R3 values of volunteer 2 decrease in the cycle but the R3 value of volunteers 2 and 3 are bigger than R2. The t_2/t_1 value of volunteer 3 would be usually larger than volunteer 4.

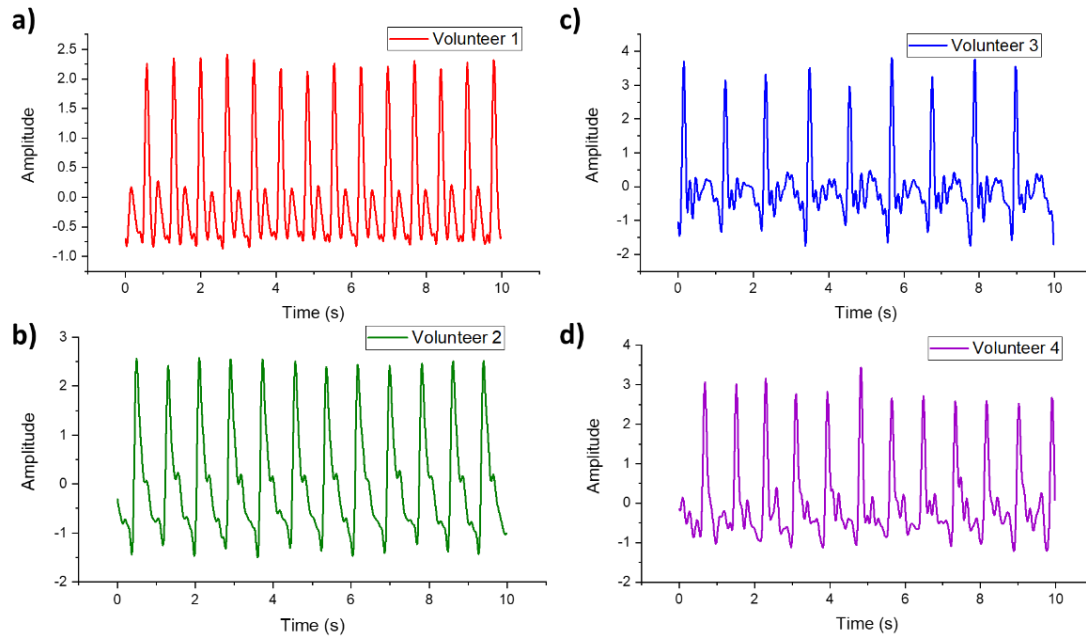


Figure 3.15: The schematics of collected wrist pulse signals on time domain of (a) volunteer 1, (b) volunteer 2, (c) volunteer 3 and (d) volunteer 4.

The difference in volunteer pulse patterns can be also found in the frequency domain plot in Fig. 3.16. The different positions and amplitude of peak points of volunteer pulses are observed. Although the frequency domain signals are possible for human eyes to qualitatively differentiate in the example figure, the data-driven intelligent pulse diagnosis system requires computational quantitative analyses.

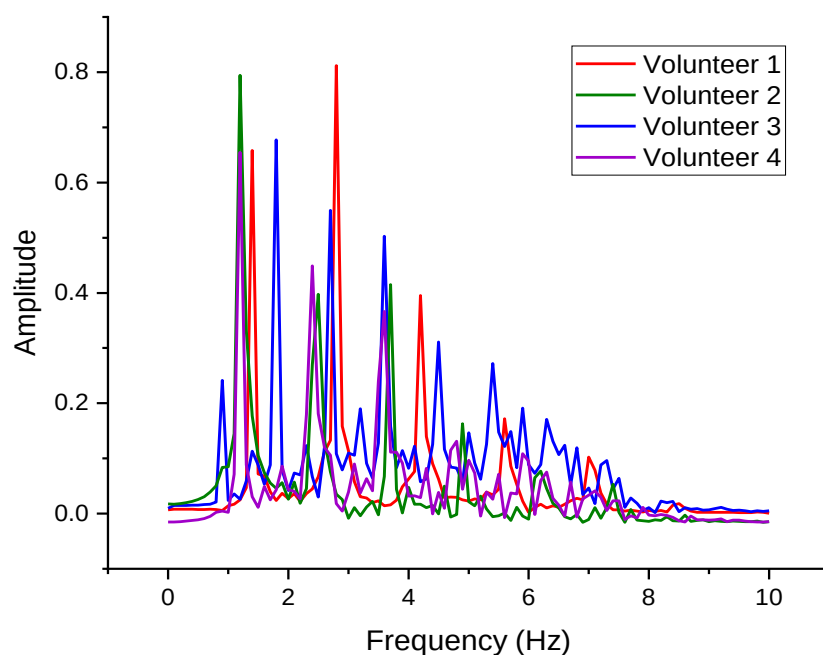


Figure 3.16: The schematics of collected wrist pulse signals on frequency domain while different colors denote different volunteers.

For the data visualization of extracted pulse features, the three-dimensional Principal Component Analysis (PCA) plot of the sampled pulse wave signal is shown in the Fig. 3.17a, from which one can hardly observe the clusters of sample points with the same label. On the other hand, after the feature extraction and selection, the new PCA demonstration is shown in Fig. 3.17b. The data point clusters become clearer as the intelligent feature extraction and selection process are effective in preserving critical statistical information. For this case study, there 29 features are selected (FI0-FI28). The Pearson correlation matrix among selected features is shown in Fig. 3.18, where more than half of the feature pairs have an absolute correlation value under 0.5 (under the threshold for strong correlation strength⁸⁸). This result also indicates that these selected features are highly independent with each other and less likely to be redundant for the later classification tasks.

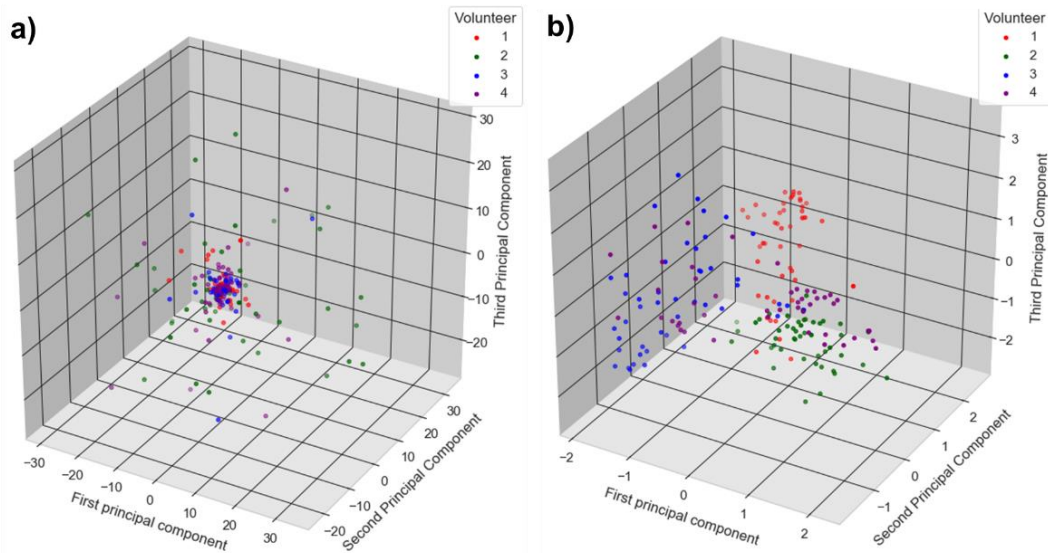


Figure 3.17: The three-dimensional PCA visualization of **(a)** the original time series dataset samples and **(b)** the feature extracted dataset with different colors denote different volunteers.

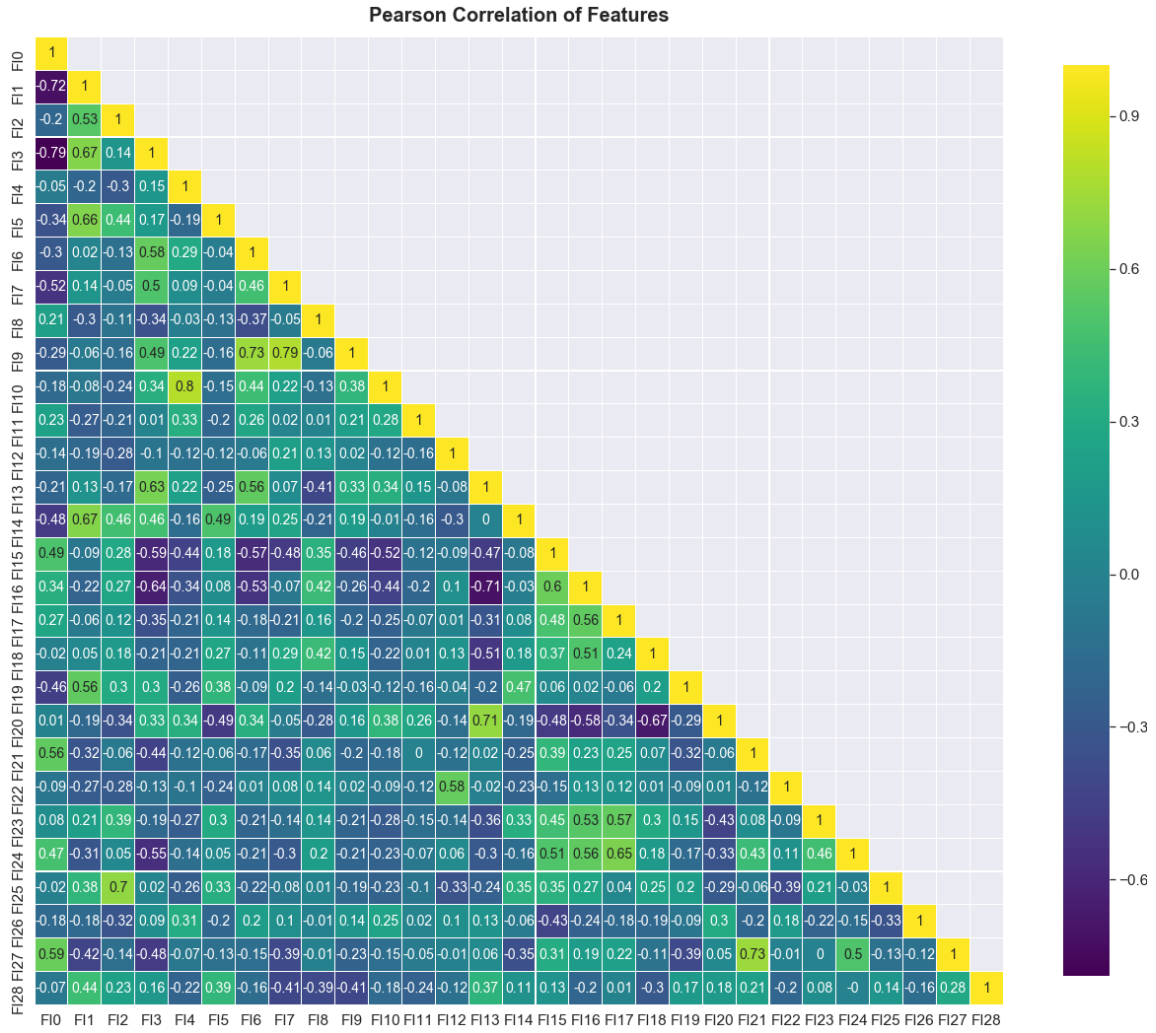


Figure 3.18: Pearson correlation matrix for user identification based on wrist pulses, with 29 selected features (FI0-FI28).

In Fig. 3.19a, the selected features are ranked through averaged impurity importance metrics and the more important the feature, the higher the ranking. The detailed explanations of the 29 selected features are described in the Appendix notes of this chapter. In this task, the top 3 contributors (the importance larger than 0.05) are the number of peaks of at a certain support on time domain (FI0), the variance of absolute consecutive change of time series between two certain quantiles (FI1) and the absolute value of FFT coefficient of a certain position (FI2). Although the features are ranked, the importance values are very close to each other, and all the features would be essential to secure the classification performance within different machine learning models. The value distributions of features FI0-FI28 are visualized in the Figs. S1, S2 of the Appendix figures. The large group variances suggest the importance of the feature and result in the easy classification task for a the strong vote in the decision making process.

For the final ML algorithm performance evaluation, the overall classification accuracies of different classification models are demonstrated in In Fig. 3.18b. It can be observed that for most machine learning models, both training and testing accuracies can reach above 95%. The highest score is achieved by NN, with its training and testing accuracy reaching 99.9 (± 0.024)% and 99.5 (± 0.60)% respectively. To avoid the unbalanced classification accuracy over each category, the F1 scores of testing samples are further

investigated. As shown in Fig. 3.18c, most of the ML algorithms have balanced F1 scores over four categories. The F1 scores of NN are 99.3 (± 0.98)%, 99.4 (± 0.73)%, 99.9 (± 0.18)%, 99.6 (± 0.81)% for volunteer 1-4 respectively. The results are already near perfect even though the hyperparameter settings of all ML algorithms are set as default, which also indicates the final selected features are of high quality. We notice that the GNB algorithms still have an obvious performance difference with the other chosen ML algorithms. This is because the GNB algorithm has a preset assumption as the distributions of feature values can be describe as the Gaussian normal distribution. However, from Figs.S1-S2 we found that if the sample distributions are processed with kernel smoother, most of the actual distribution shapes don't satisfy the assumption. As such, the GNB classifier doesn't fit in the case study context, but the rest of classifiers are suitable for resolving the task. It should be noted that the above evaluation results are obtained via the random cross validation process repeated 10 times, with 330 samples tested each time. The summarized confusion matrixes for the different ML classifiers are shown in Figs. 3.20 a-h. The dark blue colors of the four squares at the diagonal lines imply the truth positive cases, and more positive cases indicates better classification performance for the corresponding classifier.

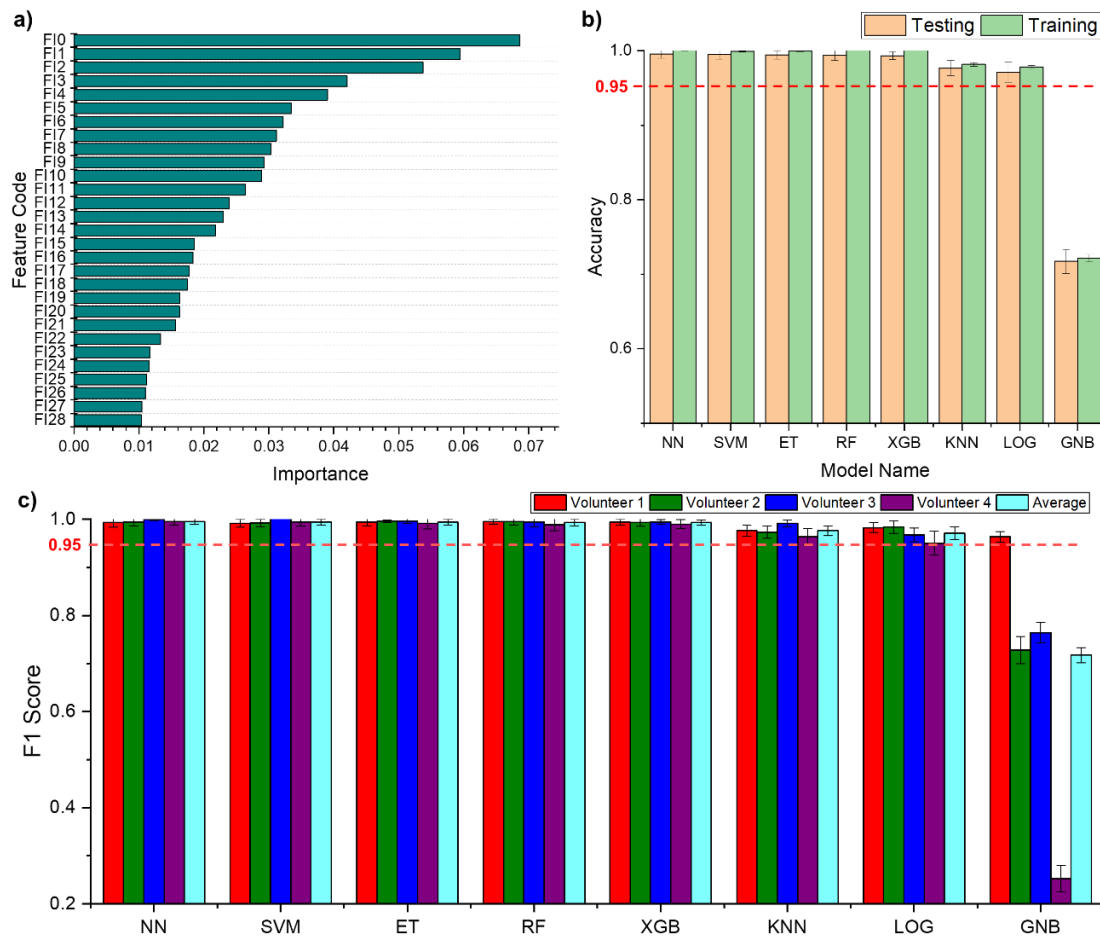


Figure 3.19: (a) The feature importance ranking based on the impurity test. **(b)** The overall training and testing accuracies of investigating ML models. **(c)** The testing data F1 scores of different volunteer categories and the averages for investigated ML models.

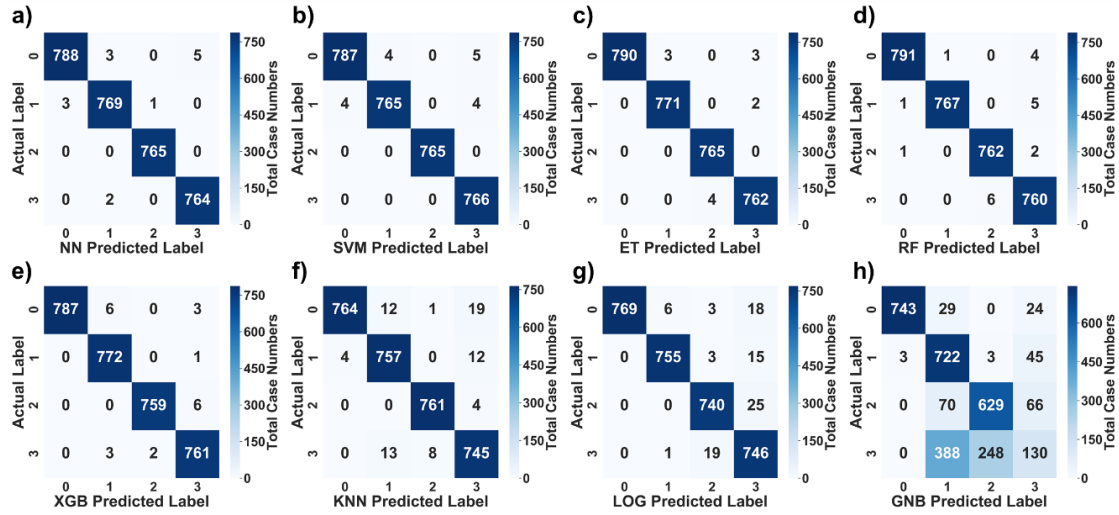


Figure 3.20: The summarized confusion matrixes of different classifiers after cross validations for results from (a) NN model, (b) SVM model, (c) ET model, (d) RF model, (e) XGB model, (f) KNN model, (g) LOG model, and (h) GNB model.

3.5 Conclusions of Chapter 3

In this chapter, a wearable human wrist pulse monitoring and diagnosis system has been demonstrated based on the sandwich-structured piezoelectret sensor and the artificial intelligent signal analysis system. The designed sensor can stably record strong pulse wave signals and with the proper hardware and software signal preprocessing, the high-quality time series data are obtained. The comprehensive time series features are extracted based on computational wavelet analysis algorithms and the identical features are selected with the statistical hypothesis tests. Based on these features, the ML algorithms can achieve the efficient and near-perfect prediction results on the user identification task. The proposed systematic schematics have the potential to extend on other applications such as the glucose level prediction and mental state prediction. In the future, by integrating the wireless module and minimizing the sensor system, there could be a wider application for the proposed schematics.

3.6 Appendix: Explanations and Value Distributions of Final Selected Features

FI0: number_peaks__n_50

Calculates the number of peaks of at least support n in the input time series x, where n=50.

FI1: change_quantiles__f_agg_"var"__isabs_True__qh_0.8__ql_0.2

The change of quantiles first fixes a corridor given by the quantiles ql and qh of the distribution of x. Then calculates the average, absolute value of consecutive changes of the series x inside this corridor. Hereby, the aggregator function f_{agg} that is applied to the differences in the bin is the variance, the absolute differences are taken, qh is 0.8 and ql is 0.2.

FI2: fft_coefficient__attr_"abs"__coeff_50

Calculates the Fourier coefficients of the one-dimensional discrete Fourier Transform for real input by Fast Fourier Trasformation (FFT) algorithm. Hereby, the feature takes the absolute values of the FFT complex outputs and as the list, then select the 50th data point in the list as the final return.

FI3: ratio_beyond_r_sigma__r_0.5

Ratio of values that are more than $r * \text{std}(x)$ (so r times sigma) away from the mean of time series x , where r value is selected as 0.5 for this feature.

FI4: fft_coefficient__attr_"abs"__coeff_74

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 74th data point in the list as the final return.

FI5: change_quantiles__f_agg_"var"__isabs_True__qh_0.8__ql_0.0

For the change of quantiles, the aggregator function f_{agg} that is applied to the differences in the bin is the variance, the absolute differences are taken, qh is 0.8 and ql is 0.

FI6: quantile__q_0.7

Calculates the q quantile of input time series x . This is the value of x greater than $q\%$ of the ordered values from x . In this specific feature, q is 0.7.

FI7: change_quantiles__f_agg_"mean"__isabs_True__qh_0.6__ql_0.4

For the change of quantiles, the aggregator function f_{agg} that is applied to the differences in the bin is taking the mean, the absolute differences are considered, qh is 0.6 and ql is 0.4.

FI8: change_quantiles__f_agg_"mean"__isabs_False__qh_0.4__ql_0.2

For the change of quantiles, the aggregator function f_{agg} that is applied to the differences in the bin is taking the mean, the differences are remaining its original value, qh is 0.4 and ql is 0.2.

FI9: change_quantiles__f_agg_"var"__isabs_True__qh_0.6__ql_0.4

For the change of quantiles, the aggregator function f_{agg} that is applied to the differences in the bin is the variance, the absolute differences are taken, qh is 0.6 and ql is 0.4.

FI10: fft_coefficient__attr_"abs"__coeff_37

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 37th data point in the list as the final return.

FI11: fft_coefficient__attr_"abs"__coeff_70

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 70th data point in the list as the final return.

FI12: fft_coefficient__attr_"abs"__coeff_83

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 83rd data point in the list as the final return.

FI13: partial_autocorrelation__lag_1

Calculates the value of the partial autocorrelation⁹⁴ function at the given lag =1.

FI14: number_crossing_m__m_-1

Calculates the number of crossings of input time series x on the threshold value m. A crossing is defined as two sequential values where the first value is lower than m and the next is greater, or vice-versa. In this feature, m is -1.

FI15: change_quantiles__f_agg_"mean"__isabs_False__qh_0.6__ql_0.4

For the change of quantiles, the aggregator function f_{agg} that is applied to the differences in the bin is taking the mean, the differences are remaining its original value, qh is 0.6 and ql is 0.4.

FI16: agg_autocorrelation__f_agg_"median"__maxlag_40

Calculates the value of an aggregation function f_{agg} over the autocorrelation $R(l)$ for different lags l , and defined as $R(l) = \frac{1}{(n-l)\sigma^2} \sum_{t=1}^{n-l} (X_t - \mu)(X_{t+l} - \mu)$. Where X_t are the values of the input time series and n is its length. σ^2 and μ are its variance and mean. The feature finally outputs $f_{agg}(R(1), \dots, R(m))$ where $m = \max(n, maxlag)$ and $maxlag$ is the maximal number of lags to consider. Hereby, the aggregation function f_{agg} is taking the median and $maxlag$ is 40.

FI17: fft_coefficient__attr_"abs"__coeff_55

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 55th data point in the list as the final return.

FI18: approximate_entropy__m_2__r_0.3

Calculates the approximate entropy (ApEn)⁷⁷ value with length of compared run of data m=2 and filtering level r=0.3.

FI19: lempel_ziv_complexity__bins_5

The input time series data is first binned into the given number of bins, then calculate a complexity estimate of the binned data based on the Lempel-Ziv compression algorithm⁹⁵. For this feature, the bin number is selected as 5.

FI20: friedrich_coefficients__coeff_2__m_3__r_30

Fitting the input time series data in to a polynomial $h(x)$ with the deterministic dynamics of Langevin model⁹⁶ and obtain the coefficients of polynomial. During the polynomial fitting, m is the order of polynomial to fit for estimating fixed points of dynamics, r is the number of quantiles to use for averaging. For this feature, m=3 and r=30, the final returned value is the second coefficient (coeff=2) of the polynomial $h(x)$.

FI21: fft_coefficient__attr_"abs"__coeff_59

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 59th data point in the list as the final return.

FI22: fft_coefficient__attr_"abs"__coeff_82

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 82nd data point in the list as the final return.

FI23: `fft_coefficient__attr_"abs"__coeff_53`

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 53rd data point in the list as the final return.

FI24: `fft_coefficient__attr_"abs"__coeff_56`

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 56th data point in the list as the final return.

FI25: `fft_coefficient__attr_"abs"__coeff_99`

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 99th data point in the list as the final return.

FI26: `fft_coefficient__attr_"abs"__coeff_77`

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 77th data point in the list as the final return.

FI27: `fft_coefficient__attr_"abs"__coeff_29`

The feature takes the absolute values of the FFT complex outputs and as the list, then select the 29th data point in the list as the final return.

FI28: `ratio_beyond_r_sigma__r_1.5`

Ratio of values that are more than $r * \text{std}(x)$ (so r times sigma) away from the mean of time series x , where r value is selected as 1.5 for this feature.

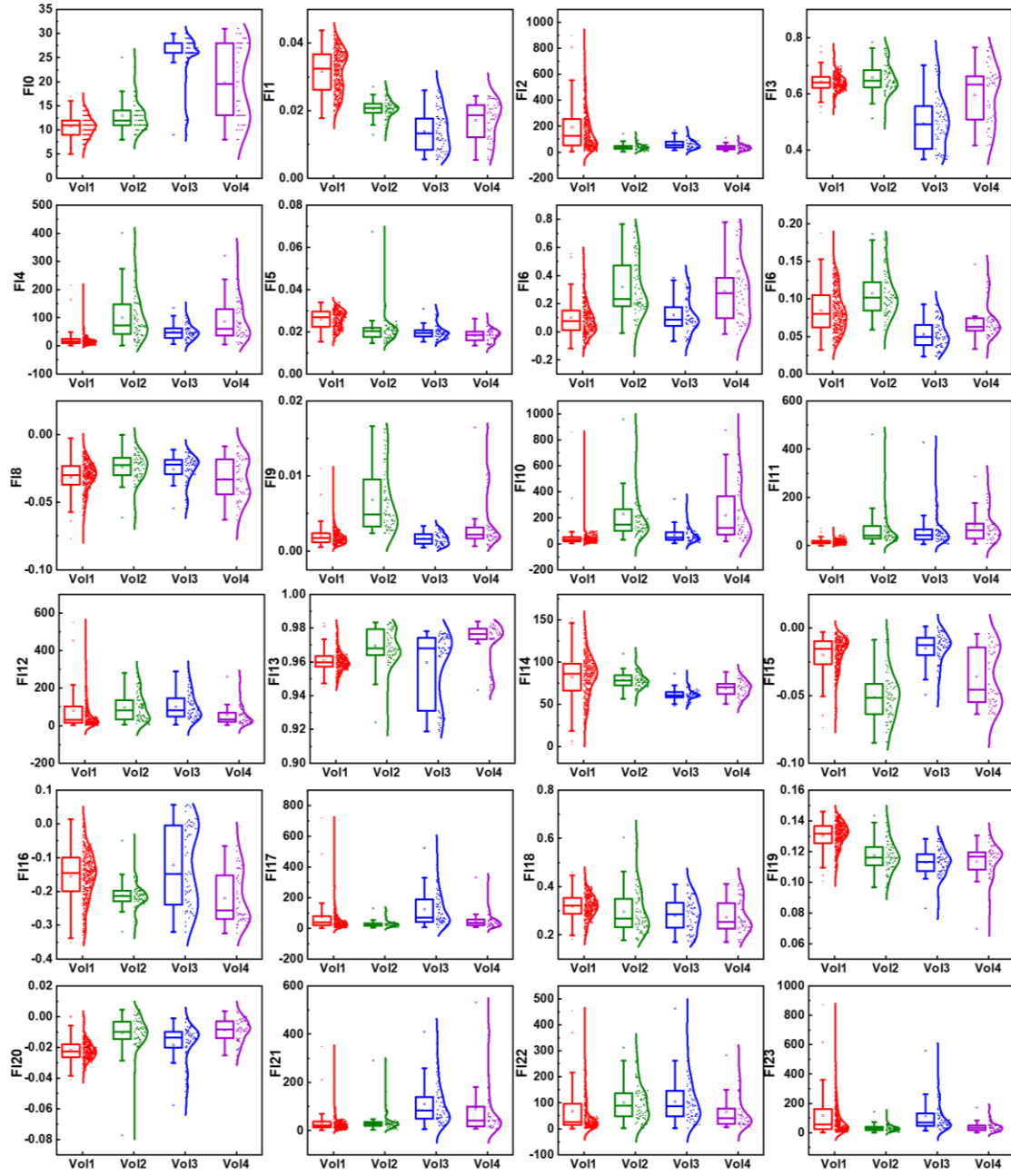


Figure S1: The value distribution and boxplot of final selected features F10-FI28.

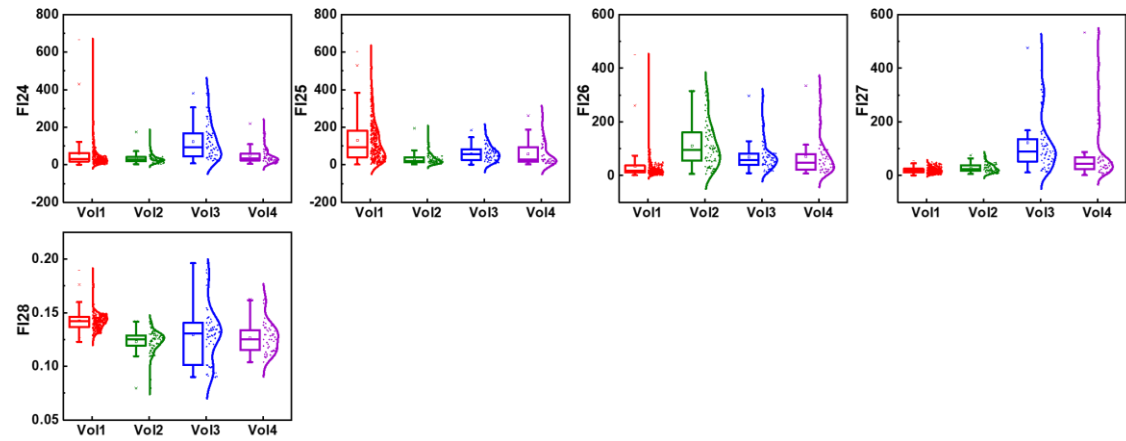


Figure S2: The value distribution and boxplot of final selected features FI24-FI28.

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Chapter 4: Summary and Future Works

4.1 Summary

The progresses in advanced sensing, data transmission, and computation analytics have made dramatic impacts in the “big data” society in recent years. For example, MEMS structural designs and sensing signal analyses are two important research directions that could benefit from the big data approach. This thesis focuses on two areas: (1) MEMS structural design assisted with ML techniques to guide the design and optimization of next generation intelligent sensing systems, and (2) the combination of flexible and wearable sensors, signal processing, computational analytics, and ML techniques toward future mobile health applications.

Chapter 2 demonstrates two major ML-based results: (1) representing MEMS structure with the free-form binary-images, and (2) high speed & accurate physical property prediction of MEMS devices. The proposed systems are found to accurately calculate the modal frequencies and quality factors of disk-shape resonators as well as the frequency bands and open-circuit voltages of energy harvesters after adequate training processes. Furthermore, this system can save orders of magnitude computation time as compared to the conventional numerical methods such as Finite Element Analysis.

Chapter 3 shows a wrist pulse taking flexible sensor with an intelligent time series signal diagnosis analytics to identify specific volunteers. The sandwich structured piezoelectret sensor shows strong and stable outputs as the high-quality raw pulse data are obtained with adequate signal preprocessing techniques. Inspired by the TCM approaches, the identical wavelet features are extracted and selected by computational and statistical approaches. Finally, the a near perfect user identification performance is achieved with ML algorithms.

4.2 Future Works

The future works of the thesis include two aspects: (1) ML-centered data-driven design innovations and automation to explore the optimal solutions for MEMS structural designs, and (2) ML for future precision health and virtual reality (VR) applications, including the signal monitoring and actuation control of the multi-channel, multimodal E-skin systems.

The ML-centered structural design method should require the combination of ML Enabled Structure Generator and the High-speed ML-Analyzer. In this work, the pattern generator can only generate random design configurations, while the ML enabled structure generator can adjust the structural generation policy according to the previous experiences to increase the design optimization efficiency. As shown in Fig. 4.1, the blue colored arrows illustrate the training process of the High-speed ML-Analyzer, which is very similar to the process described in Chapter 2. Since the weighting parameters are initialized randomly in the ML Enabled Generator, the training samples are randomly generated. After training the ML-Analyzer with enough samples, the inverse design cycle connected with the red-colored arrows can be activated. The inverse design is to use an optimization algorithm to generate a solution for a desired physical performance. There are some state-of-art generative

models such as the genetic algorithm¹, generative neural networks² and deep reinforcement learning models³. The proposed sample designs are generated with the generative model and evaluated with the ML-Analyzer. The role of the generative model is to update the structural generation policies by comparing the design performance of different samples and new samples for the next round of operation. By repeating the inverse design cycle for many iterations, the proposed system could discover better designs by learning from the “Big Data Samples”. This future task can benefit many other engineering applications where the structural design is required.

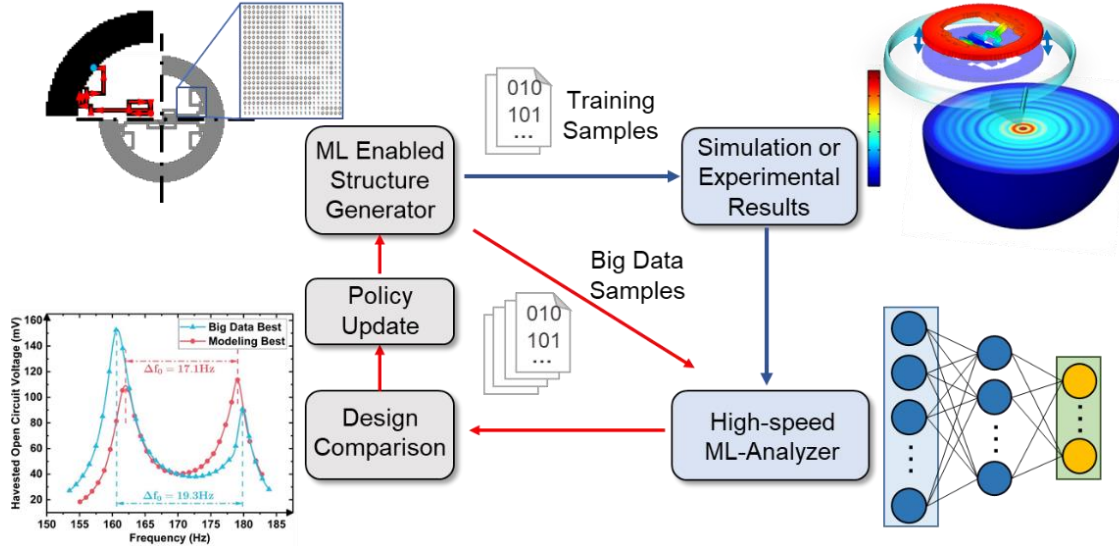


Figure 4.1: The system pipeline for the next-generation high throughput autonomous structure design system, where the blue arrows are the training processes of the ML-Analyzer and the red arrows indicate the inverse design cycle to discover the optimal structures.

One major focus of this thesis is the non-invasive wrist pulse signal diagnosis, while the same wearable device can be mounted on other body positions to acquire different types of biological information⁴ (Fig. 4.2, left). Commercial wearable devices have been developed to fit accessories or clothing without interfering the users’ daily activities. However, motion artifacts and sensor misalignments are challenging issues for the continuous monitoring of medical-grade signals. The approach of electronic skin (E-skin) could be an interesting approach to alleviate these issues by tightly fixing the sensing units on the specific locations on the human body. For example, state-of-art E-skin biomarkers are designed to be imperceptibly attached to human skins with stretchable, ultra-thin, and breathable structures^{5,6} (Fig. 4.2, right). As such, the multimodal, multichannel, and non-invasive E-skin systems could be an important part of the biomedical landscape, as they provide a miniaturized and conformal solution for health monitoring than those of the traditional wearable devices.

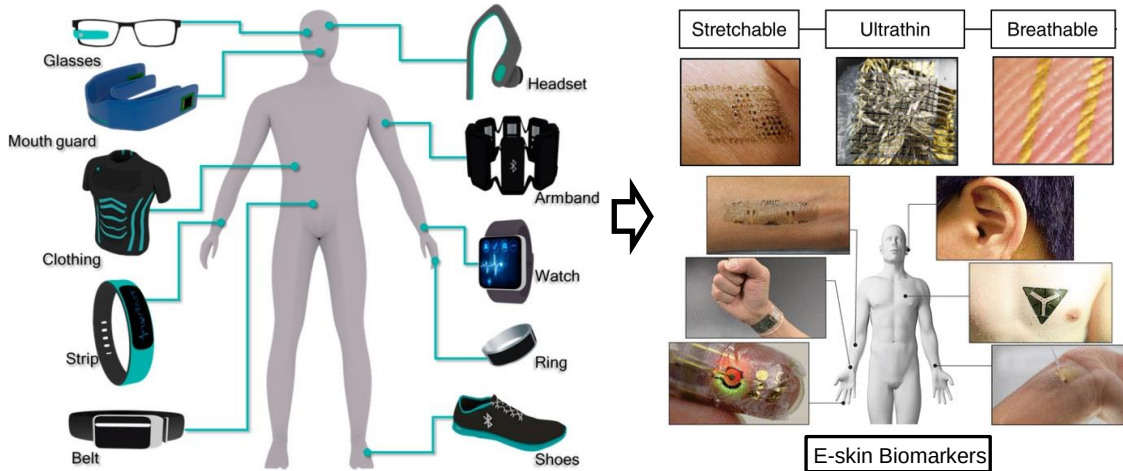


Figure 4.2: Transition from wearable devices to E-skin electronics for the future precision health services⁴⁻⁶.

Besides the sensing mechanism, the proposed piezoelectret structures can be used for the actuation purpose and the integration of the sensing and actuation mechanism have a promising potential in Augmented Reality(AR) and Virtual Reality(VR) applications. As shown in Fig. 4.3 a, a haptic human-machine interface device has been developed based on the flexible electret materials⁷. The stable electromechanical stimulation can be generated by applying external driving voltage. However, it is difficult to precisely control the actual haptic sensation effect since the epidermal condition varies significantly across different individuals, and the body motion will also influence the results. As shown in Fig. 4.3b, by integrating piezoelectret sensor and actuator arrays on the flexible E-skin substrate, adaptive control of the haptic module can be realized. For the sensing module, the electric pulses are detected with responses to the mechanical deformations, and the exact amount of deformation can be calibrated with the total amount of transferred charges. Afterward, the output power of the actuator array can be controlled accordingly.

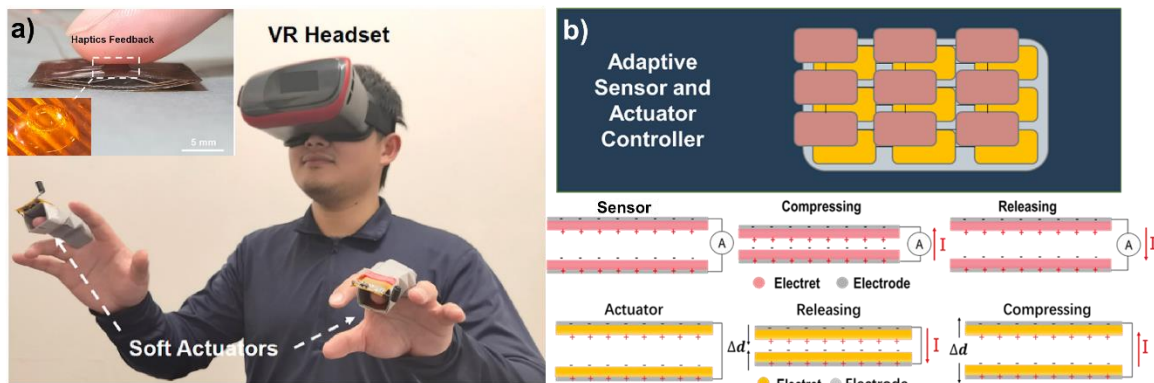


Figure 4.3: The piezoelectret structure for future AR/VR applications. **(a)** The haptic human-machine interface based on soft piezoelectret actuators⁷. **(b)** The future adaptive sensor and actuator device arrays based on piezoelectret structures, with the sensing and actuation mechanism demonstrated underneath.

From the system level perspective, there are also challenges in the E-skin sensing and actuation applications such as uncertainties in failure modes and qualities of each transducer, the integration of heterogeneous big data streams, and the insufficient decision making accuracy/speed. As such, one approach is to calibrate sensing and actuating results with data-driven learning approaches, instead of manually setting the decision-making thresholds. As demonstrated in Fig. 4.4, the latest ML techniques can be introduced to the embedded intelligent system for the E-skin applications. The raw data inputs can be preprocessed with the data-driven techniques such as denoising autoencoders⁸. Training the DL predictive models, such as the CNN-LSTM model⁹ with the preprocessed data can make decisions according to the sensing inputs. Finally, model compression techniques¹⁰ together with signal preprocessing and decision making models can be compressed to a small form-factor and deployed on computation edges for low latency, real-time operations.

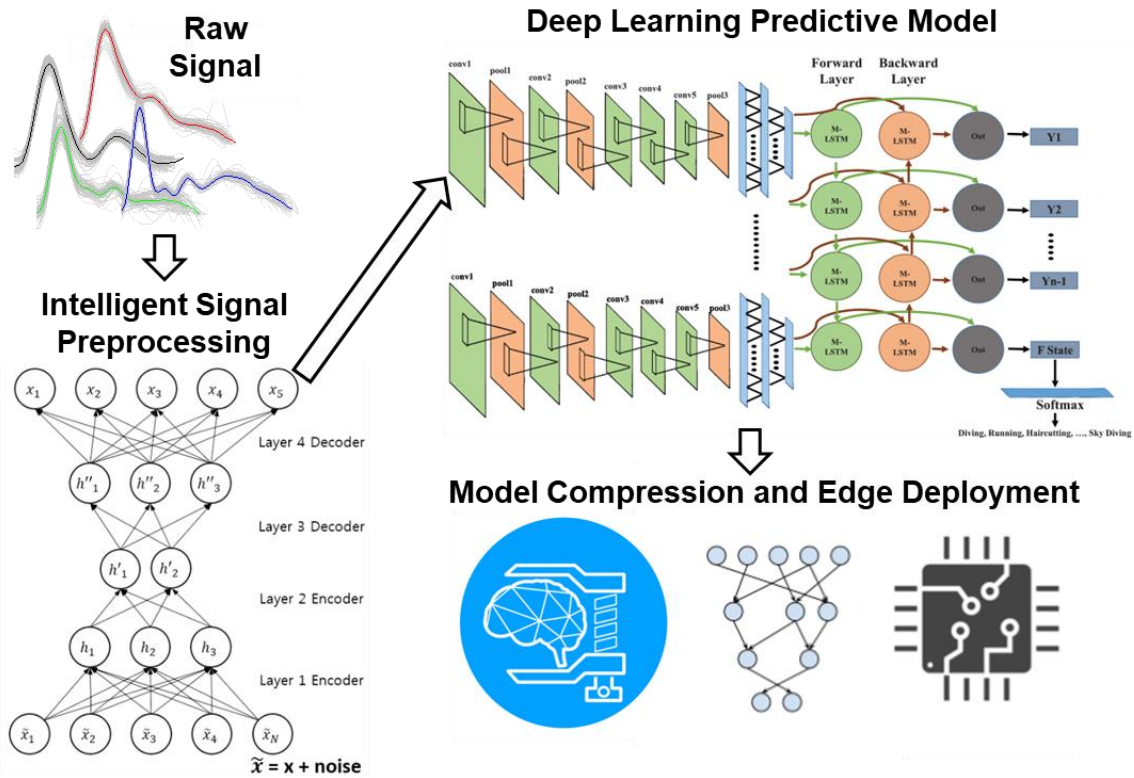


Figure 4.4: The system pipeline of the embedded intelligent decision making models for future E-skin applications, where the raw signals are passed to the intelligent signal preprocessing model⁸, and analyzed by the deep learning predictive model⁹. These models are deployed on computation edges through model compression¹⁰ techniques.

The future intelligent E-skin systems should also be portable to operate both online and offline. As shown in Fig. 4.5, this E-skin system should be integrated with wireless and edge computing modules to communicate with mobile devices. The light-weighted ML algorithms should be embedded in edge computing units to realize data analysis or actuator action control and the diagnosis results or suggested actions could be visualized on mobile devices. After storing enough amount of healthcare data, the key information would be uploaded to the cloud for the big data analysis and update the software systems on both

mobile and edge sides. We believe these proposed future functionalities will benefit diverse populations around the world.

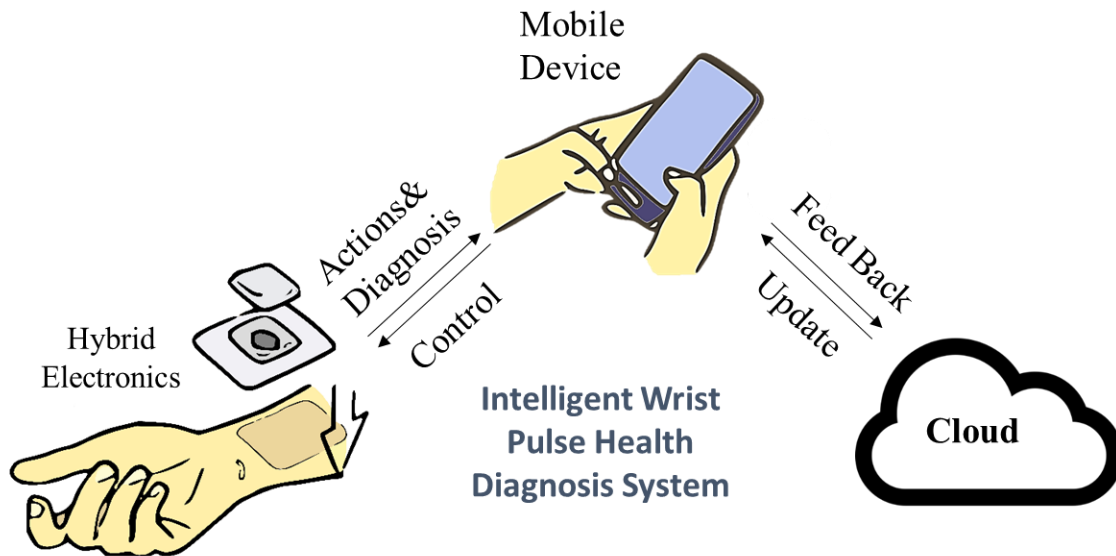


Figure 4.5: The schematic of the future intelligent E-skin health diagnosis system, including the interactions between the hybrid electronics, mobile devices and cloud side.

References of Chapter 4

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