Multiplex Detection with Multispectral Sensors and Machine Learning

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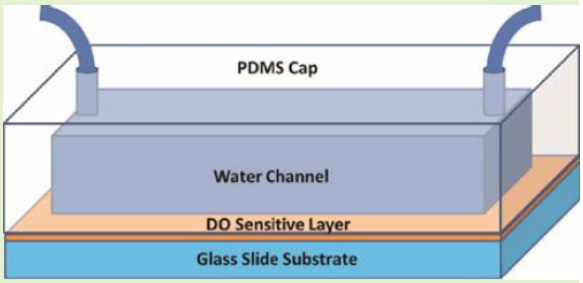

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B. Multi-spectral sensor in bio-assays

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C. Machine learning background

I think here is where we discuss background on Multiplex QD predictions and the benefit in using raspberry pi vs smart phone?

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S. B. Author, Jr., was with Rice University, Houston, TX 77005 USA. He is now with the Department of Physics, Colorado State University, Fort Collins, CO 80523 USA (e-mail: author@lamar.colostate.edu).

T. C. Author is with the Electrical Engineering Department, University of Colorado, Boulder, CO 80309 USA, on leave from the National Research Institute for Metals, Tsukuba, Japan (e-mail: author@nrim.go.jp).

II. Methods

Use either SI (MKS) or CGS as primary units. (SI units are strongly encouraged.) English units may be used as secondary units (in parentheses). This applies to papers in data storage. For example, write "15 Gb/cm^2 (100 Gb/in^2)." An exception is when English units are used as identifiers in trade, such as "3½-in disk drive." Avoid combining SI and CGS units, such as current in amperes and magnetic field in oersteds. This often leads to confusion because equations do not balance dimensionally. If you must use mixed units, clearly state the units for each quantity in an equation.

A. Multispectral sensing system

The SI unit for magnetic field strength H is A/m. However, if you wish to use units of T, either refer to magnetic flux density B or magnetic field strength symbolized as $\mu_0 H$. Use the center dot to separate compound units, e.g., "A·m^2."

B. Set up for testing our sensing system

The SI unit for magnetic field strength H is A/m. However, if you wish to use units of T, either refer to magnetic flux density B or magnetic field strength symbolized as $\mu_0 H$. Use the center dot to separate compound units, e.g., "A·m^2."

C. Description of Machine learning algorithms

We have used supervised machine learning to predict the QD concentration from the eight wavelength intensities. For each observation x_i for $i = 1, 2, .., n$ there is an associated response measurement y_i. The goal during training, is to approximate a mapping function from the input x to the output y variable, so that when given a new set of unknown input data, the algorithm can correctly predict the correct output variable. To avoid potential overfitting of the data, we have used 10fold-cross validation scheme.

We have tried 5 distinct types of ML algorithms to predict the QD concentration. In this section we provide a shot description and key properties of each ML algorithm. (following the style of Subhendu Pandit paper)

1) Univariate Models: One possible appraoch to predict multiple QD types is to train a model for each emitter. During inference time we run both models in sequence.

"Gaussian process regression is nonparametric (i.e. not limited by a functional form), so rather than calculating the probability distribution of parameters of a specific function, GPR calculates the probability distribution over all admissible functions that fit the data. However, similar to the above, we specify a prior (on the function space), calculate the posterior using the training data, and compute the predictive posterior distribution on our points of interest."

"Regression NN predict an output variable as a function of the inputs. The input features (independent variables) can be categorical or numeric types, however, for regression NN, we require a numeric dependent variable. If the output variable is a categorical variable (or binary) the ANN will function as a classifier"

TABLE I
MACHINE LEARNING MODELS

Model	Type	Accuracy*	Trainable Parameters
Gaussian Process Reggression	Univariate	4.5	N/A**
Linear Regression	Univariate	4.5	1
Bayesian Regression	Univariate	4.5	1
Random Forest Regession	Univariate	4.5	1
Neural Network	Univariate	4.5	1
Neural Network	Multiivariate	4.5	1

*Accuracy is measure of MSE for 10-fold Cross val. All models were tested using the same cross validation dataset breakdown. For univaraite models accuracy is the average between the two models
**Bayesian methods are non-parametric and therefore have no trainable parameters

" random forest is a meta estimator that fits a number of classifying decision trees on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is controlled with the max samples parameter if bootstrap=True (default), otherwise the whole dataset is used to build each tree"

" Support Vector Regression is a supervised learning algorithm that is used to predict discrete values. Support Vector Regression uses the same principle as the SVMs. The basic idea behind SVR is to find the best fit line. In SVR, the best fit line is the hyperplane that has the maximum number of points."

"Linear regression is a linear model, e.g. a model that assumes a linear relationship between the input variables (x) and the single output variable (y). More specifically, that y can be calculated from a linear combination of the input variables (x).

When there is a single input variable (x), the method is referred to as simple linear regression. When there are multiple input variables, literature from statistics often refers to the method as multiple linear regression."

2) Multivariate Models: Here we briefly discuss the extensions required to make some of the models multivariate

3) Frequentist vs Bayesian Models: here we discuss the key differences in assumptions and applications between bayesian methods and frequentist methods. Also discuss confidence intervals, and some considerations when comparing models.

D. Training Details

Here we can discuss general training details. Epochs, libraries we used. and other compute details

1) Hyper-parameter Optimization: Every algorithm attempted here has various hyper-parameters that affect the corresponding optimization process. These can have a significant difference in learning, so its important we employ a search to find optimal hyper-parameters. I think we can make a table in appendix showing optimal hyperparameters

III. Results

A. Characterizing the limit of detection

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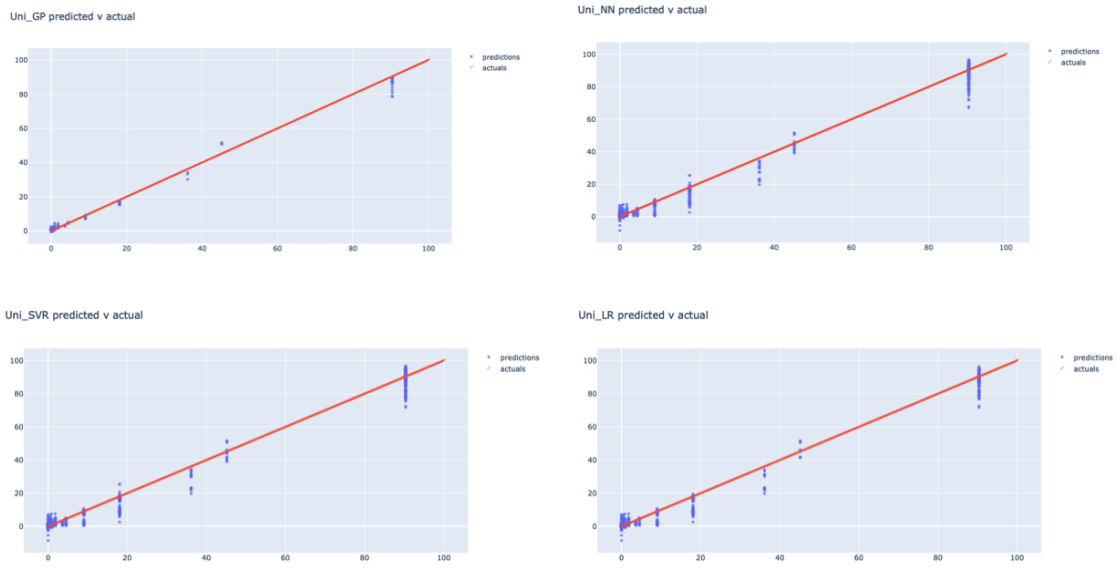

Fig. 1. Magnetization as a function of applied field. It is good practice to explain the significance of the figure in the caption.

B. Model Selection

1) Metrics: Figures that are composed of only black lines and shapes. These figures should have no shades or half-tones of gray, only black and white.

Here we discuss cross validation accuracy and BIC, AIC criterial?

2) Confidence interval for Bayesian Methods: Figures that are composed of only black lines and shapes. These figures should have no shades or half-tones of gray, only black and white.

C. Making Predictions

1) Raspberry Pi Details: Figures that are composed of only black lines and shapes. These figures should have no shades or half-tones of gray, only black and white.

2) Confidence Intervals for retraining: Figures that are composed of only black lines and shapes. These figures should have no shades or half-tones of gray, only black and white.

IV. Conclusion

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Appendixes, if needed, appear before the acknowledgment.

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The second paragraph uses the pronoun of the person (he or she) and not the author's last name. It lists military and work experience, including summer and fellowship jobs. Job titles are capitalized. The current job must have a location; previous positions may be listed without one. Information concerning previous publications may be included. Try not to list more than three books or published articles. The format for listing publishers of a book within the biography is: title of book (publisher name, year) similar to a reference. Current and previous research interests end the paragraph. The third paragraph begins with the author's title and last name (e.g., Dr. Smith, Prof. Jones, Mr. Kajor, Ms. Hunter). List any memberships in professional societies other than the IEEE. Finally, list any awards and work for IEEE committees and publications. If a photograph is provided, it should be of good quality, and professional-looking. Following are two examples of an author's biography.

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