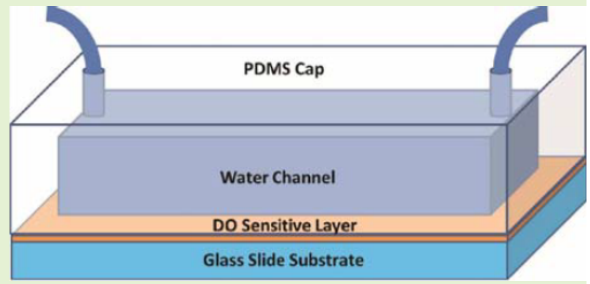
Multiplex Detection with Multispectral Sensors and Machine Learning

First A. Author, *Fellow, IEEE*, Second B. Author, and Third C. Author, Jr., *Member, IEEE*



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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).

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III. Machine learning implementation

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.

A. Model Definitions

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"

" 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."

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

"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.

B. 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

C. 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.

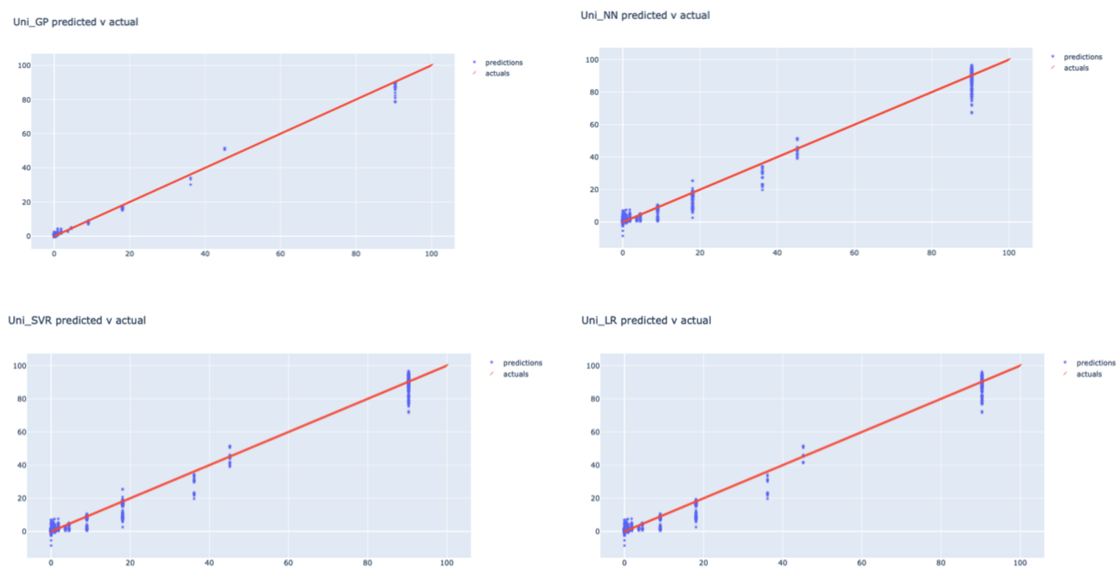

Fig. 1. Magnetization as a function of applied field. It is good practice to explain the significance of the figure in the caption.

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Second B. Author was born in Greenwich Village, New York, NY, USA in 1977. He received the B.S. and M.S. degrees in aerospace engineering from the University of Virginia, Charlottesville, in 2001 and the Ph.D. degree in mechanical engineering from Drexel University, Philadelphia, PA, in 2008.

From 2001 to 2004, he was a Research Assistant with the Princeton Plasma Physics Laboratory. Since 2009, he has been an Assistant Professor with the Mechanical Engineering Department, Texas A&M University, College Station. He is the author of three books, more than 150 articles, and more than 70 inventions. His research interests include high-pressure and high-density nonthermal plasma discharge processes and applications, microscale plasma discharges, discharges in liquids, spectroscopic diagnostics, plasma propulsion, and innovation plasma applications. He is an Associate Editor of the journal *Earth, Moon, Planets*, and holds two patents.

Dr. Author was a recipient of the International Association of Geomagnetism and Aeronomy Young Scientist Award for Excellence in 2008, and the IEEE Electromagnetic Compatibility Society Best Symposium Paper Award in 2011.

Third C. Author, Jr. (M'87) received the B.S. degree in mechanical engineering from National Chung Cheng University, Chiayi, Taiwan, in 2004 and the M.S. degree in mechanical engineering from National Tsing Hua University, Hsinchu, Taiwan, in 2006. He is currently pursuing the Ph.D. degree in mechanical engineering at Texas A&M University, College Station, TX, USA.

From 2008 to 2009, he was a Research Assistant with the Institute of Physics, Academia Sinica, Tapei, Taiwan. His research interest includes the development of surface processing and biological/medical treatment techniques using nonthermal atmospheric pressure plasmas, fundamental study of plasma sources, and fabrication of micro- or nanostructured surfaces.

Mr. Author's awards and honors include the Frew Fellowship (Australian Academy of Science), the I. I. Rabi Prize (APS), the European Frequency and Time Forum Award, the Carl Zeiss Research Award, the William F. Meggers Award and the Adolph Lomb Medal (OSA).