Visualization for Machine Learning models

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There is a lot of basic plots

FIGURE 2.1 The visuals I use most

Knaflic, C.N. *Storytelling with data: A data visualization guide for business professionals*. John Wiley & Sons, 2015

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We need specific plot for particular application areas

They are just basic plots, but with
specific curves or points displayed

We consider machine learning as an example

Main problem statements in Machine Learning

- Regression
- Classification
- Clustering
- Dimension reduction

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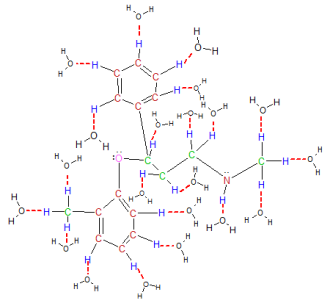
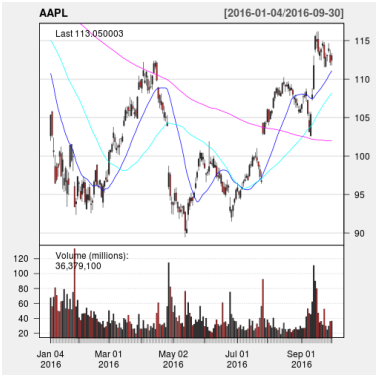
For regression target is continuous

We want to predict the target continuous value

Examples:

- Predict solubility of a molecule
- Predict price of a house
- Predict performance of a portfolio





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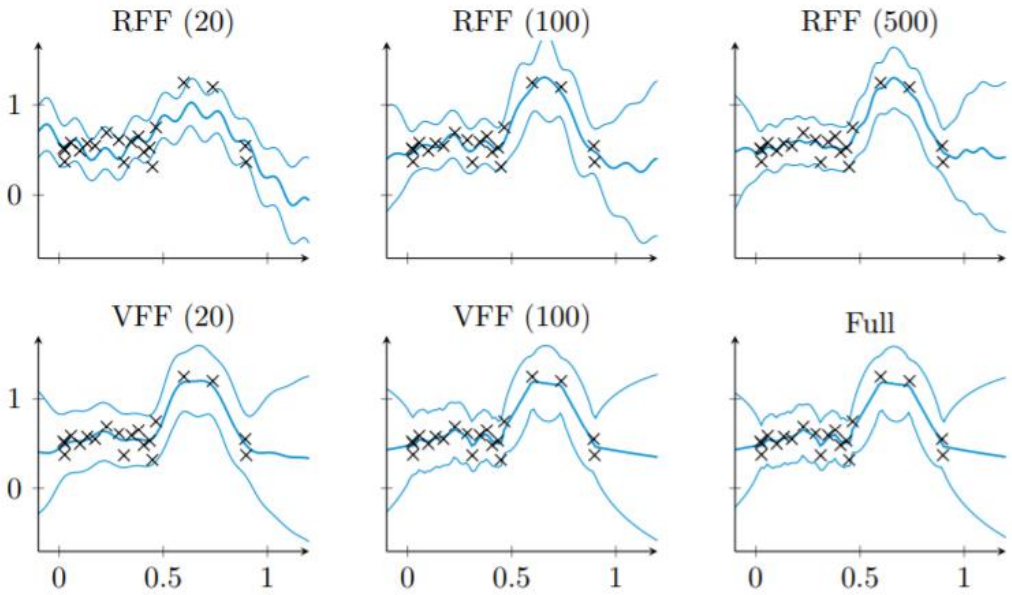
Simplest way: measure errors for different approach and get table

N	10,000		100,000		1,000,000		5,929,413	
	MSE	NLPD	MSE	NLPD	MSE	NLPD	MSE	NLPD
VFF	0.89 ± 0.15	1.362 ± 0.091	0.82 ± 0.05	1.319 ± 0.030	0.83 ± 0.01	1.326 ± 0.008	0.827 ± 0.004	1.324 ± 0.003
Full-RBF	0.89 ± 0.16	1.349 ± 0.098	N/A	N/A	N/A	N/A	N/A	N/A
Full-additive	0.89 ± 0.16	1.362 ± 0.096	N/A	N/A	N/A	N/A	N/A	N/A
SVIGP	0.89 ± 0.16	1.354 ± 0.096	0.79 ± 0.05	1.299 ± 0.033	0.79 ± 0.01	1.301 ± 0.009	0.791 ± 0.005	1.300 ± 0.003
String GP†	1.03 ± 0.10	N/A	0.93 ± 0.03	N/A	0.93 ± 0.01	N/A	0.90 ± 0.01	N/A
rBCM†	1.06 ± 0.10	N/A	1.04 ± 0.04	N/A	N/A	N/A	N/A	N/A

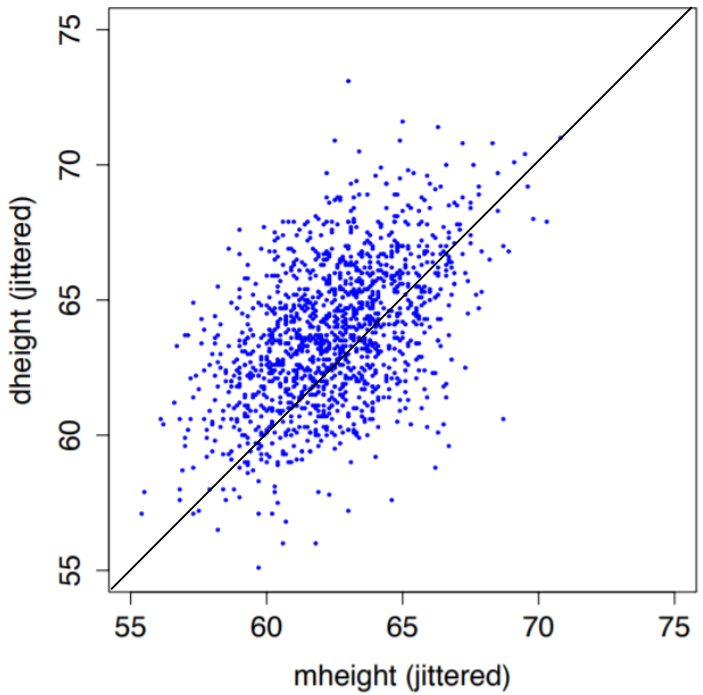
Hensman, James, Nicolas Durrande, and Arno Solin. "Variational Fourier features for Gaussian processes." *Journal of Machine Learning Research* 18, no. 151 (2018): 1-52.

Another simple way is to plot the model itself



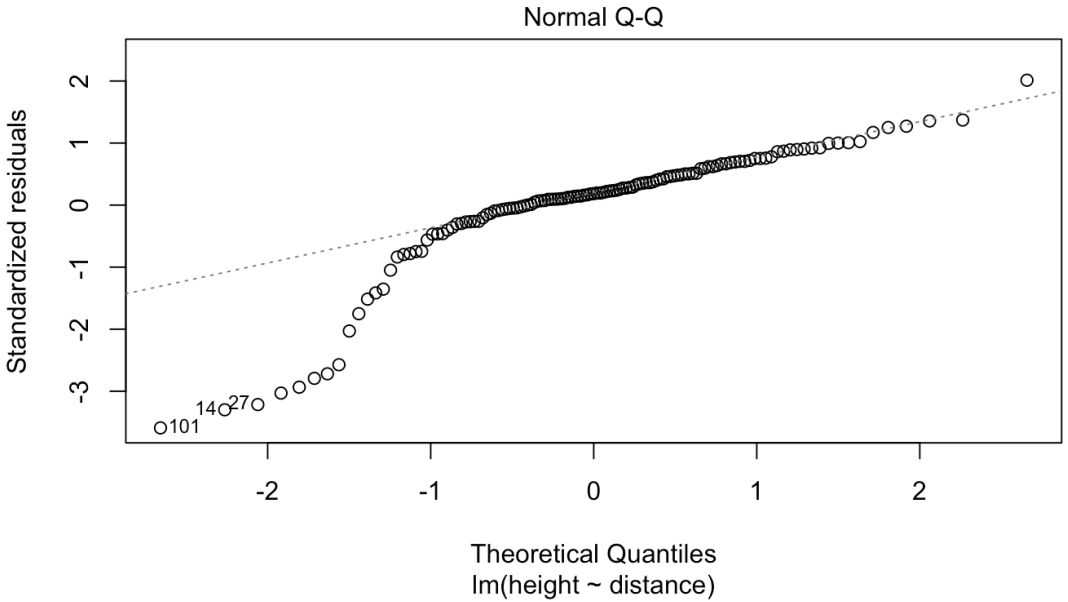
Hensman, James, Nicolas Durrande, and Arno Solin. "Variational Fourier features for Gaussian processes." *Journal of Machine Learning Research* 18, no. 151 (2018): 1-52.

Scatter plot



http://staff.washington.edu/dbp/s423/PDFs/01-chapter-ALR-for-printing.pdf

QQ plot



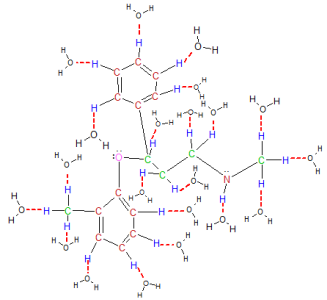
https://stats.stackexchange.com/questions/253916/what-does-this-q-q-plot-indicate-about-my-data

For classification target is discrete

We want to predict the target class of an object

Examples:

- Is the molecule a good drug?
- Will the customer pay a mortgage?
- What dog breed is at the figure?



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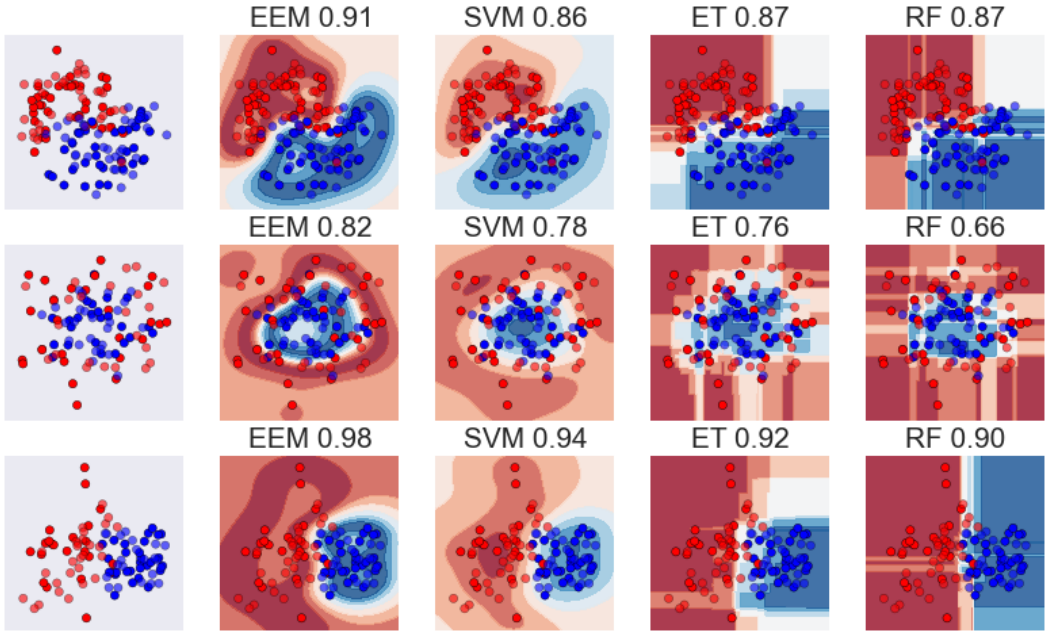
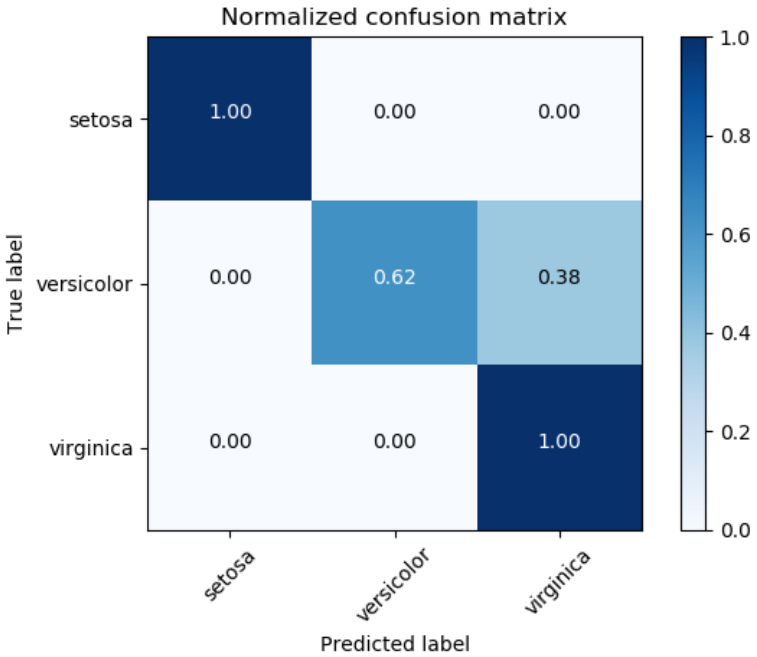
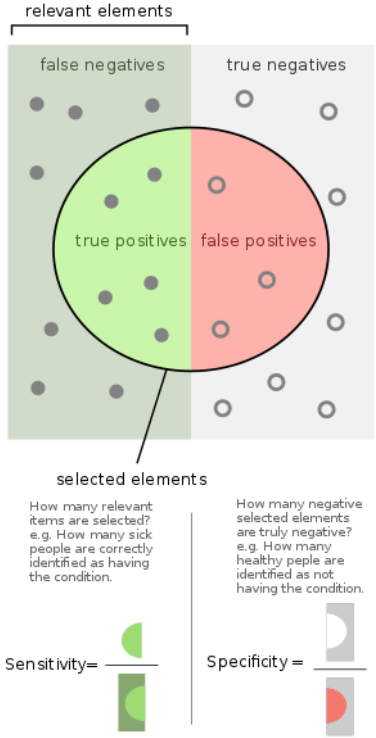
If data is 2D we can plot the model



https://www.researchgate.net/publication/283740661_Extremely_Randomized_Machine_Learning_Methods_for_Compound_Activity_Prediction

Simplest way: calculate errors

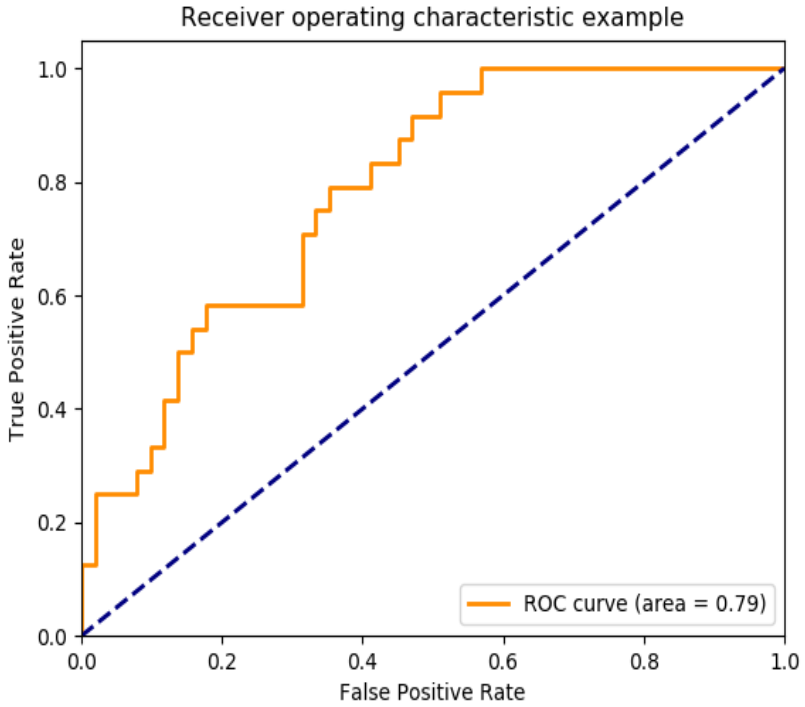


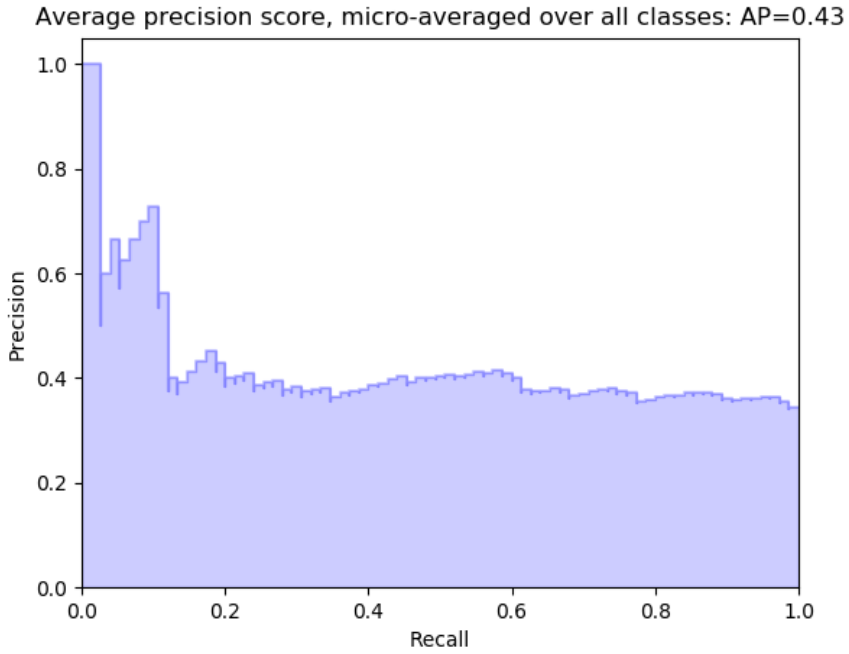


https://scikit-learn.org/stable/auto_examples/model_selection/plot_confusion_matrix.html

https://en.wikipedia.org/wiki/File:Sensitivity_and_specificity.svg

Simplest way: ROC & Precision Recall curves





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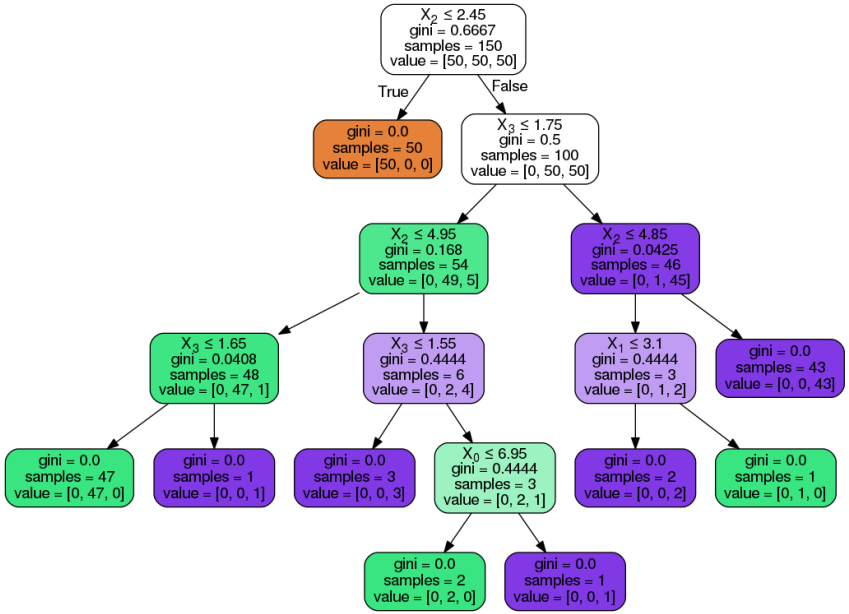
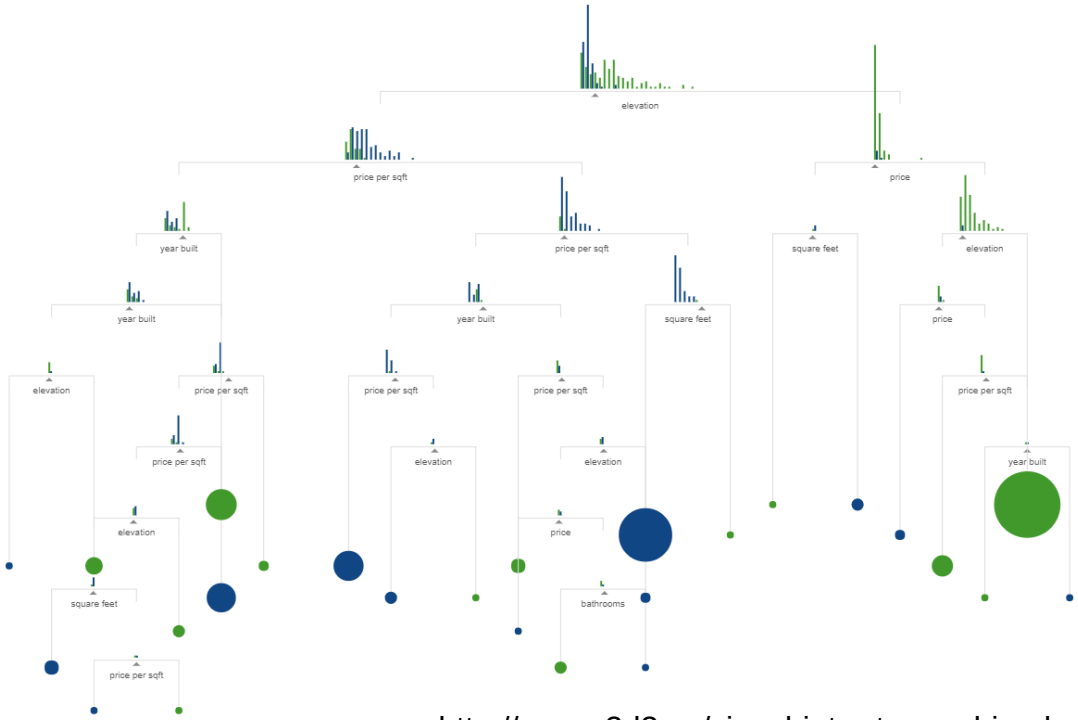
Visualize the model: decision tree



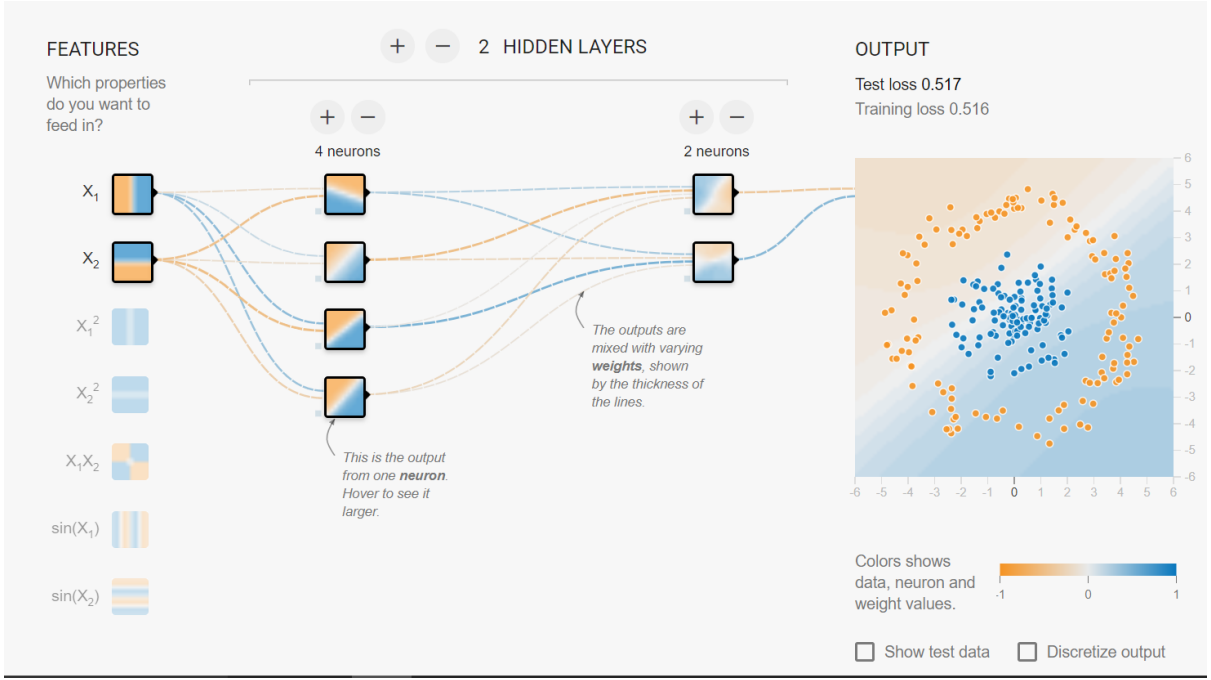
https://medium.com/@rnbrown/creating-and-visualizing-decision-trees-with-python-f8e8fa394176

Visualize the model: decision tree



http://www.r2d3.us/visual-intro-to-machine-learning-part-1/

Visualize the model: Neural Network



https://playground.tensorflow.org/

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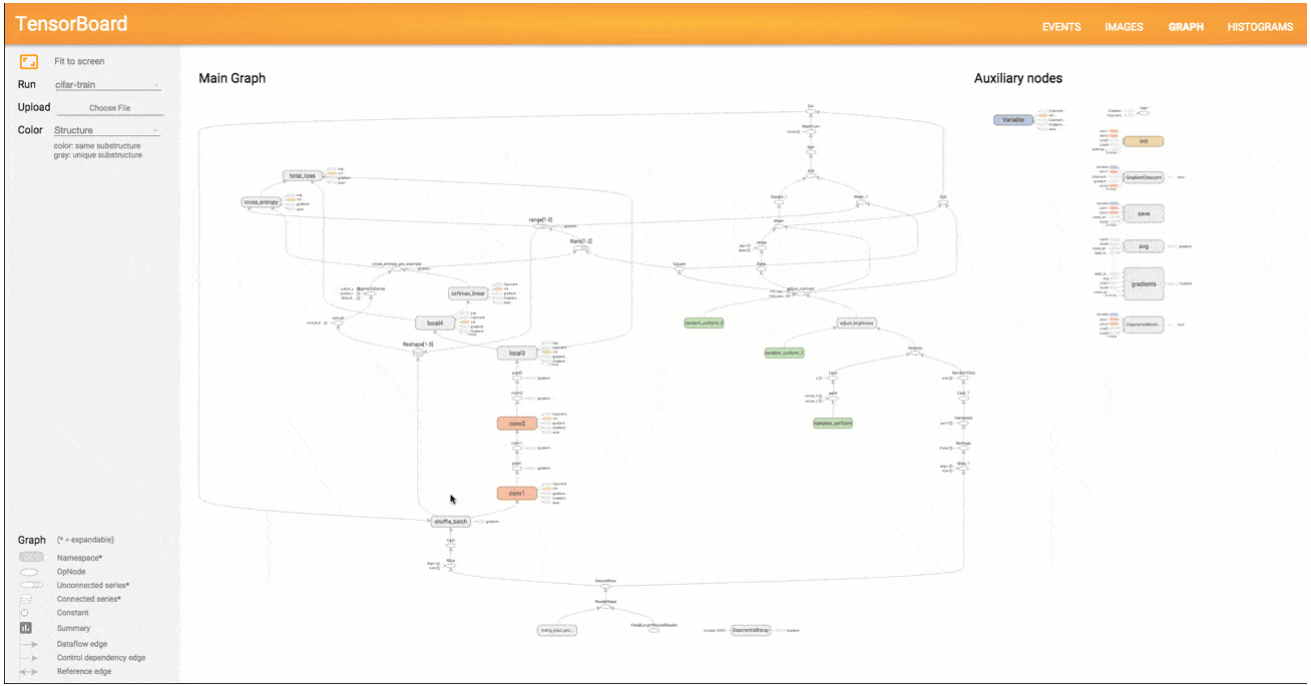
Visualize the model: Neural Network with Tensorboard



https://www.tensorflow.org/guide/graph_viz

Linear regression

```
print(results.summary())
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.075
Model:                            OLS   Adj. R-squared:                  0.026
Method:                 Least Squares   F-statistic:                     1.532
Date:                Sat, 02 Jul 2016   Prob (F-statistic):              0.216
Time:                        15:16:59   Log-Likelihood:                -725.57
No. Observations:                  61   AIC:                             1459.
Df Residuals:                      57   BIC:                             1468.
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
const      -7990.8552   1.18e+04     -0.679      0.500     -3.16e+04  1.56e+04
x1          6704.9269   6546.017      1.024      0.310     -6403.245  1.98e+04
x2           549.6695    458.838      1.198      0.236      -369.138  1468.477
x3          1.819e+04   1.48e+04      1.227      0.225     -1.15e+04  4.79e+04
==============================================================================
Omnibus:                      103.868   Durbin-Watson:                   2.058
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             2650.260
Skew:                           5.181   Prob(JB):                         0.00
Kurtosis:                      33.584   Cond. No.                         63.4
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

http://www.michaeljgrogan.com/statsmodels-sklearn-linear-regression/ols-regression-results/

Summary

- If you are into Machine learning there are specific plots
  - For regression it is scatter plot or box plot for cross-validation runs
  - For classification there are ROC and PR AUC curves

- There a lot of ways to visualize your machine learning models
  - Decision trees
  - Neural networks
  - Linear regression
  - …