

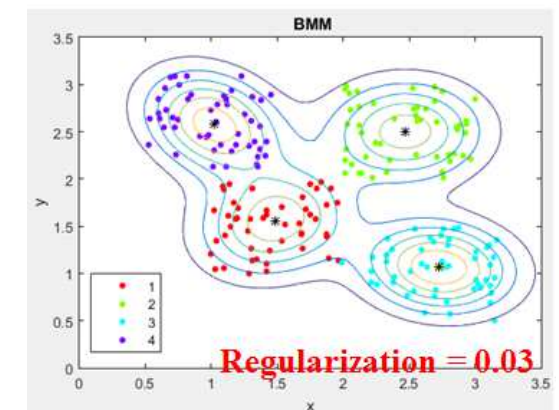
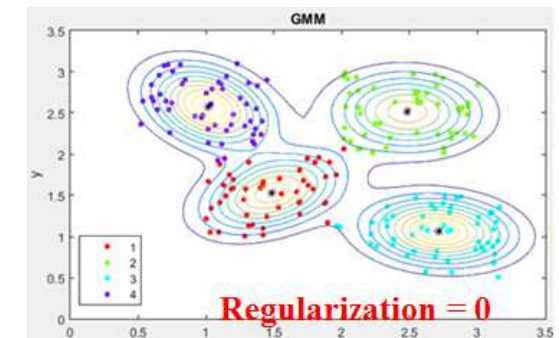
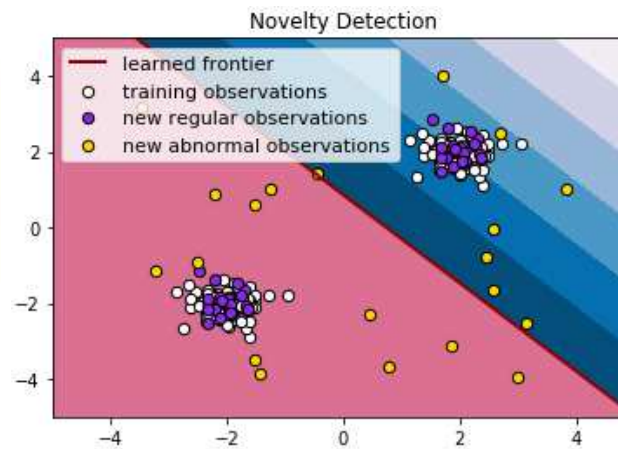
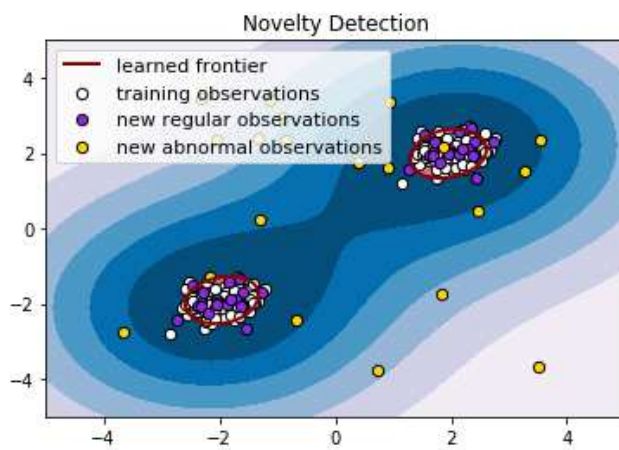
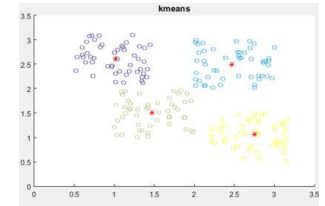
SVM One Class Classification

■ Matlab `fitcsvm()` or Sklearn `svm.OneClassSVM()`

- An unsupervised method to learn a decision function for novelty detection.
- Classify new data as how similar or how different to the training set. **kNN??**

- **Like clustering???** Compare either to *k-means* or *GMM* (Gaussian Mixture Model).

- <http://scikit-learn.org/stable/modules/generated/sklearn.svm.OneClassSVM.html#sklearn.svm.OneClassSVM>
- http://scikit-learn.org/stable/auto_examples/covariance/plot_outlier_detection.html#sphx-glr-auto-examples-covariance-plot-outlier-detection-py
- http://scikit-learn.org/stable/auto_examples/svm/plot_oneclass.html



```
# kernel must be one of 'linear', 'poly', 'rbf', 'sigmoid'
clf = svm.OneClassSVM(nu=0.1, kernel="rbf", gamma=0.1)
clf.fit(X_train); y_pred_test = clf.predict(X_test)
```

One-Class SVM Experiments

■ sklearn dataset

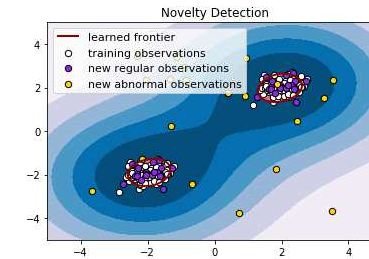
- Build **only 1 one**-class SVM from ...
- Data of (**one** class (majority) + outliers (minority)).

% one-class SVM

yy = Y * 0; %% make all labels = 0

mdl_c1 = fitsvm(X, yy, , 'KernelFunction', 'rbf');

[~, scores_c1] = predict(mdl_c1, X);



■ Iris dataset

- Build **2 one**-class SVMs from ...
- Unbalanced data of (**two** classes).
- Compare to **1 two**-class SVM.



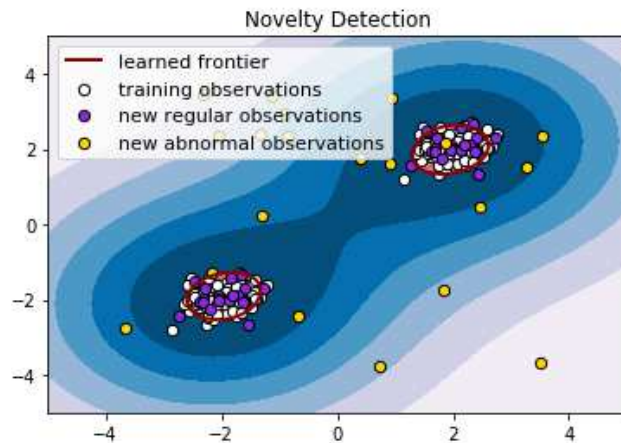
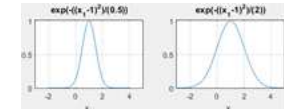
■ Ovarian cancer dataset

- Build **2** one-class SVMs from ...
- **Super** unbalanced data of (**two** classes).
- **4,000**-dimension data.



SVM RBF One Class, NO Kernel Scale

- http://scikit-learn.org/stable/auto_examples/svm/plot_oneclass.html#sphx-glr-auto-examples-svm-plot-oneclass-py

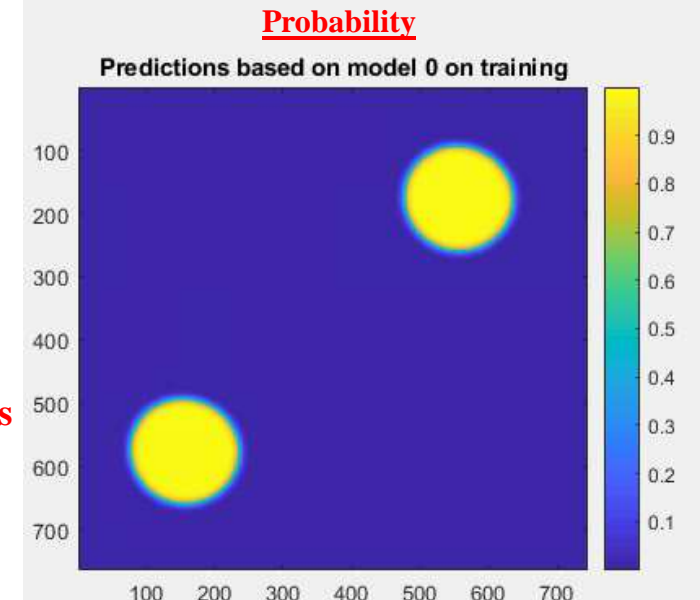
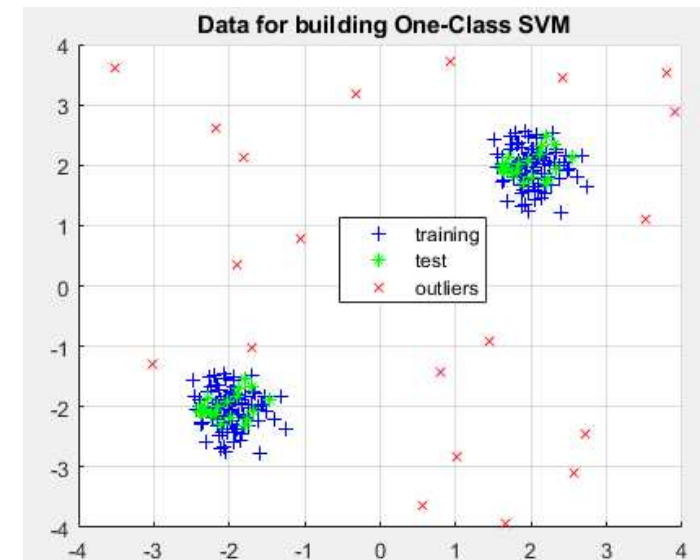


```
# data
rng(10)

XX = 0.3 * randn(100, 2);
X = [XX + 2; XX - 2];
Y = zeros(size(X, 1), 1);

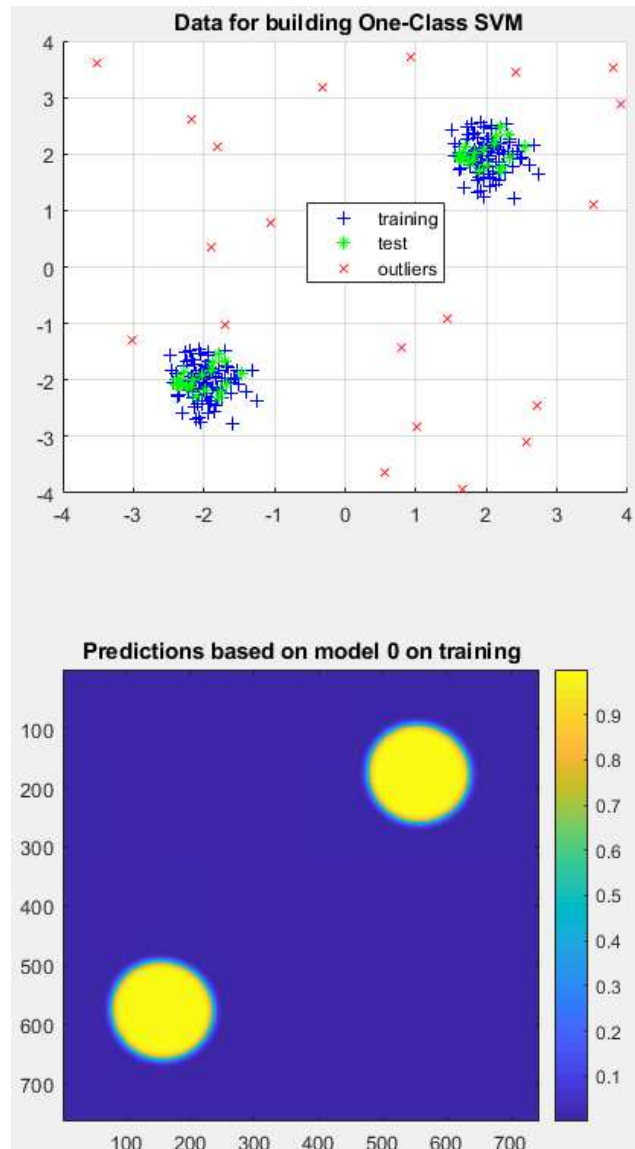
XX = 0.3 * randn(20, 2);
X_test = [XX + 2; XX - 2];

% Generate outliers
a = -4; b = 4;
X_outliers = (b-a).*rand(20,2) + a;
```

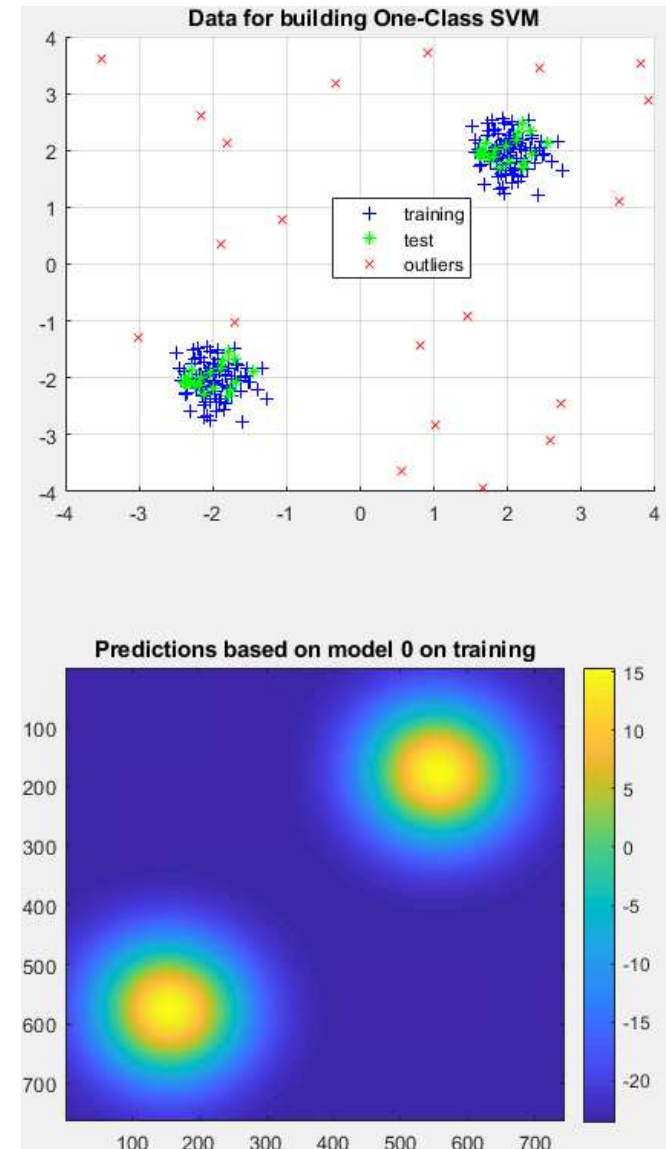


SVM RBF One Class, NO Kernel Scale

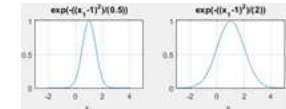
Probability



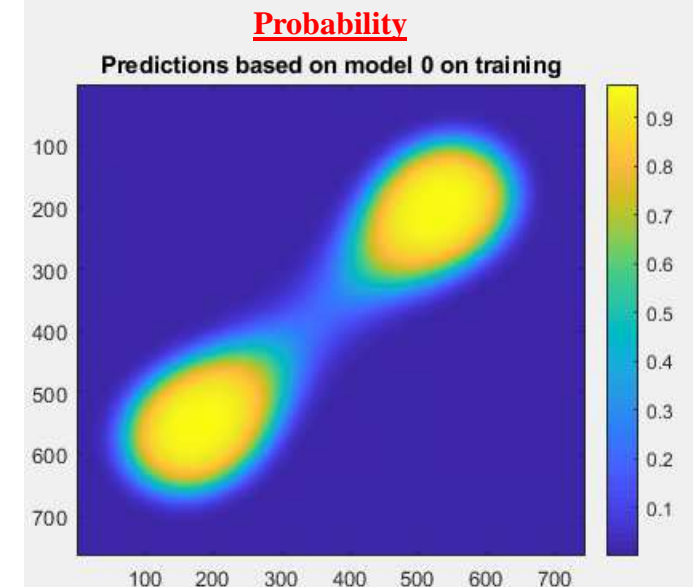
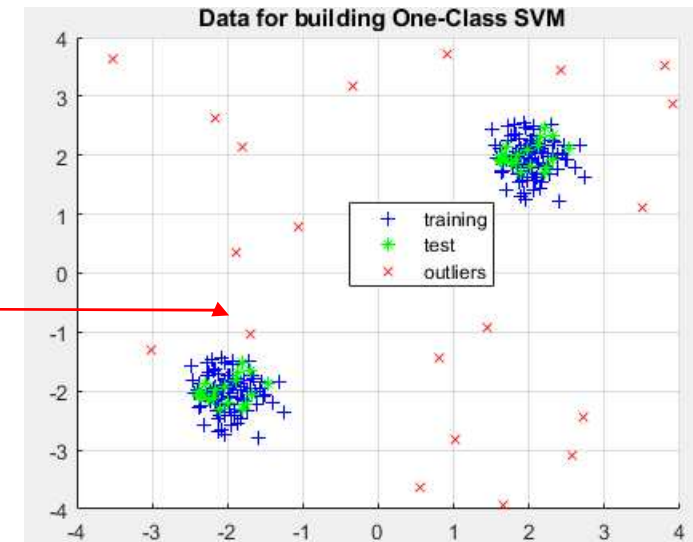
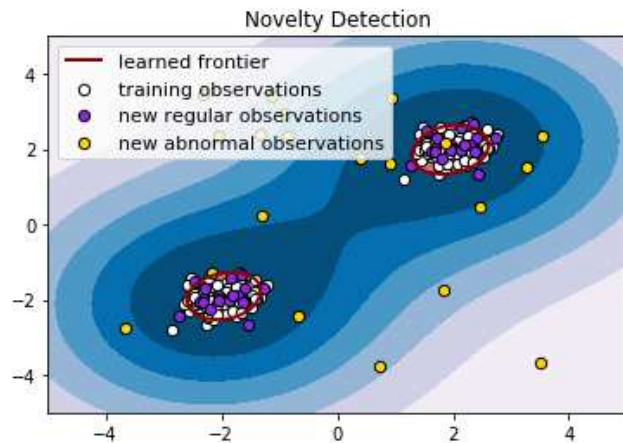
$W^T X$



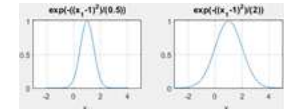
SVM RBF One Class, **Kernel Scale = 3.5**



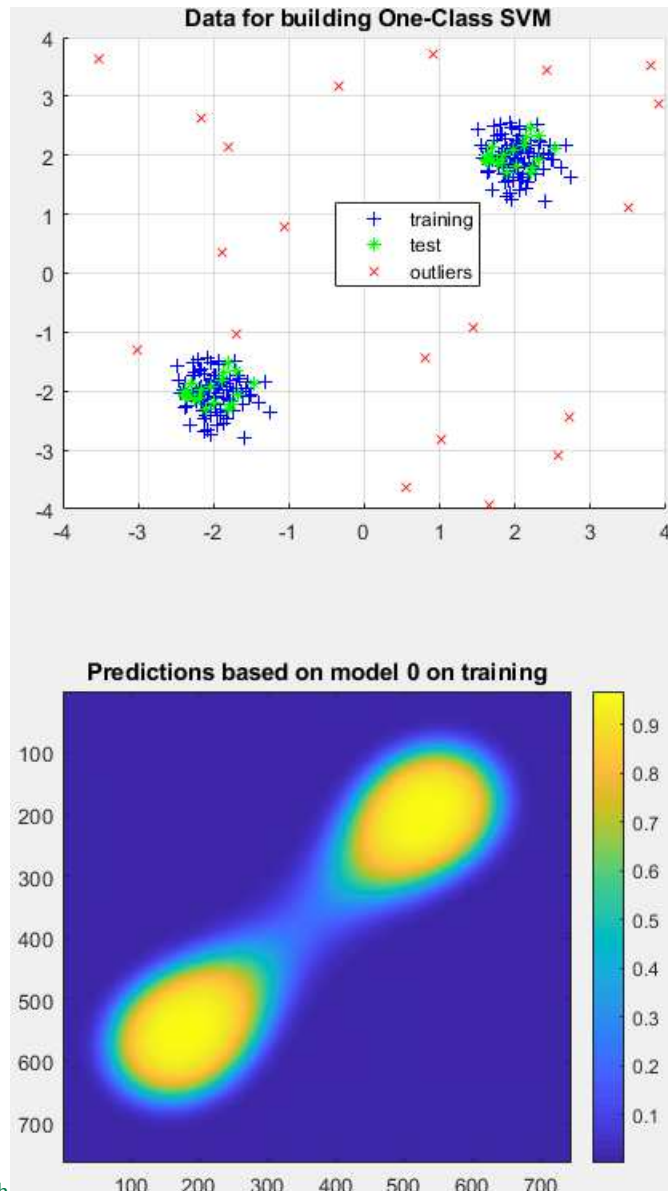
- http://scikit-learn.org/stable/auto_examples/svm/plot_oneclass.html#sphx-glr-auto-examples-svm-plot-oneclass-py



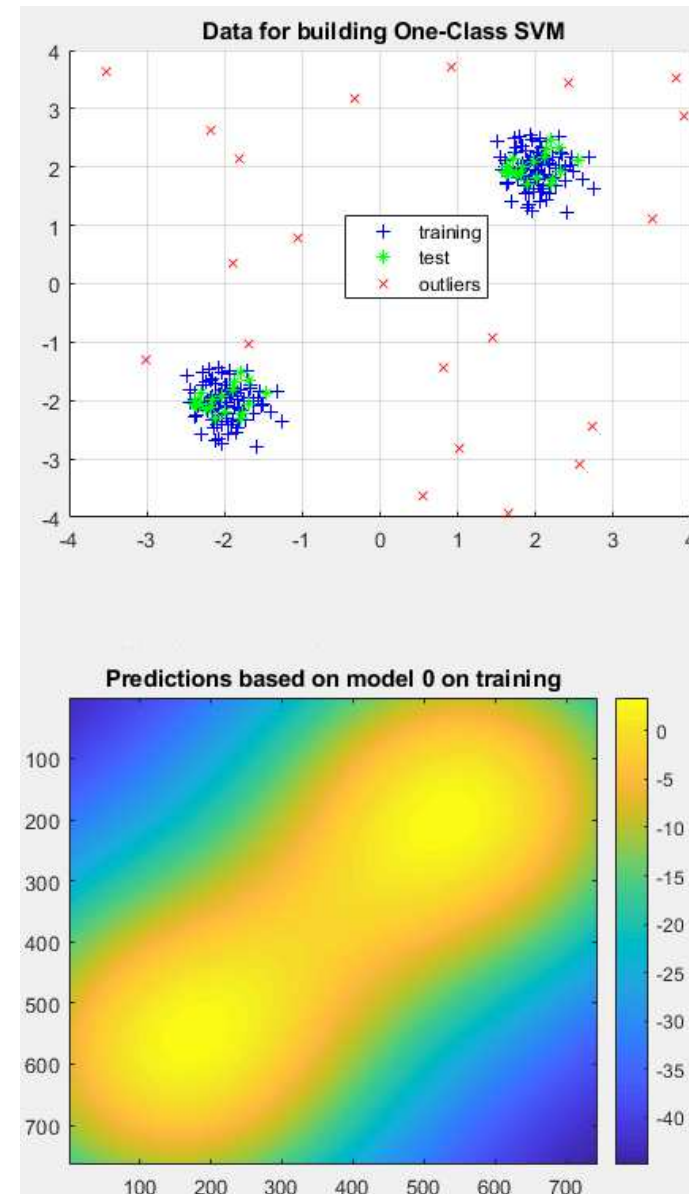
SVM RBF One Class, **Kernel Scale = 3.5**



Probability



$W^T X$



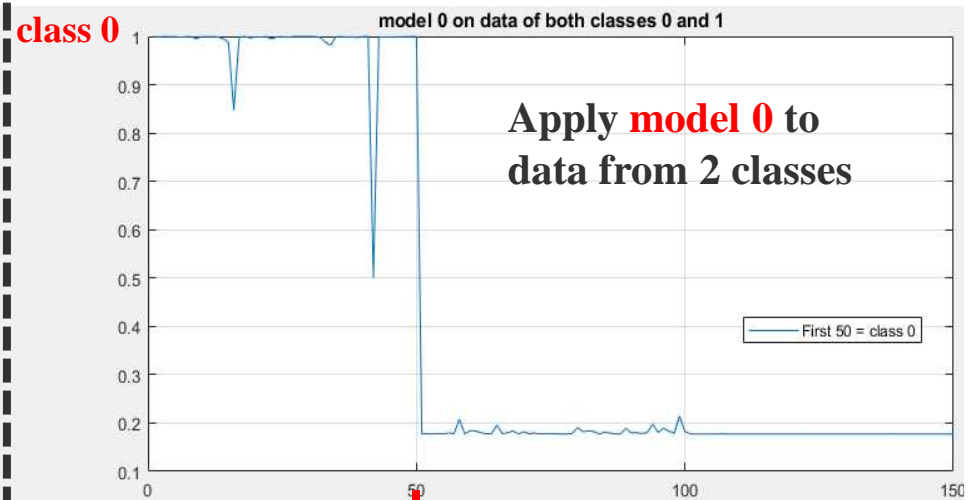
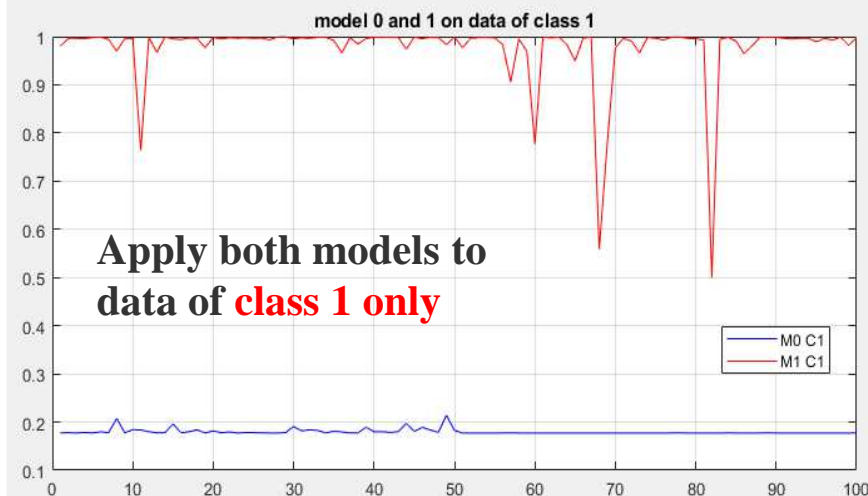
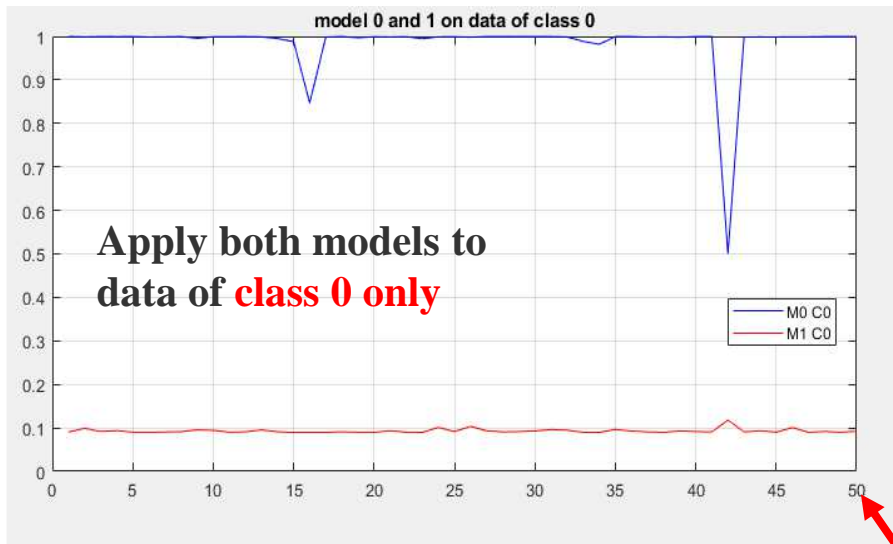
Iris Dataset



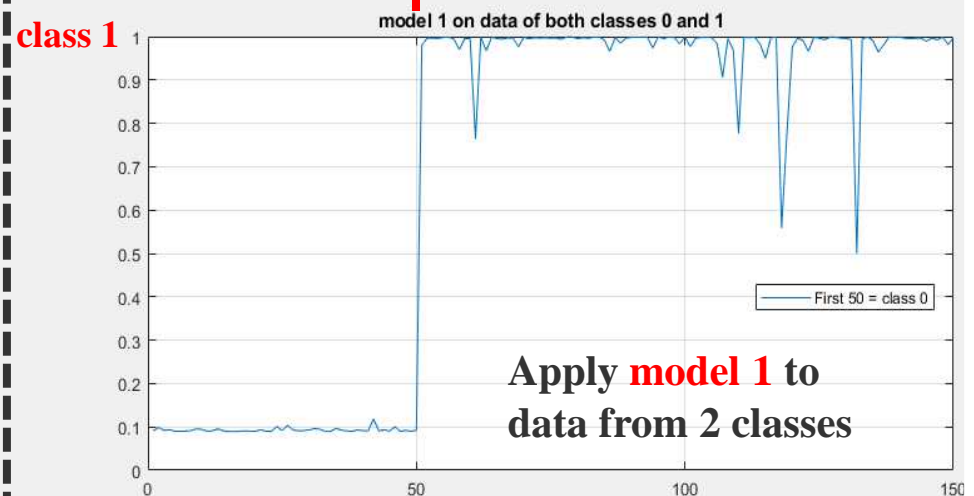
```
idx1 = find(Y);    idx0 = find(Y == 0);  
x0 = X(idx0,:);    y0 = Y(idx0);  
x1 = X(idx1,:);    y1 = Y(idx1);  
  
% for class 0  
mdl_c0 = fitsvm(x0, y0, , 'KernelFunction', 'rbf');  
[~, scores_c0] = predict(mdl_c0, x0);  
  
% for class 1 ...
```

SVM / RBF One Class for Unbalanced Iris (50 vs. 100) Dataset

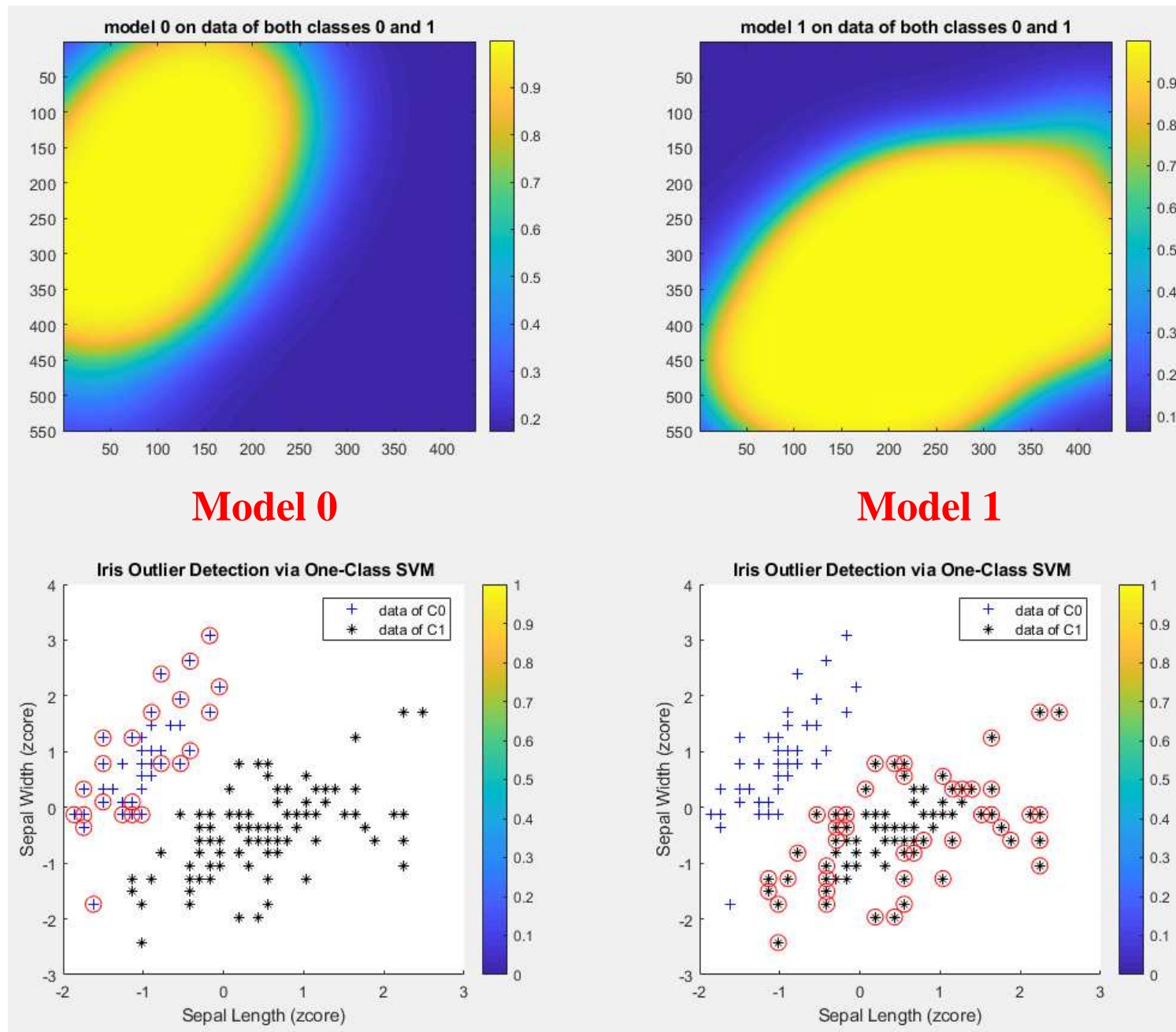
- Build model 0 (M0) from data of class 0 (first 50 rows) only.
- Build model 1 (M1) from data of class 1 (100 rows) only.



class 0 \longleftrightarrow class 1



SVM / RBF One Class for Unbalanced Iris (50 vs. 100) Dataset– Cont'd



SVM / RBF for Unbalanced Iris (50 vs. 100) Data– One 2-Class SVM

- Build ****ONE**** 2-Class model from both classes.



Ovarian Cancer Dataset

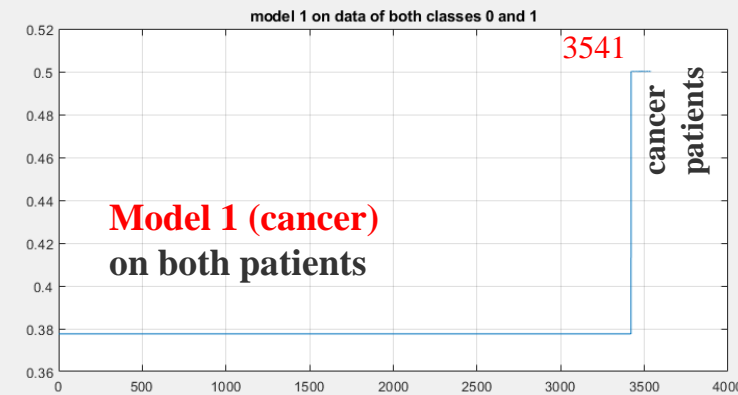
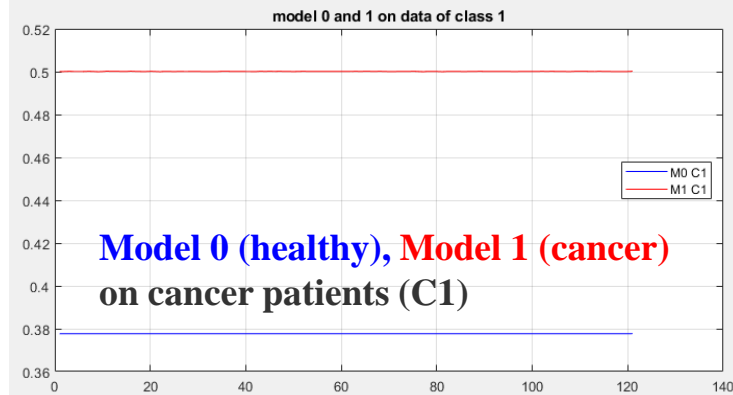
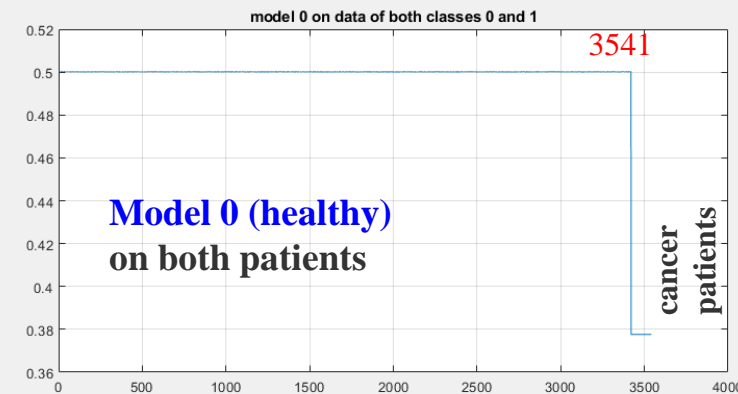
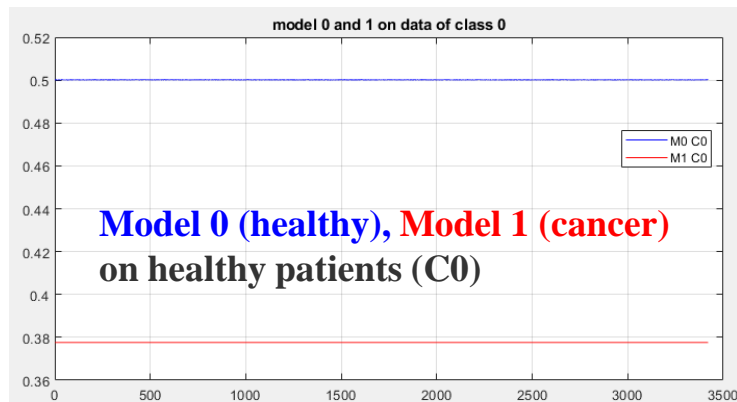


Detecting Super Unbalanced Ovarian Cancer Patients (One-Class)

- M0 was trained on healthy patients (C0).
- M1 was trained on ovarian cancer patients (C1).
- Duplicate healthy records couple times to create a skewed dataset
 - Original data, total 261, Cancer = 121 (46%).

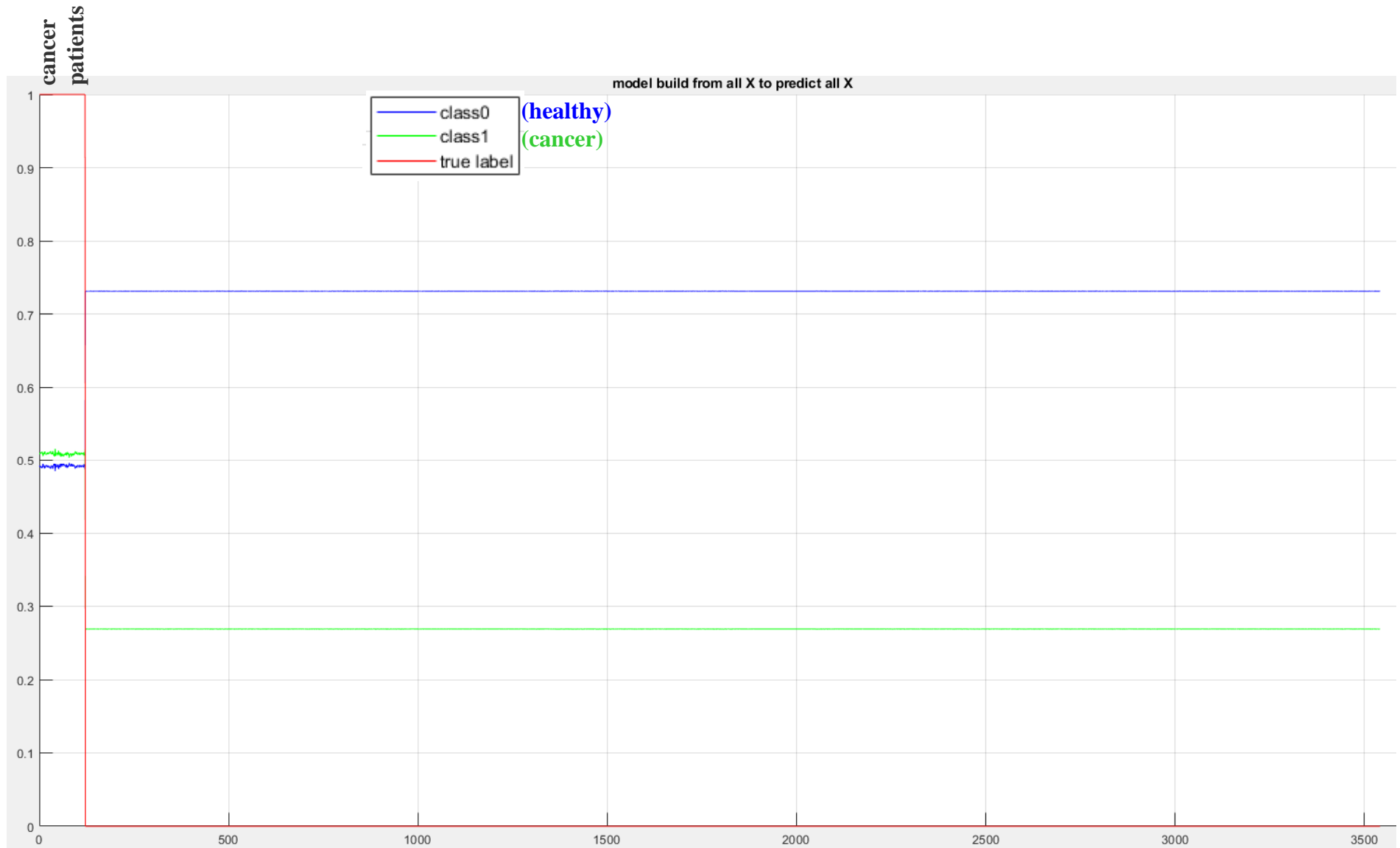
```
idx1 = find(Y);    idx0 = find(Y == 0);
x0 = X(idx0,:);    y0 = Y(idx0);
x1 = X(idx1,:);    y1 = Y(idx1);
mdl_c0 = fitsvm(x0, y0, , 'KernelFunction', 'rbf');
[~, scores_c0] = predict(mdl_c0, x0);
```

Duplicate data, total 3662, Cancer = 121 (3.4%)



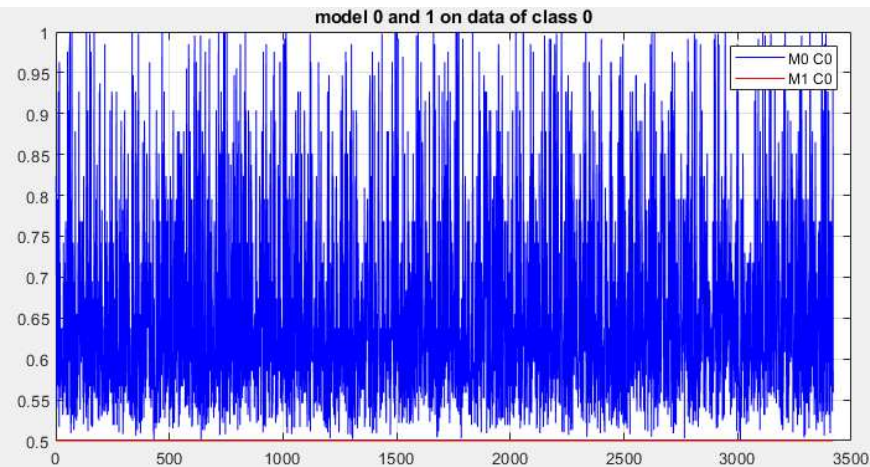
Build One 2-Class SVM

- Build one 2-class SVM model from ****ALL**** (unbalanced) patients.

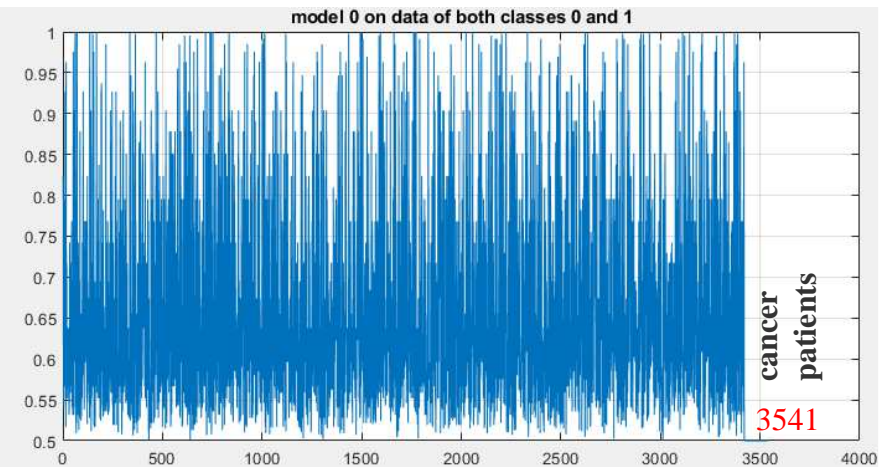


Super Unbalanced Ovarian Cancer Patients (1-Class), **Kernel Scale = 0.1**

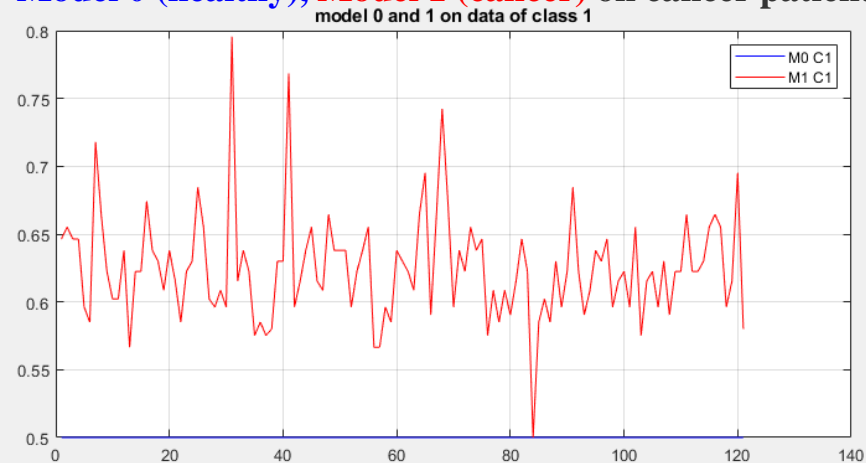
Model 0 (healthy), Model 1 (cancer) on healthy patients



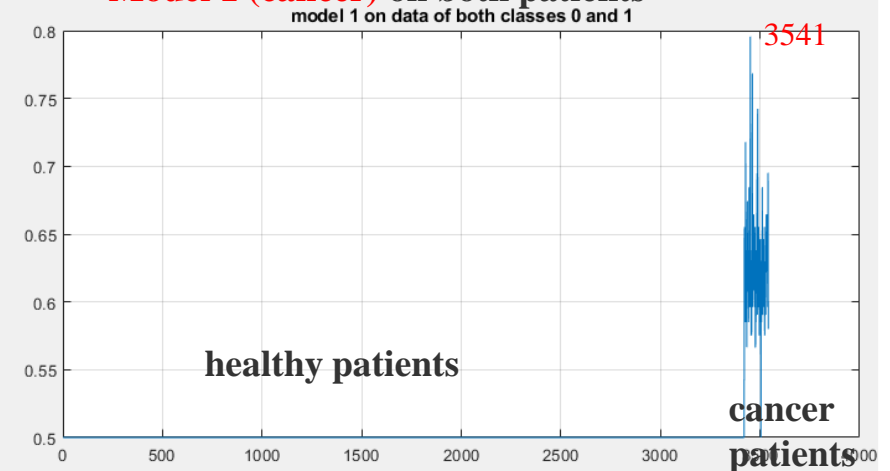
Model 0 (healthy) on both patients



Model 0 (healthy), Model 1 (cancer) on cancer patients



Model 1 (cancer) on both patients

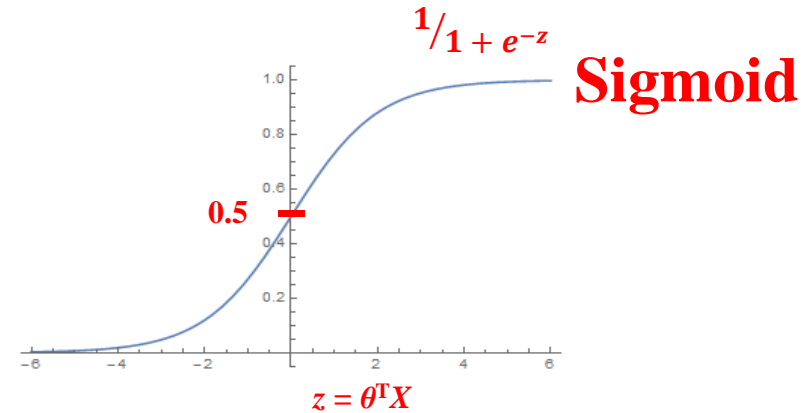


Apply One-Class Classification Using Logit??

■ Objective Function for Logistic Regression

- minimize *negative log likelihood*

$$\frac{-1}{m} \sum_{i=1}^m [Y_i \log(P_i) + (1 - Y_i) \log(1 - P_i)]$$



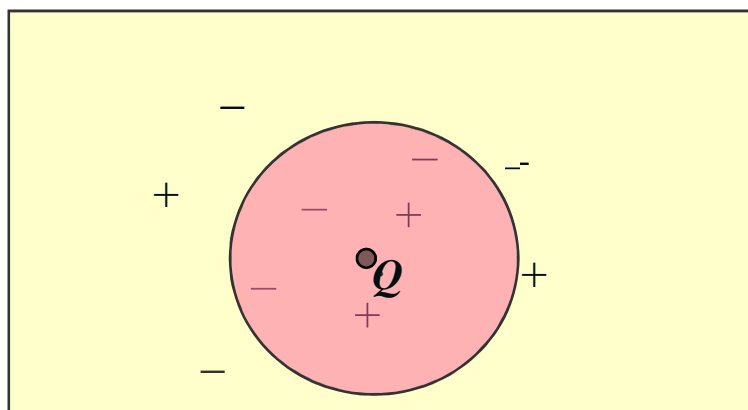
■ Object function for SVM Kernel

- Min $L_D = \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j - \sum_{i=1}^m \alpha_i$ (Dual form)
- Min $L_D = \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \Phi(\mathbf{x}_i) \Phi(\mathbf{x}_j) - \sum_{i=1}^m \alpha_i$

Instance-Based Methods

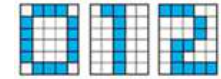
- **Eager** instance-based learning, like SVM-RBF.
- **Lazy** instance-based learning. Store past data, **NO** model construction.
 - Approach 1– *k*-nearest neighbor (*k*NN)
 - All instances (records) are represented as points in the n -D Euclidean space.
 - Assign the majority class of the nearest neighbors to the new (unseen) data.
 - For each query, finding *k*NN can be very time consuming.
 - ➡ *k*-nearest neighbors can be far away (very dissimilar) from Q .
 - Approach 2– *range query*

+ $k=11$



Outlook	Temp.	Humid	Windy	Play
S	W	H	F	N
S	W	H	T	N
O	W	H	F	Y
R	M	H	F	Y
R	C	L	F	Y
R	C	L	T	N
O	C	L	T	Y
S	M	H	F	N
S	C	L	F	Y
R	M	L	F	Y
S	M	L	T	Y
O	M	H	T	Y
O	W	L	F	Y
R	M	H	T	N

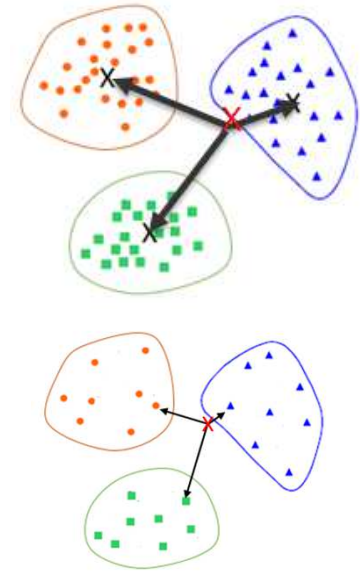
kNN for Digit Recognition



- Compute distance between each test instance against **ALL** training data
 - Predict query image based on majority of k NN digits. Slow to run.

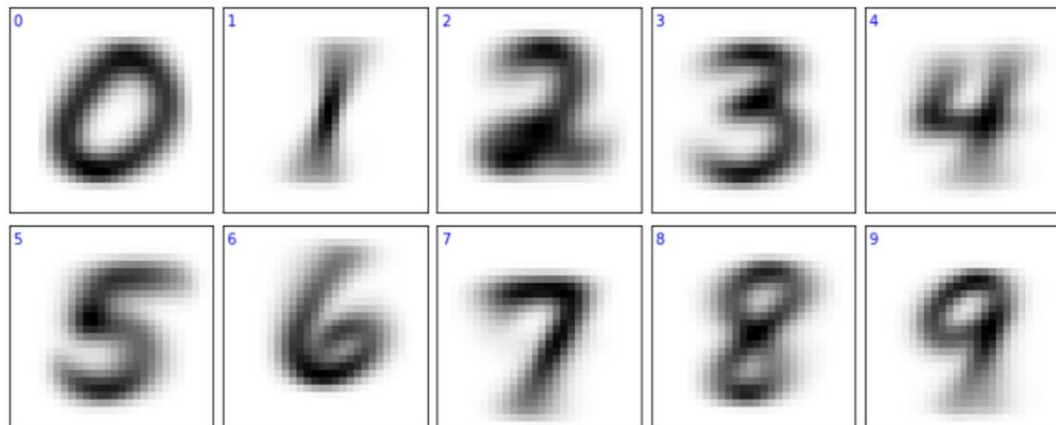
- Improvements?

- **Idea 1:** classifying based on distance to the **center** of each class.
 - **What is the center of each class?**
- **Idea 2:** using smaller samples of the dataset.



- Data Source: <https://www.kaggle.com/c/digit-recognizer/data>

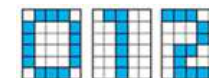
center of each class



Digit Recognition, DM-02-18S

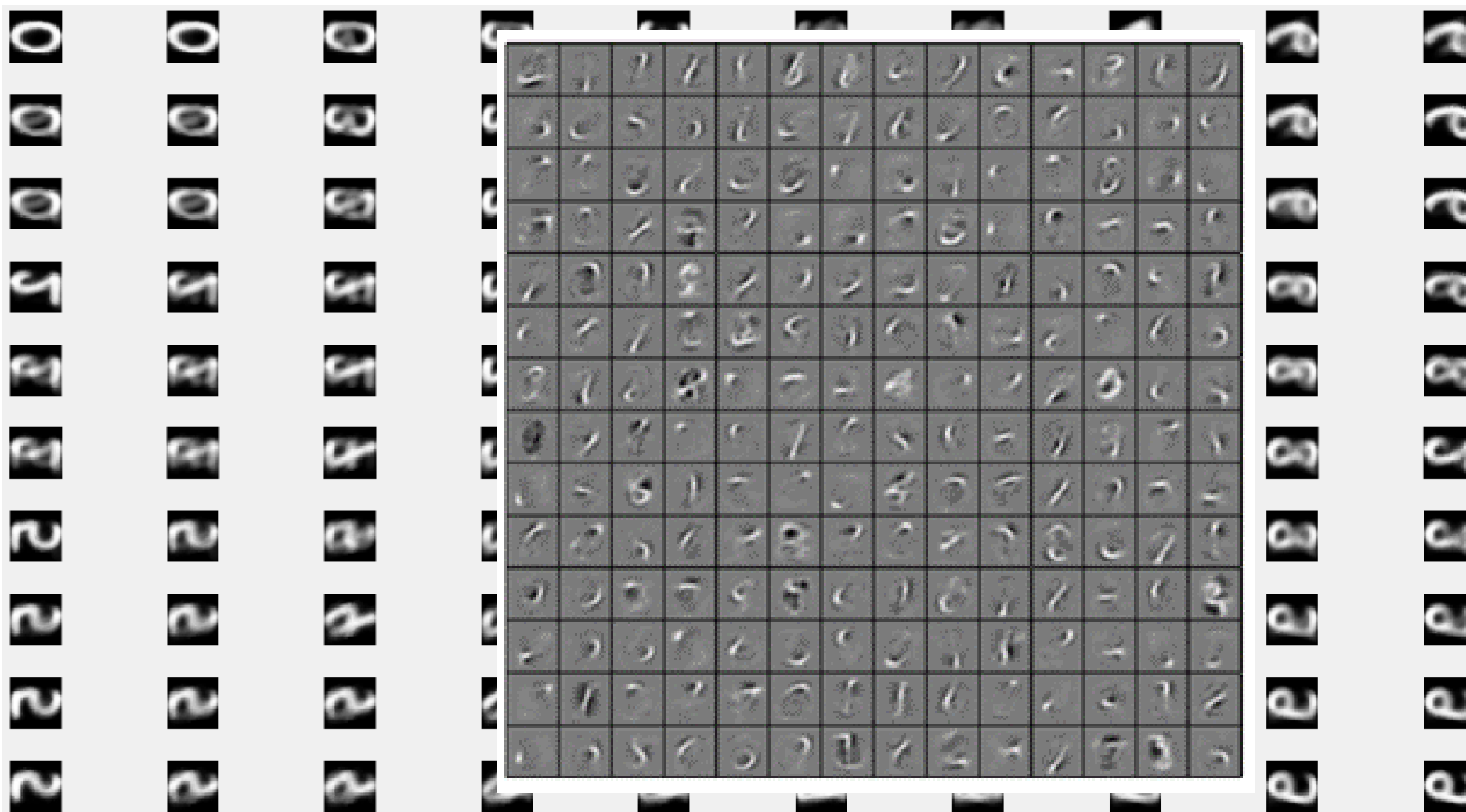
Alreshidi Abdulaziz, Yogita Singh
Bader Albulayhis, Sidi Mohamed,

Self Organizing Map (SOM)



- MUCH “better” alternative → **Convolutional Neural Network** (CNN).
 - Less recognizable patterns. They are no longer centers. They are *features*.

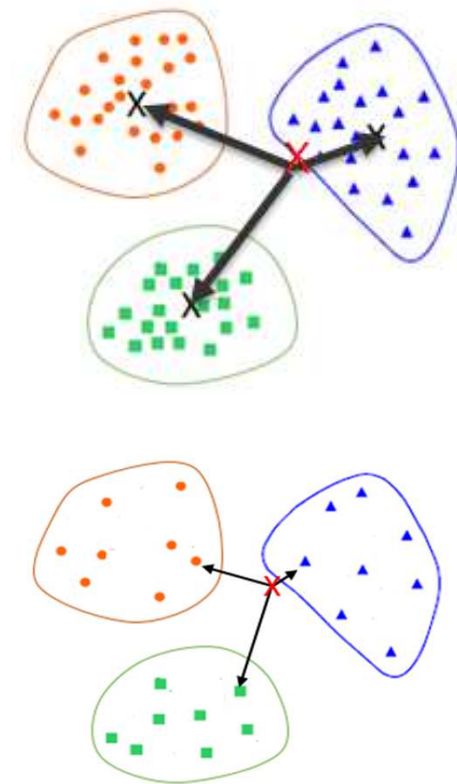
10×10 SOM neurons



Idea 2: Using Smaller Samples from Training Data

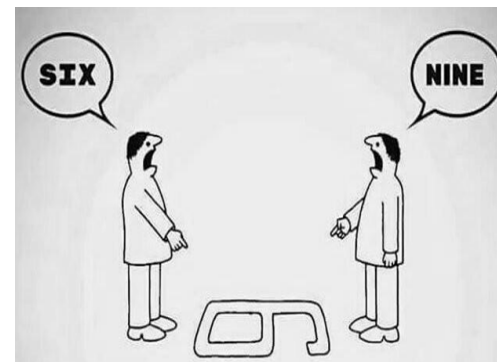
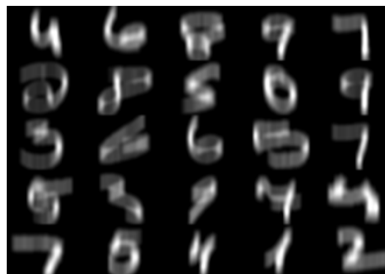
- Much faster with accuracy tradeoff.

data size used in kNN	Accuracy	Exe Time
400 (1% of the data)	84%	1sec
2000 (5% of the data)	91%	20 sec
5000 (12.5% of the data)	93%	50 sec
10000 (25% of the data)	95%	2min



Digit Recognition, DM-02-18S

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Bader Albulayhis, Sidi Mohamed,



Compare kNN Classification Quality to Other Methods

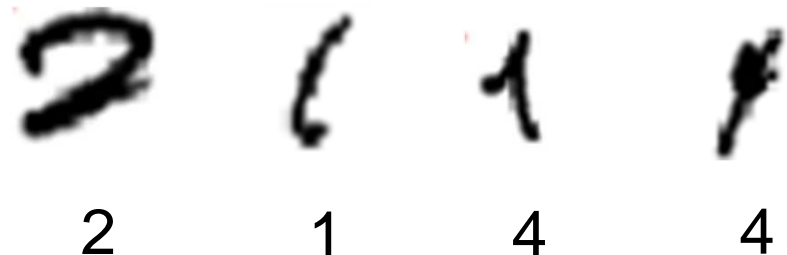
- Computing time is bit longer. But, kNN produce not bad result.
- How about executing time and quality of SVM or SVM+RBF?
- **How about advanced NN (i.e. CNN)???**

Algorithm	Accuracy (%)
Decision Tree	85
Naïve Bayes	82.55
KNN	96.0
Random Forest	96
MLP ← Regular NN	94

Digit Recognition, DM-02-18S

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Bader Albulayhis, Sidi Mohamed,

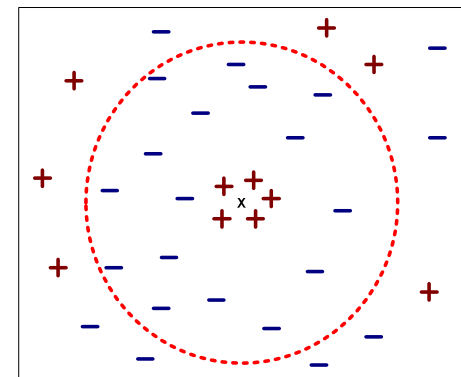
- Some writings are difficult to classify...



Issues in k NN, or Instance-Based Learning

■ Difficult choosing right k value

- If k is too small, sensitive to noise points
- If k is too large, neighborhood may include points from other classes



■ Numeric attributes with different scales.

- Distance measures may be dominated by one of the attributes
 - Heights of persons vary from 1.5m to 1.8m. \$\$ of persons vary from \$100K to \$100B.

■ Binary attributes.

$$\begin{array}{l} \text{R1} = (0 \quad 0 \quad 0) \\ \text{R2} = (1 \quad 1 \quad 0) \\ \text{R3} = (1 \quad 0 \quad 1) \end{array}$$

■ Categorical attributes. (e.g. diseases, states...)

- Convert them to dummy variables...
- **That's it??!!**
- Before **RBF**, we **never** compare distance btwn records.
 - We only derive θ to compute $\theta^T X$.

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

Lazy vs. Eager Learning

■ Lazy evaluation

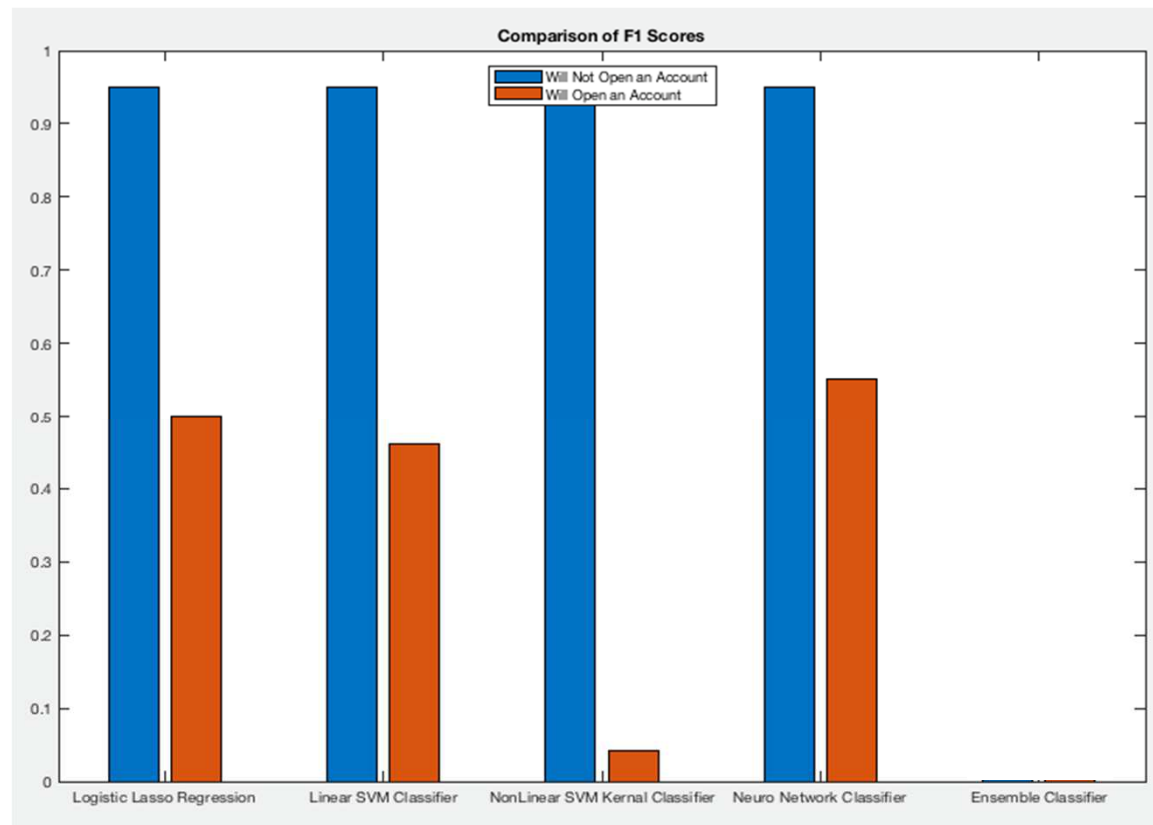
- kNN or Naïve Bayes (**instance-based learner**).
- **Less time training but more time predicting** **need to carry all instances**
- Generalize beyond the current training data.

■ Eager evaluation

- Decision-tree, logistic, LDA, SVM, **SVM RBF** (**instance-based learner**)
- **More time in training but less time in predicting**
- Commit to a fixed / static model.

Reminder

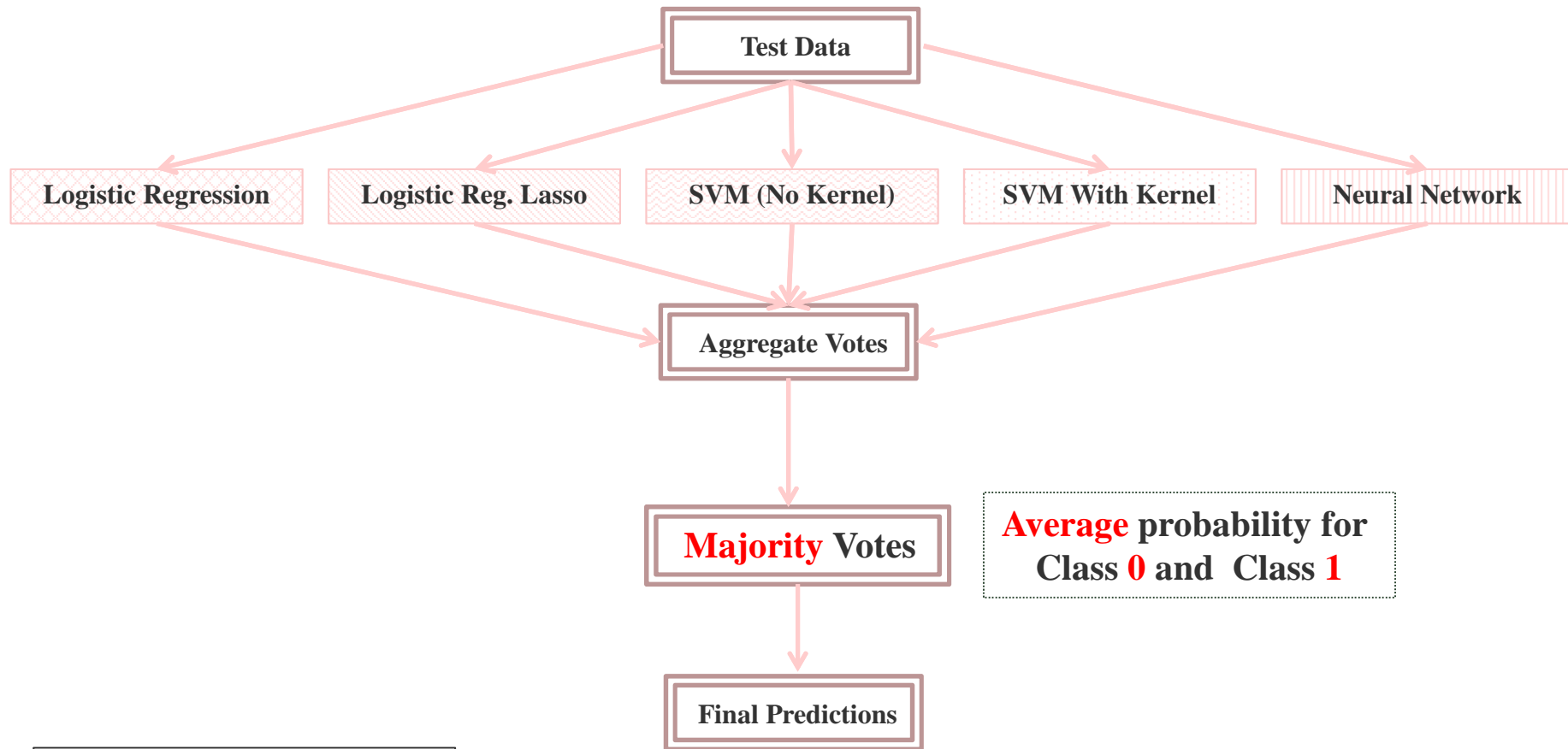
- We discussed many machine learning techniques.
- Try to use all or multiple methods.
- Not only you can compare their performance, but also... WHAT???



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Ronald E Twite
Leela Sowjanya Chippada
Ahmad K Lubnani
Mowlid Abdillahi
Nathan Adams

Ensemble Hard / Soft Voting



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Ronald E Twite
Leela Sowjanya Chippada
Ahmad K Lubnani
Mowlid Abdillahi
Nathan Adams

Characteristics of Classification Algorithms

■ SVM

- Speed & memory usage are good w/ few support vectors, poor if too many. Difficult to interpret how SVM classifies data w/ kernels. Easy for linear SVM.

■ Naive Bayes

- Speed & memory usage are good for simple distributions, but poor for kernel distributions and large data sets.

■ Nearest Neighbor

- Good predictions in low D, but poor predictions in high D. Need kd-trees for speed. Vars can be either continuous or categorical, not both.

■ Discriminant Analysis

- Accurate when normal dist. Otherwise, accuracy varies.

Algorithm	Predictive Accuracy	Fitting Speed	Prediction Speed	Memory Usage	Easy to Interpret	Handles Categorical Predictors
Trees	Medium	Fast	Fast	Low	Yes	Yes
SVM	High	Medium	*	*	*	No
Naive Bayes	Medium	**	**	**	Yes	Yes
Nearest Neighbor	***	Fast***	Medium	High	No	Yes***
Discriminant Analysis	****	Fast	Fast	Low	Yes	No
Ensembles	See Suggestions for Choosing an Appropriate Ensemble Algorithm and General Characteristics of Ensemble Algorithms					

Appendix

Why RBF $\in \infty$ -Space?



- $K(a, b) = \exp(-\|a - b\|^2) / 2\sigma^2 = e^{\frac{-\|a-b\|^2}{2\sigma^2}}.$
- $K(x, y) = \exp(-\|x - y\|^2) = \exp(-(x_1 - y_1)^2 - (x_2 - y_2)^2)$
 $= \exp(-x_1^2 + 2x_1y_1 - y_1^2 - x_2^2 + 2x_2y_2 - y_2^2)$
 $= \exp(-\|x\|^2) \times \exp(-\|y\|^2) \times \mathbf{\exp(2x^Ty)}$

$$k(x, y) = \exp(-\|x\|^2) \exp(-\|y\|^2) \sum_{n=0}^{\infty} \frac{(2x^Ty)^n}{n!}$$

- **Taylor series for e .**

- Raise x & y to n -dimension, divide it by n -factorial, and sum to infinity.

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$