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STAT 666 Project

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Introduction

- SVMs are built for binary classifications.
- We want to extend to problems of multiple classes
- Compare 3 different methods common in literature
- Apply to real-life example (star classication) and simulation.

Star Types

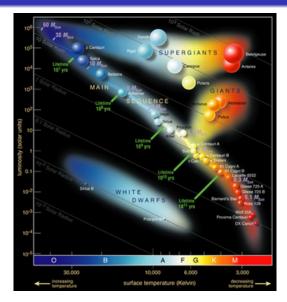


Table: Averages for the covariates across each star class

Star Class	N	Temperature (K)	Radius (R_{\odot})	Luminosity (L_{\odot})
Brown Dwarf	40	2997.9	0.110	6.933×10^{-4}
Red Dwarf	40	3283.8	0.348	$5.405 imes 10^{-3}$
White Dwarf	40	13931.4	0.010	2.433×10^{-3}
Main Sequence	40	16018.0	4.430	3.206×10^{4}
Supergiant	40	15347.8	51.150	3.018×10^{5}
Hypergiant	40	11405.7	1366.897	3.092×10^{5}

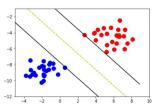
- Balanced Classes
- = Relative to the Sun

- It would be nice if computers could label thousands of stars for us
- Build a SVM classifier to predict star type
- Compare across 3 different multi-class techniques:
 - One vs One
 - One vs All
 - 3 Divide-by 2

(Brief) SVM review

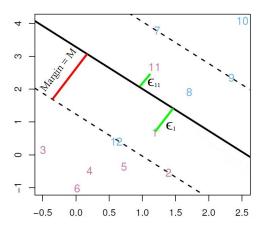
Main idea: Find the hyperplane that best separates the data into 2 classes

- Hyperplane Equation $\mathcal{H} = \{ \boldsymbol{x} : \beta_0 + \boldsymbol{x}' \boldsymbol{\beta} = 0 \}$
 - ullet $\beta s
 ightarrow$ estimated hyperplane coefficients
- Classifier function: $f(x_0) = \beta_0 + x_0'\beta$
 - If $eta_0 + extbf{\emph{x}}_0^{'} oldsymbol{eta} \geq 0
 ightarrow ext{Class A}$
 - If $\beta_0 + \mathbf{x_0'} \boldsymbol{\beta} < 0 \rightarrow \text{Class B}$
- Decision Value: $\beta_0 + x_0' \beta$
- More positive → more like Class A



SVMs Review

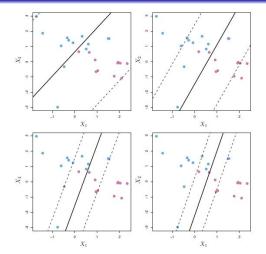
SVM terms



- Each datapoint x_i gets a slack value ε_i (residual)
- SVM seeks to maximize the margin (M) while minimizing slacks ϵ_i 's.
- x_i on wrong side: $\epsilon_i \geq 1$
- x_i is on right side & inside M: $\epsilon \in (0,1)$
- x_i is on correct side and outside M: $\epsilon_i = 0$

SVMs Review

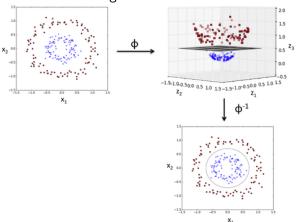
C (Tuning parameter) - e1071 library



Cost (C) determines how much to penalize slack variables Low C values (top right) high C (bottom left)

Kernels

Sometimes a straight line doesn't cut it...



4 types of kernels: Linear, Radial, Polynomial and Sigmoid (tuning parameter γ)

One vs One (OvO)

Introduction

Suppose we have k classes

- Build $\binom{k}{2}$ classifiers for each pair of classes
- Generate predictions for each classifer and take majority

ex. suppose k = 4

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Classifier	Prediction
1 vs 2	2
1 vs 3	1
1 vs 4	4
2 vs 3	2
2 vs 4	2
3 vs 4	3

 \rightarrow Predict Class 2

Note: Default in e1071 library in R for multi-class SVMs

One vs All (OvA)

- Build k classifiers. Compare each class with everything else.
- Generate predictions for each classifer and take maximum decision value $(\beta_0 + \mathbf{x}' \boldsymbol{\beta})$

ex.
$$k=4$$
 | Classifier | Decision Value | 1 vs Not1 | -3.01 | 2 vs Not2 | 0.01 | 3 vs Not3 | 1.01 | 4 vs Not4 | 0.87 | \rightarrow Predict Class 3

Divide by 2 (DB2)

Vural and Dy $(2004)^1$ suggest splitting the classes into 2 subsets until each subset has a single class.

- ullet "Tree method" o Build a decision tree that separates classes.
- ullet Classifier for each split o k-1 classifiers

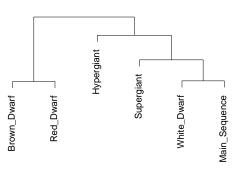
ex. Using star data (k = 6):

- Is this a dwarf star or giant/main sequence? (1)
- If it's a Dwarf:
 - Is this a brown/red dwarf or white dwarf? (2)
 - If not white: is this brown dwarf or red dwarf? (3)
- If it's not a dwarf:
 - Is this a giant star or main-sequence? (4)
 - If it's a giant star: is it super- or hyper-? (5)

DB2 data splits

- Splitting the classes is left to the user.
- One idea is to do hierarchical clustering on class centroids.
- Seek to find "even" splits → minimizes average # of classifiers needed to get to a single class (Ward's linkage)

DB2 Class Split



Results

- Split data into train (75%) and test sets.
- Using 10-fold cross validation, do a grid search on tuning parameters (C, γ , and the kernel) using training set.
- Predict accuracy on test set

Method	Kernel	C	γ	Accuracy
OvO	Linear	5×10^8	0.01	95.0%
OvA	Raidal	1×10^7	0.1	90.0%
DB2	Sigmoid	2×10^5	0.075	96.7%

Star dataset is very separable. DB2 and OvO do the best.

Confusion Matrix (Test set)

Truth (top) vs predicted (left)

Class	BD	RD	WD	MS	SG	HG
Brown Dwarf	13	1	0	0	0	0
Red Dwarf	1	7	0	0	0	0
White Dwarf	0	0	7	0	0	0
Main-Seq	0	0	0	11	0	0
Supergiant	0	0	0	0	9	0
Hypergiant	0	0	0	0	0	11

SVM only has "trouble" with separating Brown and red dwarfs.

Simulation

We wish to see how the 3 methods perform under levels of:

- Class Separation (Low, Med, High)
- Class Balances (Balanced, Varied, Imbalanced)

Simulation Plan

- Simulate 240 datapoints with Balanced, Varied, and imbalanced class counts.
 - Varied = (20,40,50,60,40,30)
 - Unbalanced = (12, 20, 50, 110, 30, 18)
- Give each group its own mean for 3 covariates. Change separation (Low, Med, High) by scaling these means.
 - Scale group means by 0.5 (Low), 1 (Moderate) and 2 (High)
 - I used:
 - Covariate 1: Each group mean $\sim N(0,1)$
 - Covariate 2: (0,0,-.2, 1, 1, 3)
 - Covariate 3: (-.5, 0, 0, 1, 2, 2)
 - Covariate 4: N(0,1) noise
 - Normal data, $\sigma=1$
- 9 Datasets total. Keep the same data across 3 methods and test performance.

Introduction

Simulation Results

(a) OvO Test set accuracy

OvO	Bal	Varied	Unbal
Low	33.3%	55.0%	51.7%
Moderate	50.0%	66.7%	71.7%
High	75.0%	80.0%	86.7%

(b) OvA Test set accuracy

OvA	Bal	Varied	Unbal
Low	45.0%	45.0%	58.3%
Moderate	59.7%	58.3%	74.6%
High	63.3%	78.3%	90.0%

(c) DB2 Test set accuracy

DB2	Bal	Varied	Unbal
Low	40.0%	45.0%	65.0%
Moderate	60.0%	68.3%	76.7%
High	73.3%	78.3%	78.3%

Green=Best, Orange=Worst by 2%

- Higher accuracy for unbalanced classes \rightarrow predicting everything in common classes
 - All methods struggle to predict well in rare classes
- Mixed bag results → all have utility?
- High Separability, balanced classes → DB2 and OvA do well
- OvO and DB2 were actually faster. Most classifiers do not need the full data.

Class prediction accuracy example

Table: Class test set accuracy rates for OvA Moderate spread. The (Size) represents the class distribution in the entire dataset.

Classes	1	2	3	4	5	6
Balanced	20.0%	60.0%	57.1%	88.9%	83.3%	50.0%
(Size)	40	40	40	40	40	40
Varied	33.3%	36.4%	37.5%	92.3%	76.9%	44.4%
(Size)	20	40	50	60	40	30
Unbalanced	40.0%	33.3%	60.0%	96.0%	100.0%	16.7%
(Size)	12	20	50	110	30	18

Maybe a result of a low sample size? Rare classes have super low accuracies. (Overall 74.6% for unbalanced)

Conclusion

- DB2 and OvO performed best on star dataset
 - See how it performs on thousands of stars
- Mixed bag of results for simulation. All methods have some utility
- Rare classes were hard for all 3 methods.
 - Future work: Increasing sample size?

Final thoughts

- One vs One $\binom{k}{2}$
 - Easy to implement (existing software)
 - Blows up as k gets larger. If $k = 20 \rightarrow 190$ Classifiers
- One vs All (k)
 - Works well for unbalanced data?
 - Slowest for small k. All classifiers train on all the data
- Divide by 2 (k-1)
 - Fast and requires the least number of classifiers
 - Requires specification of class divisions
 - Took longer to implement

These can be generalized to any binary classifier!

references

• Vural, V. and Dy, J. (2004) A Hierarchical Method for Multi-class Support Vector Machines. In proceedings of The Twenty-First International Conference on Machine Learning (ICML), p. 831-838