

LEARNING MINIMUM VOLUME SETS WITH SUPPORT VECTOR MACHINES

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Overview

Use support vector machines to estimate *minimum volume sets (MV-sets)*

- anomaly detection
- clustering

Key idea: reduce MV-set estimation to *Neyman-Pearson classification*

- treat MV-set estimation (*one-class* problem) as a *two-class* problem like classification
- draw second class from *uniform* distribution

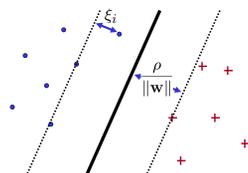
Support Vector Machines

Method for learning classifiers from training data

- Use "kernel-trick"
- Maximize the "margin"

$$\min_{\mathbf{w}, b, \xi, \rho} \frac{1}{2} \|\mathbf{w}\|^2 - \nu \rho + \frac{1}{n} \sum_{i=1}^n \xi_i \quad \nu \in [0, 1]$$

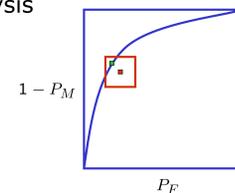
$$\text{s.t. } (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) y_i \geq \rho - \xi_i$$



Measuring Performance

Algorithms for MV/level set estimation of NP classification are typically analyzed using

ROC analysis



We want to operate at a *specific point* of the ROC curve

$$\mathcal{E}(G) := \frac{1}{1 - \beta} \max\{\beta - P(G), 0\} + \mu(G)$$

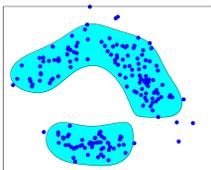
Minimum Volume Sets

Given

- Probability measure P
- Reference measure μ (typically Lebesgue)
- Target mass β

The *minimum volume set* is

$$G_\beta^* = \arg \min\{\mu(G) : P(G) \geq \beta, G \text{ measurable}\}$$



Neyman-Pearson SVMs

Consider *cost-sensitive* SVM

- Introduce class-specific weights
- Adjust weights to achieve desired error rates

Relies on accurate error estimation

- cross-validation

$$\min_{\mathbf{w}, b, \xi, \rho} \frac{1}{2} \|\mathbf{w}\|^2 - 2\nu_+ \nu_- \rho + \frac{\nu_-}{n_+} \sum_{i \in I_+} \xi_i + \frac{\nu_+}{n_-} \sum_{i \in I_-} \xi_i$$

$$\text{s.t. } (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) Y_i \geq \rho - \xi_i$$

$$(\nu_+, \nu_-) \in [0, 1]^2$$

Results: MV-set Estimation

Compare with one-class SVM

Modified LIBSVM software

Highlights:

- manifold sampling performs best
- two-class methods more reliable
- impact of discrete data

		$\mathcal{E}_\mu(G)$
banana	OC-SVM	1.36
	NP-IND	0.53
	NP-THIN	0.47
	NP-MAN	0.44
breast-cancer	OC-SVM	0.55
	NP-IND	0.29
	NP-THIN	1.75
	NP-MAN	0.06
heart	OC-SVM	0.63
	NP-IND	0.43
	NP-THIN	1.26
	NP-MAN	0.16
thyroid	OC-SVM	0.77
	NP-IND	0.63
	NP-THIN	0.79
	NP-MAN	0.7
ringnorm	OC-SVM	0.11
	NP-IND	0.17
	NP-THIN	0.11
	NP-MAN	0.06

Neyman-Pearson Classification

Given

- Probability measures Q_+ and Q_-
- Target power α

$$\text{Let } P_F(f) = Q_-(\{x : f(x) = +1\})$$

$$P_M(f) = Q_+(\{x : f(x) = -1\})$$

The *Neyman-Pearson classifier* is

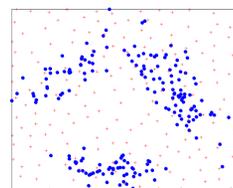
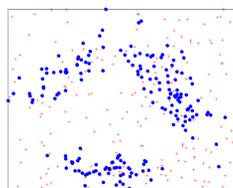
$$f_\alpha^* = \arg \min\{P_M(f) : P_F(f) \leq \alpha\}$$

Uniform Data: Thinning

In high dimensions we must confront the "curse of dimensionality"

One option is *thinning* the data to ensure a large distance between any pair of points

- results in an approximate "packing set"

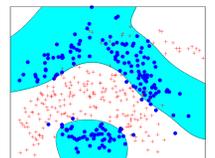
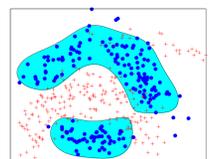


Results: Anomaly Detection

Test validity of uniform prior

Compare

- MV-set (one class)
- NP-classifier (both classes)



		$\mathcal{E}_\mu(G)$
banana	without	0.29
	with	0.24
breast-cancer	without	0.83
	with	0.99
heart	without	0.76
	with	0.50
thyroid	without	0.44
	with	0.22
ringnorm	without	0.015
	with	0.021

Reduction to Neyman-Pearson Classification

Any technique for estimating an NP classifier can be adapted to estimate an MV-set

$$\text{Set } Q_- = 1 - P$$

$$Q_+ = \mu$$

$$\alpha = 1 - \beta$$

Then, if f_α^* is the optimal NP classifier,

$$G_\beta^* = \{x : f_\alpha^* = -1\}$$

Challenge: we only have samples from P

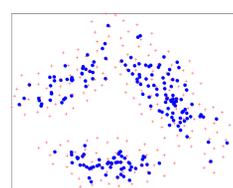
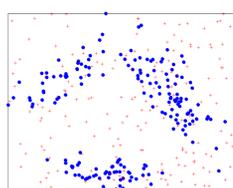
→ we can *sample* from μ

Uniform Data: Manifold Sampling

Thinning does not directly overcome the "vastness of space" in high dimensions

What if our data lies on a *manifold*?

- adapt to this structure
- do not waste samples



Conclusions

Minimum volume sets are an effective way to approach anomaly detection

We can accurately estimate minimum volume sets using Neyman-Pearson SVMs

The procedure used for generating "uniform" samples can significantly impact performance

Our approach tends to perform

- better than the one-class SVM
- often nearly as well the NP classifier trained using *both* classes

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