

# Computational Data Analysis

## Machine Learning

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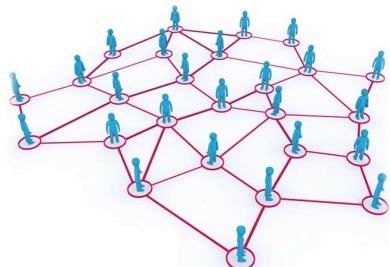
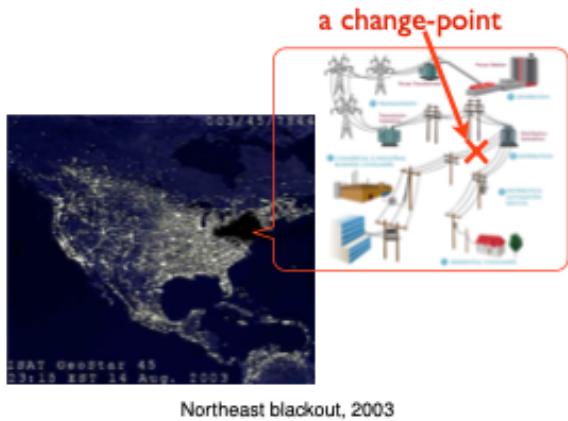
Harold R. and Mary Anne Nash Early Career Professor  
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Engineering

Anomaly detection



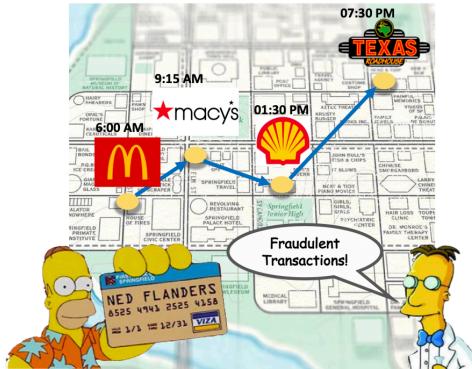
# Motivation

Power network monitoring

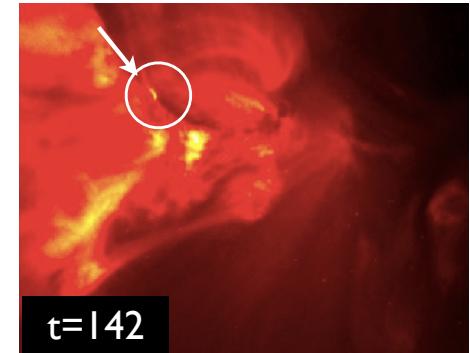


Event detection from  
social networks

Credit card fraud  
detection



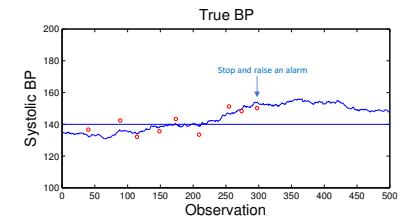
Solar flare detection



Blood pressure  
monitoring

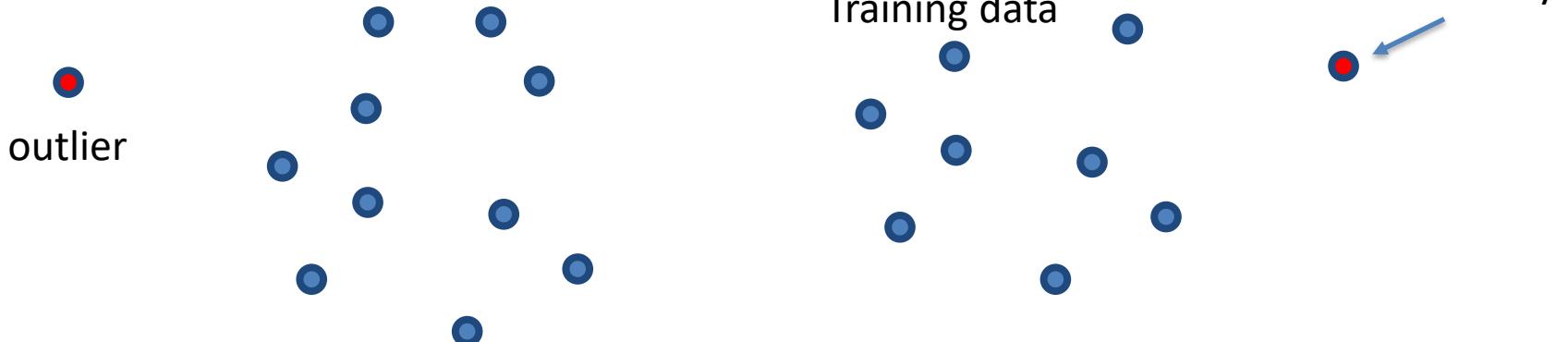


Omron Project Zero 2.0.



# Anomaly detection

- Outlier detection: identify outliers in training data, which are defined as observations that are “far” from the others in a chosen metric. --- As pre-processing step to clean data.
- Novelty detection: Detecting whether a **new** observation is an outlier. Related to change point detection (e.g., detecting change-points in time series).

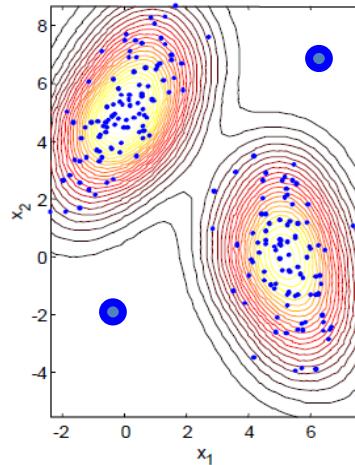
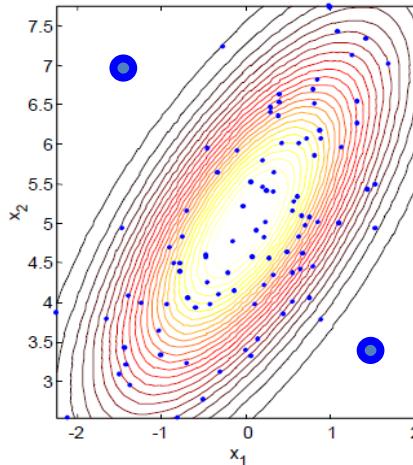


# Anomaly detection

- Statistical methods: likelihood based
- Geometric methods: one-class SVM
- Some theory

# Outlier detection: density-based

- Declare data points in low density region as outliers
  - First fit density to normal data  $\hat{f}_0(x)$ , and then set a threshold  $\epsilon$  (e.g. using kernel density estimation (KDE))
  - Data points in region with density small than  $\epsilon$ , i.e.  $\hat{f}_0(x) \leq \epsilon$



# Covariance based detector

- Multivariate Gaussian

$$f_0(x) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

- Find parameter estimation from data

$$\hat{\mu} = \frac{1}{m} \sum_{i=1}^m x^i, \hat{\Sigma} = \frac{1}{m} \sum_{i=1}^m (x^i - \hat{\mu}) (x^i - \hat{\mu})^T$$

- For a new data, having  $\hat{f}_0(x_{new}) \leq \epsilon$  is equivalent to having

$$(x_{new} - \hat{\mu})^T \hat{\Sigma}^{-1} (x_{new} - \hat{\mu}) \geq b$$

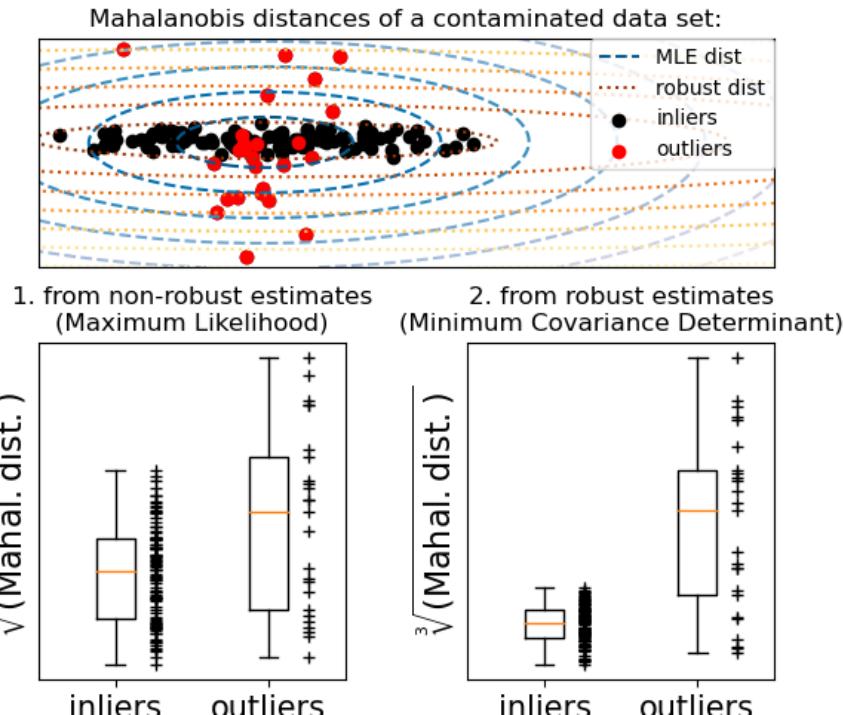
Mahalanobis distance

for some threshold  $b$

# Robust covariance estimation

- Mahalanobis distance can be affected by outliers
- Minimum Covariance Determinant estimator (MCD):

find a subset of observations whose empirical covariance has the smallest determinant  $|\hat{\Sigma}|$

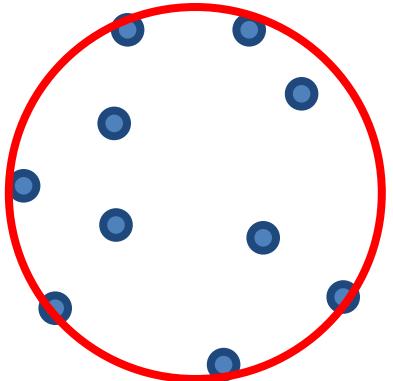


# Anomaly detection

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# Geometric method for anomaly detector

Rather than first fit density and then find threshold, directly find the boundary



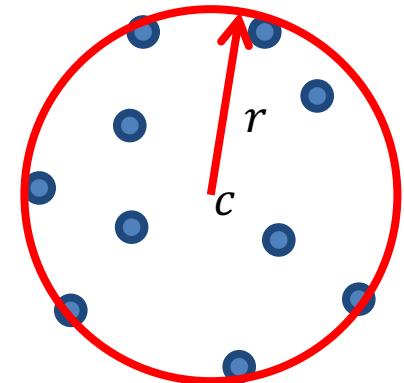
# SVM based one-class classification (OCC)

Find the smallest ball such that it include all training data points.

Parameterized the ball with a center  $c$  and radius  $r$

Optimization problem

$$\begin{aligned} & \min_{r,c} r^2 \\ \text{s.t. } & \|x^i - c\|^2 \leq r^2, \\ & r \geq 0 \\ & \forall i = 1, \dots, m \end{aligned}$$



# Solving one-class SVM

Lagrangian function

$$L(r, c, \alpha) = r^2 + \sum_{i=1}^m \alpha_i \left( (x^i - c)^\top (x^i - c) - r^2 \right), \alpha_i \geq 0$$

Set partial derivative of  $L$  to 0

$$\frac{\partial L}{\partial r} = 2r - 2 \sum_{i=1}^m \alpha_i r = 0 \Rightarrow \sum_{i=1}^m \alpha_i = 1$$

$$\frac{\partial L}{\partial c} = \sum_{i=1}^m \alpha_i (-2x^i + 2c) = 0 \Rightarrow c = \sum_{i=1}^m \alpha_i x^i$$

# Expressing Lagrangian function $L$ in $\alpha_i$

$$\max_{\alpha} g(\alpha) := L(r^*, c^*, \alpha) = \sum_{i=1}^m \alpha_i x^{i^\top} x^i - \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j x^{i^\top} x^j$$
$$s.t. \quad \sum_{i=1}^m \alpha_i = 1, \alpha_i \geq 0$$

A quadratic programming problem  $g(a) = b^\top a - a^\top A a$

Can be solved efficiently

Optimal radius can be

found based on  $c^*$

$$A_{ij} = x^{i^\top} x^j$$

$$b_i = x^{i^\top} x^i$$

$$\alpha$$

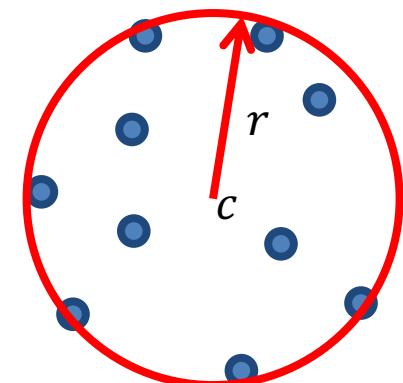
# Sparsity in $\alpha_i$

Complementary slackness (for all  $i$ ):

$$\alpha_i \left( (x^i - c)^\top (x^i - c) - r^2 \right) = 0, \quad \alpha_i \geq 0$$

Interesting observation:

- Many data points will be inside the circle
  - $(x^i - c)^\top (x^i - c) - r^2 < 0$
  - $\alpha_i = 0$
- Very few data point will be exactly on the boundary
  - $(x^i - c)^\top (x^i - c) - r^2 = 0$
  - $\alpha_i$  can be nonzero



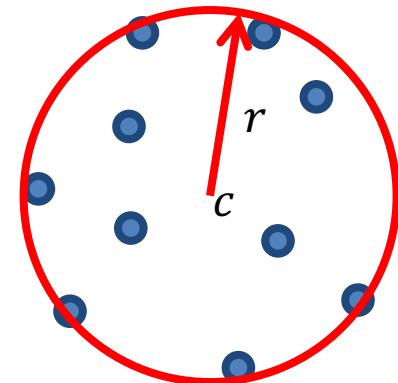
Solution in  $\alpha$  is very sparse!

# Support vectors

- Each  $\alpha_i$  is associated with a one data point
- Data points with nonzero  $\alpha_i$  are called **support vectors**. They determine the center and radius

$$c^* = \sum_{i=1}^m \alpha_i x^i$$

$$r = \min_{i:\alpha_i > 0} \|x^i - c^*\|$$



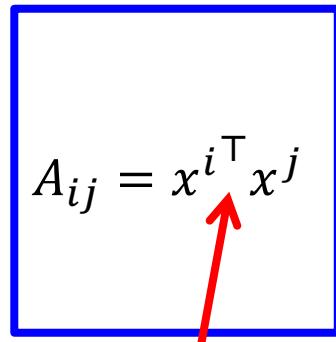
- Data points with zero  $\alpha_i$  is not affect  $c$  and  $r$

# Kernalize the algorithm

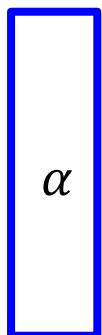
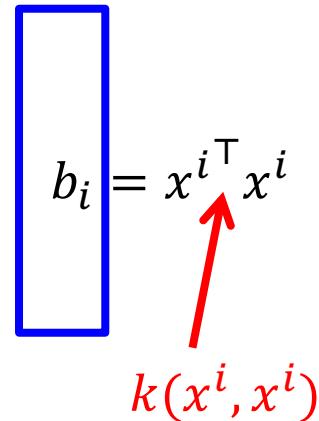
Dual problem

$$\max_{\alpha} g(\alpha) = b^\top \alpha - \alpha^\top A \alpha$$

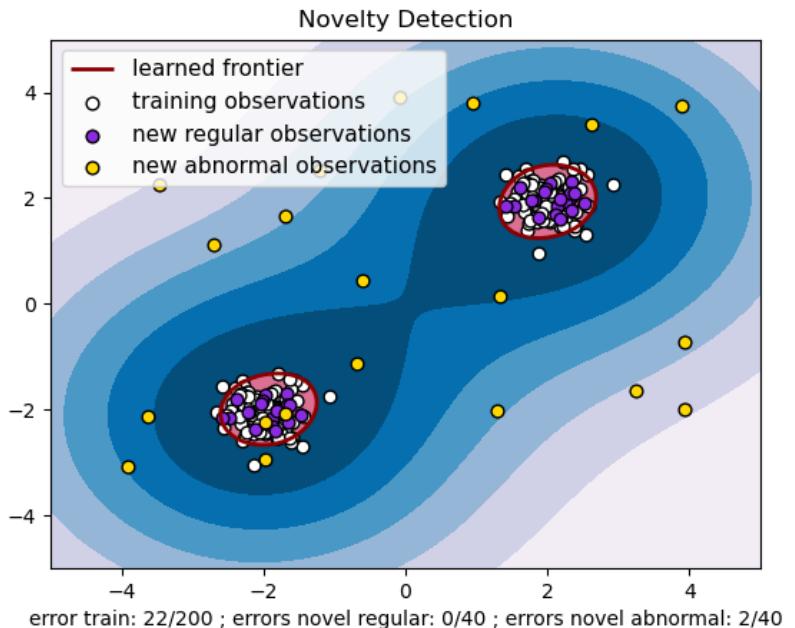
$$s.t. \sum_{i=1}^m \alpha_i = 1, \alpha_i \geq 0$$



$$k(x^i, x^j)$$



# Demo: Novelty detection



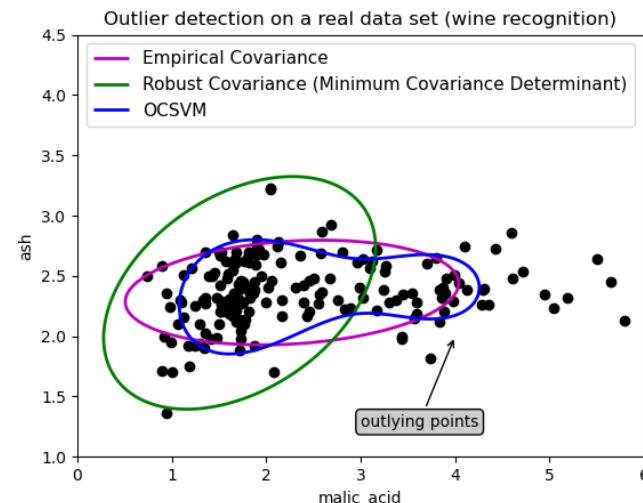
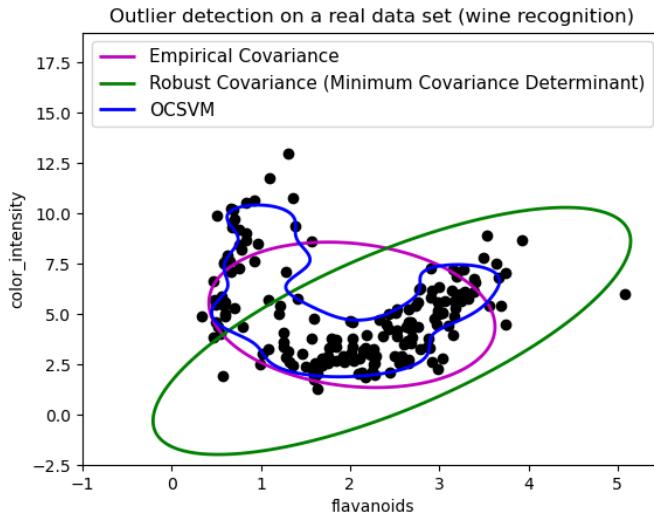
[https://scikit-learn.org/stable/auto\\_examples/svm/plot\\_onesample.html#sphx-glr-auto-examples-svm-plot-onesample-py](https://scikit-learn.org/stable/auto_examples/svm/plot_onesample.html#sphx-glr-auto-examples-svm-plot-onesample-py)

# Demo: Wine data



- The wine data set was introduced by Forina et al. (1986).
- It originally included the results of 27 chemical measurements on 178 wines made in the same region in Italy but derived from three different cultivars: Barolo, Grignolino and Barbera.

[https://scikit-learn.org/stable/auto\\_examples/applications/plot\\_outlier\\_detection\\_wine.html#sphx-glr-auto-examples-applications-plot-outlier-detection-wine-py](https://scikit-learn.org/stable/auto_examples/applications/plot_outlier_detection_wine.html#sphx-glr-auto-examples-applications-plot-outlier-detection-wine-py)



# Anomaly detection

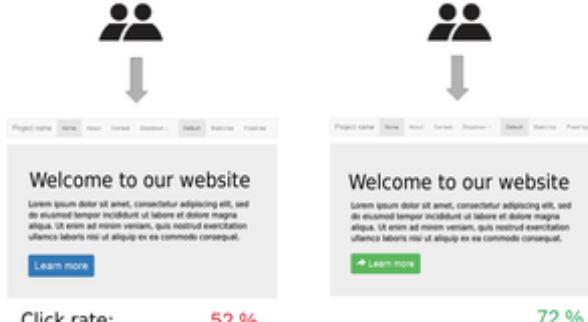
- Statistical methods: likelihood based
- Geometric methods: one-class SVM
- Some theory

# Hypothesis test

- Common hypothesis test

$$H_0: x^i \sim f_0, \quad i = 1, \dots, m$$
$$H_1: x^i \sim f_1, \quad i = 1, \dots, m$$

- A/B testing

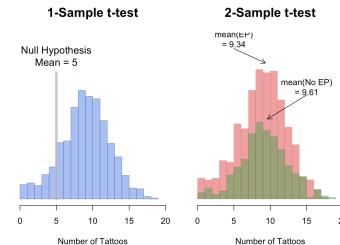


- Anomaly detection

$$H_0: x^i \sim f_0, \quad i = 1, \dots, m$$
$$H_1: x^i \neq f_0, \quad i = 1, \dots, m$$

- Two-sample test

$$H_0: x^i \sim f_0, z^i \sim f_0, \quad i = 1, \dots, m$$
$$H_0: x^i \sim f_0, z^i \sim f_1. \quad i = 1, \dots, m$$

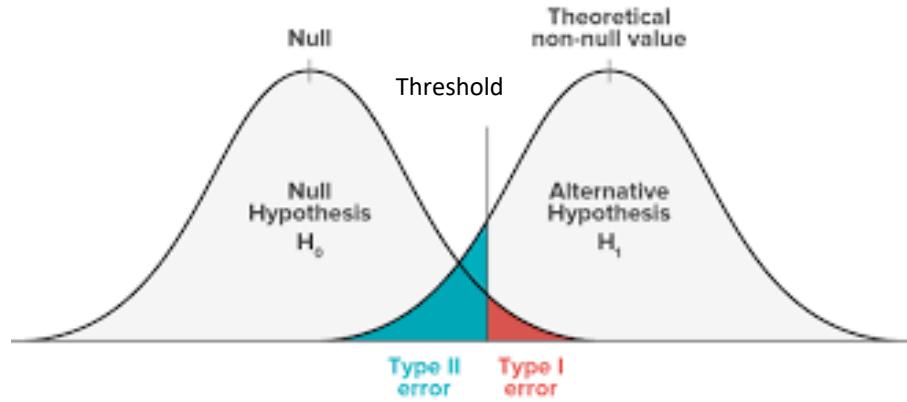


# Performance metrics

Decision making: Choose  $H_0$  or  $H_1$

Performance metrics

- Type-I error =  $P_{H_0}\{\text{reject } H_0\}$
- Type-II error =  $P_{H_1}\{\text{accept } H_0\}$



Decision	$H_0$ Is True	$H_0$ Is False
Fail to reject $H_0$	no error	type II error
Reject $H_0$	type I error	no error

# Likelihood ratio test

- The likelihood ratio test is optimal when  $f_0$  and  $f_1$  are known exactly (Neyman-Pearson lemma)

Decide  $H_1$  when  $\frac{f_1(x)}{f_0(x)} > b$

- In practice, we can estimate the distributions
- Set the threshold  $b$  to control false alarms (Type-I error)

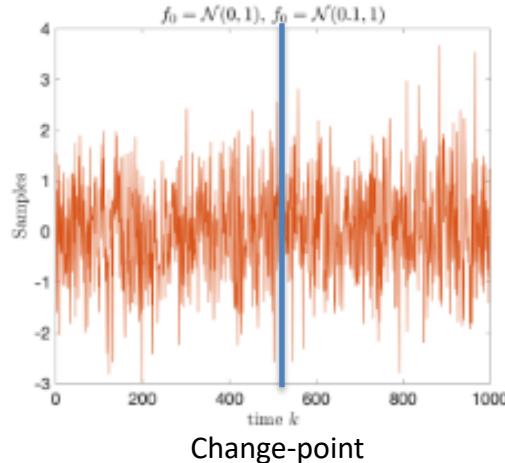
# Novelty detection for sequential data

Assume the distribution before the change:  $f_0(x)$ , after the change:  $f_1(x)$

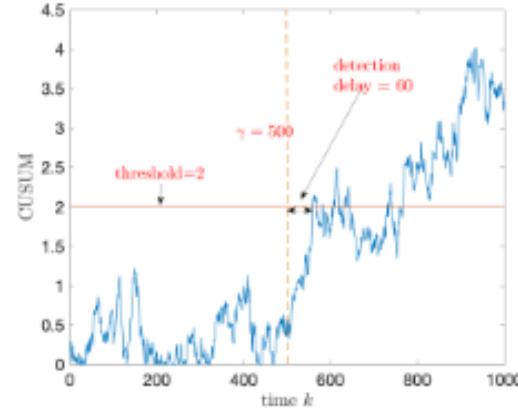
CUSUM procedure (cumulative sum over log-likelihood ratios)

$$W_0 = 0, \quad W_t = \max\left(W_{t-1} + \log \frac{f_1(X_t)}{f_0(X_t)}, 0\right)$$

Sequential data

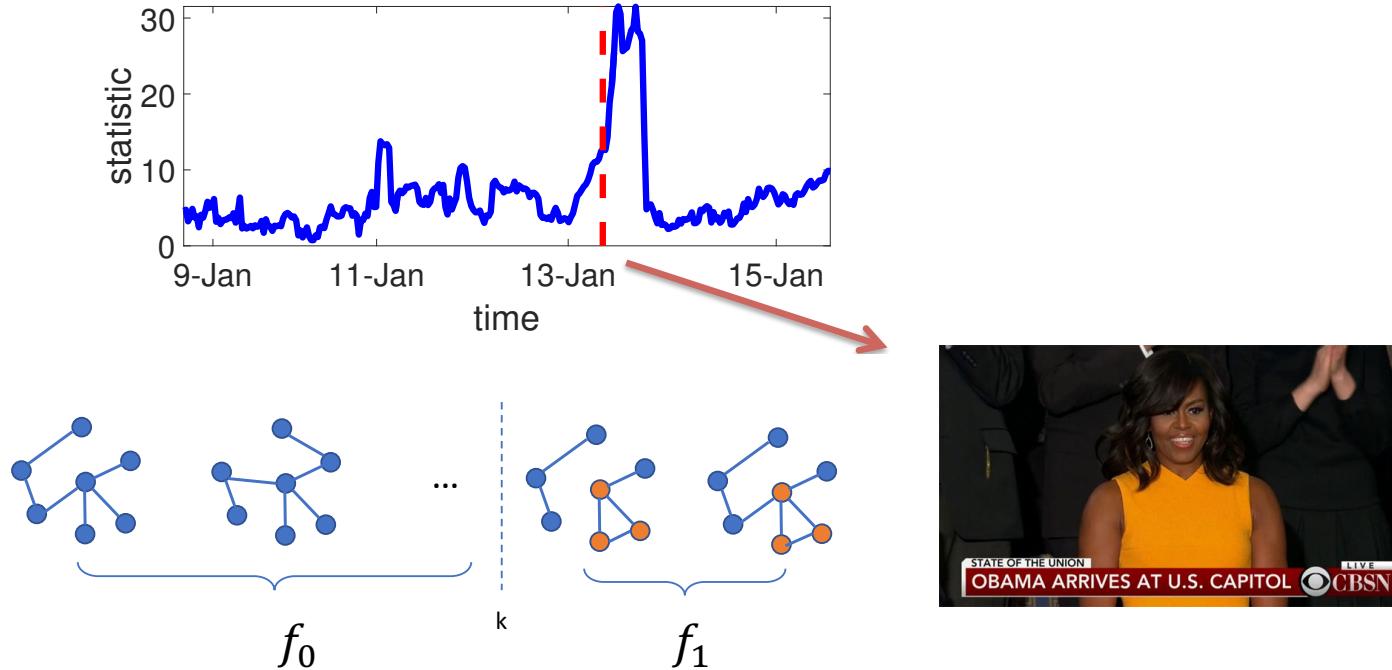


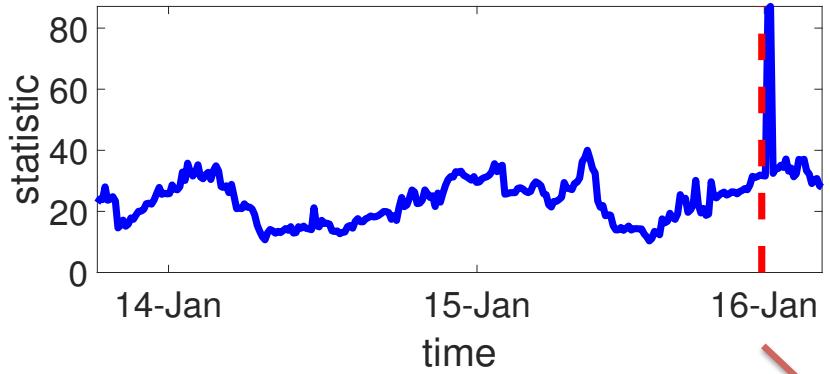
CUSUM statistics



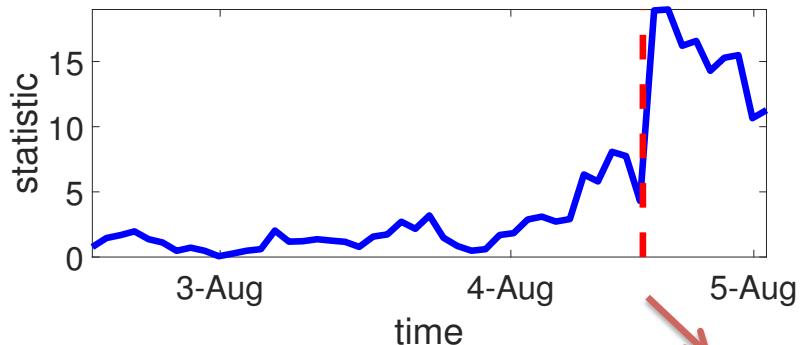
# Example: Social network change detection

Detecting change in random graph, using twitter data





Israel announces ceasefire in Gaza War in 2009



Beijing Olympic opening in 2008

# Other anomaly detection algorithms

- Local outlier factor (LOF): distance metric based
- Neural network based: e.g., anomalous sequence detection using RNN

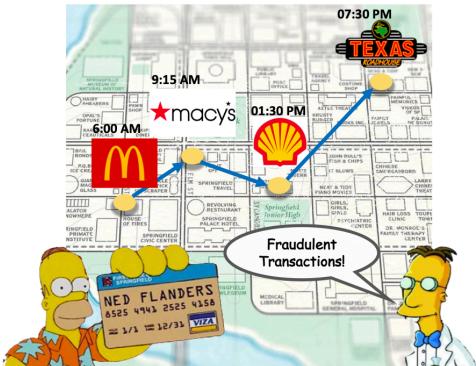
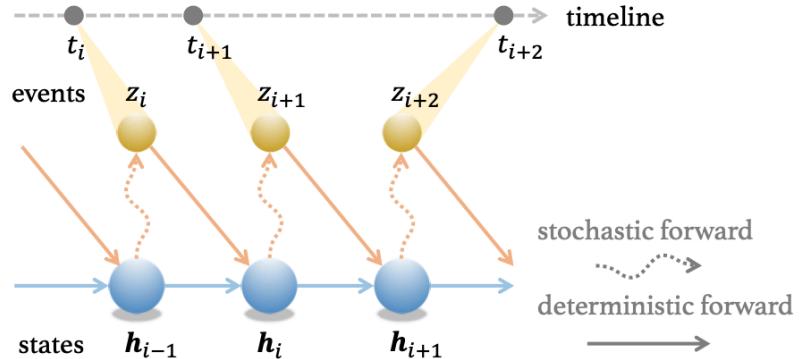


Fig. 1: An example of a sequence of anomalous events that are dependent: one leads to another.

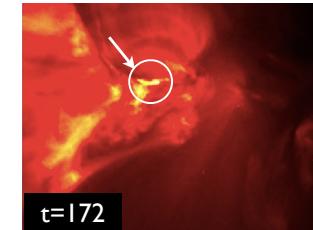
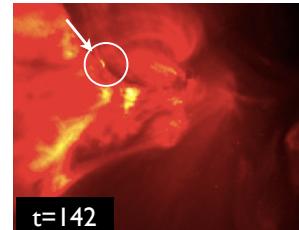
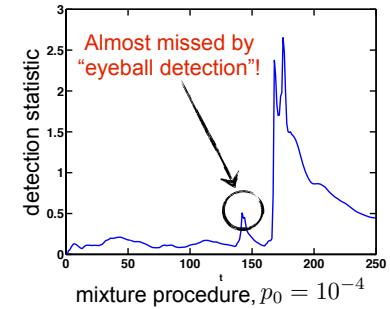
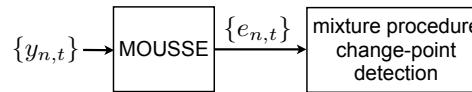
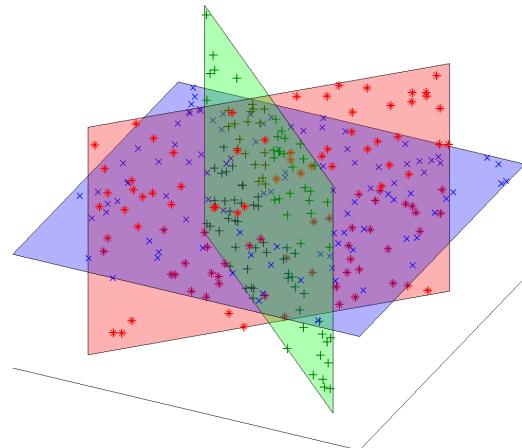


RNN-based anomalous seq. detection

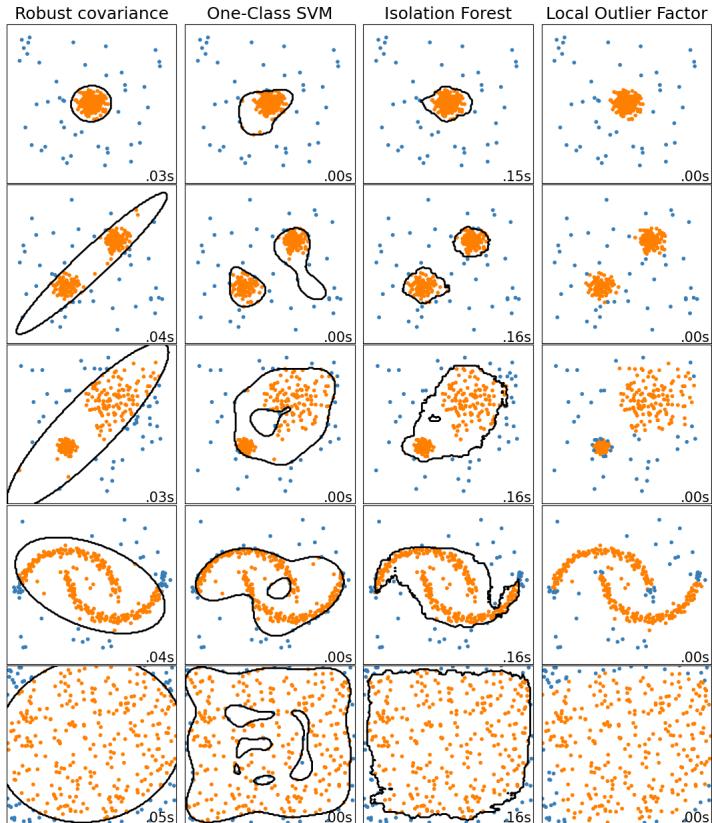
# Other anomaly detection algorithms (cont.)

- Subspace based anomaly detection

Represent normal data using subspace



# Comparison of algorithms



[https://scikit-learn.org/stable/auto\\_examples/miscellaneous/plot\\_anomaly\\_comparison.html#sphx-glr-auto-examples-miscellaneous-plot-anomaly-comparison-py](https://scikit-learn.org/stable/auto_examples/miscellaneous/plot_anomaly_comparison.html#sphx-glr-auto-examples-miscellaneous-plot-anomaly-comparison-py)

