Machine Learning for Predictive Maintenance Applications:
Feature Learning / One-Class Classifiers

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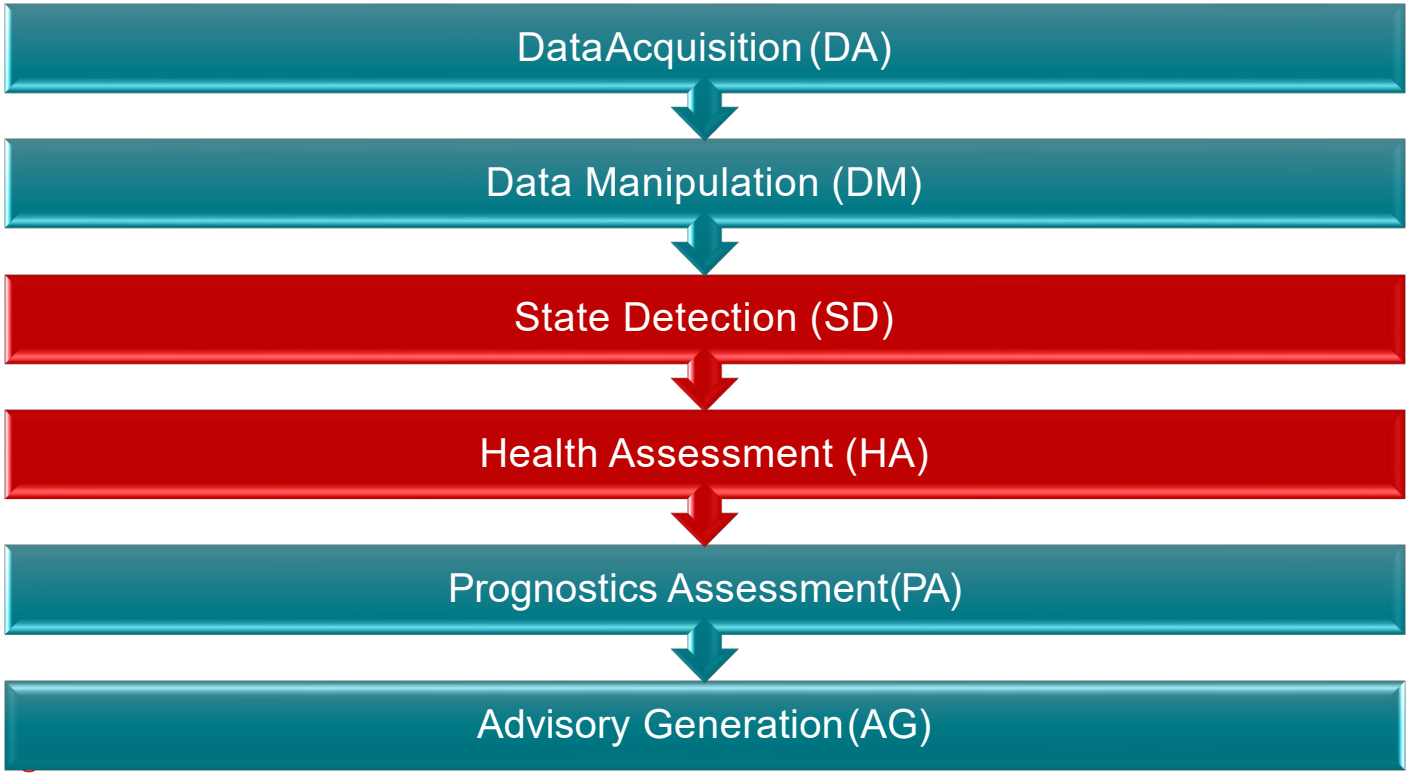
September 2025

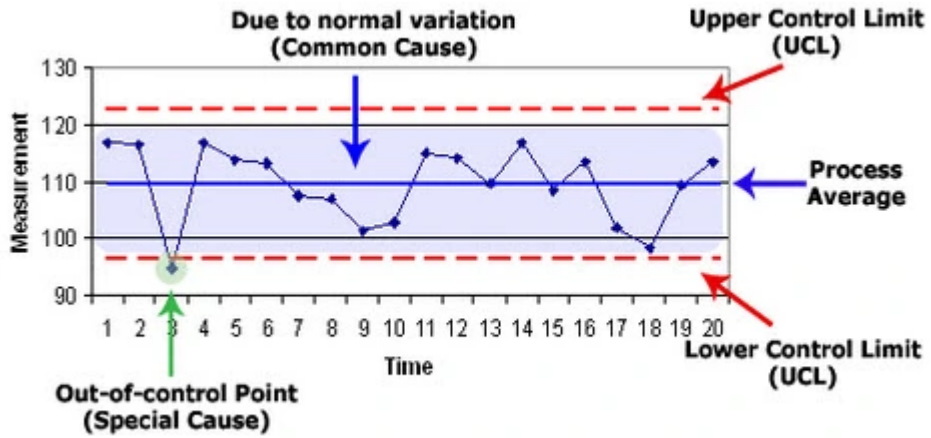
PHM Process


DataAcquisition (DA)
Data Manipulation (DM)
State Detection (SD)
Health Assessment (HA)
Prognostics Assessment(PA)
Advisory Generation (AG)

Control Charts for fault detection

Control charts

- Also known as Shewhart Charts or Statistical Process Control Charts (SPCC)
- Graphical tools used to determine if a process is in a state of statistical control, or how much variation exists in a process



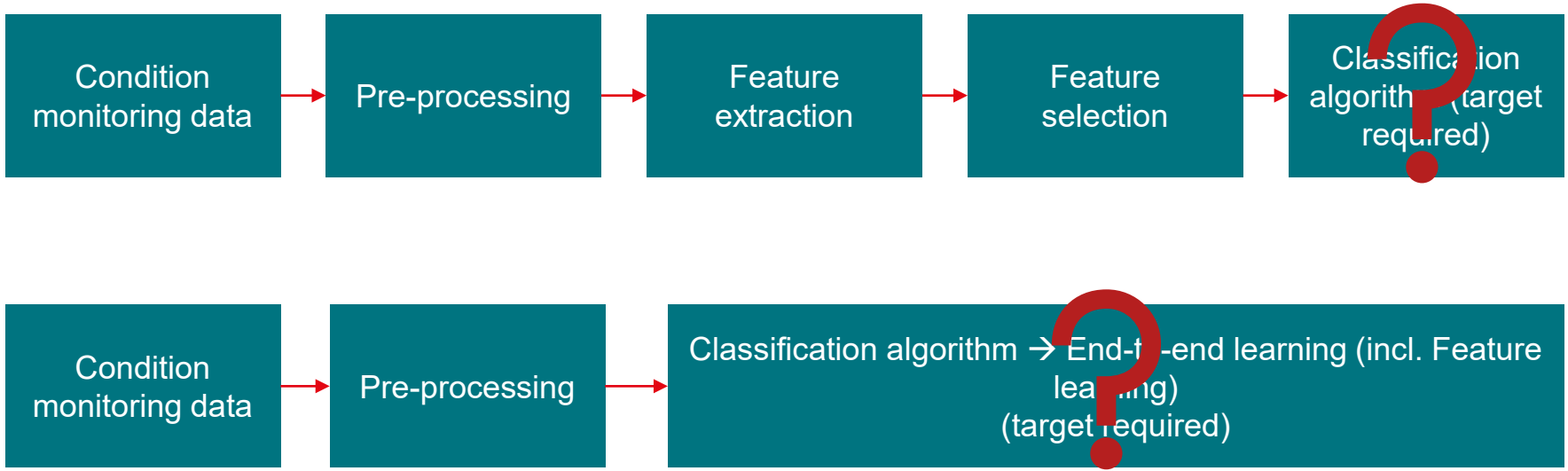
https://www.clearpointstrategy.com/

Fault detection

Fault detection

- Faults in mission-critical systems are rare → not possible to learn the fault patterns from examples
- Often only healthy data observed at the point in time of the fault detection model development !!!
- We are missing labeled data!!!

Fault detection?



Types of fault detection approaches

- (Supervised)
- **Unsupervised**
- Semi-supervised

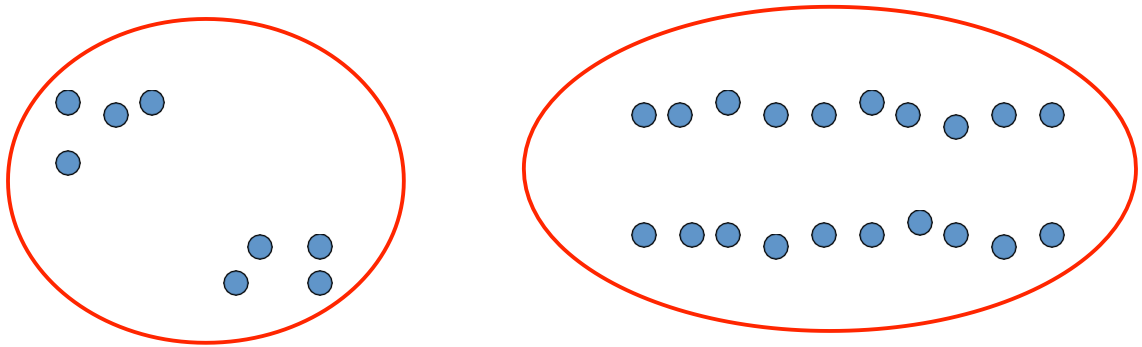
Clustering algorithms for fault detection and diagnostics

Cluster analysis

- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation, …*)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- The subgroups are chosen such that the intra-cluster differences are minimized and the inter-cluster differences are maximized.
- Unsupervised learning: no predefined classes
- Applications of cluster analysis:
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Clustering

- Basic idea: group together similar instances
- In the context of feature selection: group together similar features (and replace the groups by a «representative» feature)

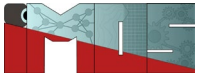


- How do we define similarity?
  - Classical: Euclidean distance, Manhatten distance
  - Correlation-based distances
  - Cosine similarity

Quality of the cluster analysis

- A good clustering method will produce high quality clusters
  - high intra-class similarity: **cohesive** within clusters
  - low inter-class similarity: **distinctive** between clusters
- The quality of a clustering method depends on
  - the similarity measure used by the method
  - its implementation, and
  - Its ability to discover some or all of the hidden patterns

Clustering as a pre-processing step for other algorithms



1. Feature Engineering and Extraction

- **Creating Cluster-Based Features:**
- After performing clustering on your dataset, each data point is assigned to a specific cluster. This cluster assignment can be used as an additional feature for supervised learning algorithms.
- **Dimensionality Reduction:**
- Clustering can help in identifying and retaining the most representative features of the data by grouping similar features together.

2. Data Cleaning and Noise Reduction

- **Identifying Outliers:**
- Clustering algorithms can help identify outliers or anomalies by highlighting data points that do not fit well into any cluster.
- **Smoothing Data:**
- Clustering can group similar data points, allowing for the smoothing of noisy data within each cluster.

3. Data Transformation and Encoding

- **Encoding Categorical Variables:**
- Clustering can be used to encode categorical variables by grouping similar categories together.
- **Enhancing Feature Space:**
- Clustering can transform the original feature space into a new space where cluster memberships or distances to cluster centroids are used as features.

Clustering as a pre-processing step for other algorithms

4. Initialization for Other Algorithms

- **Improving Algorithm Convergence:**
- Clustering can provide good initial centers or starting points for iterative algorithms, enhancing their convergence speed and accuracy.
- **Facilitating Ensemble Methods:**
- Clustering can be used to create diverse subsets of data or features, which can then be used in ensemble learning methods to build more robust models.

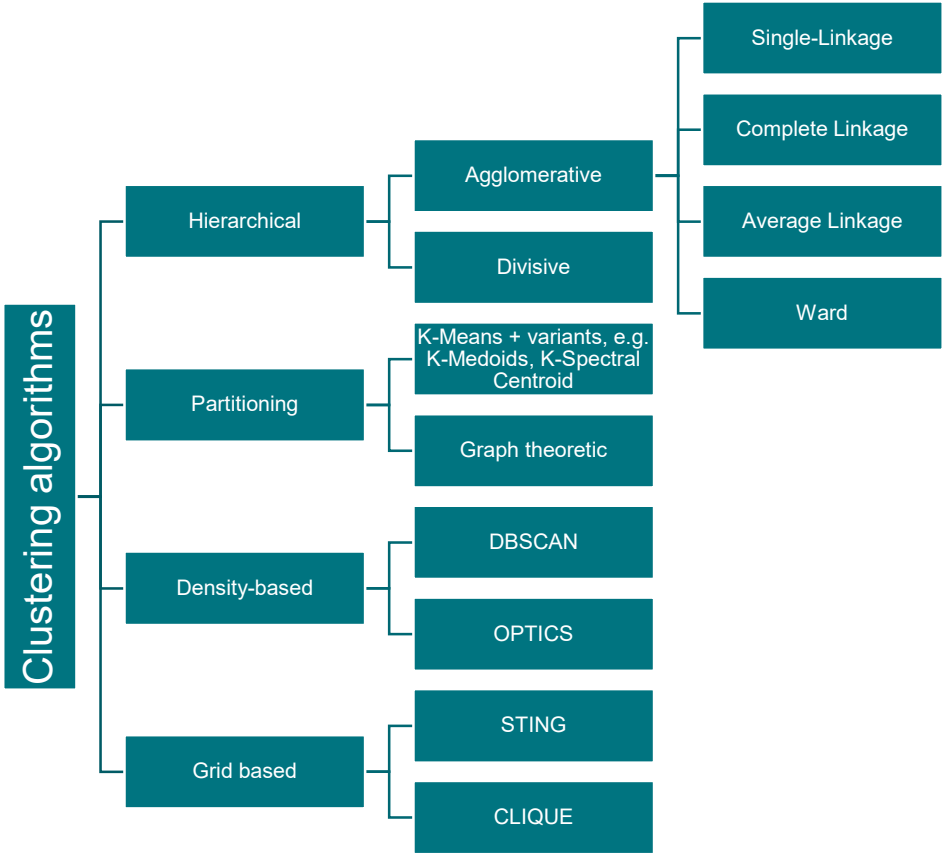
5. Handling Imbalanced Data

- **Resampling Techniques:**
- Clustering can assist in resampling techniques by ensuring that minority classes are adequately represented.

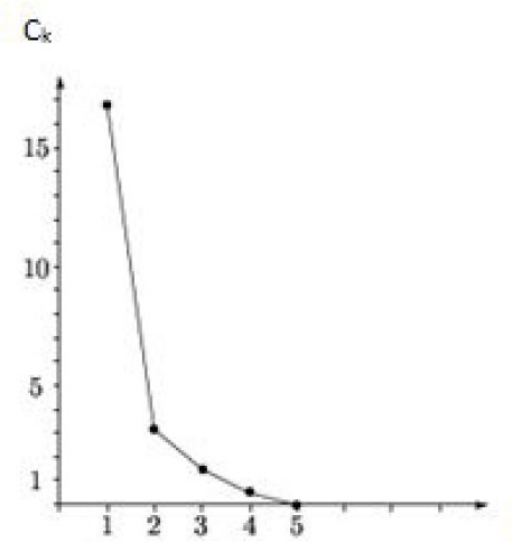
6. Enhancing Interpretability

- **Simplifying Model Interpretation:**
- By clustering similar data points, models can be built on aggregated cluster-level data, making the models easier to interpret.

Major Clustering algorithms



Number of clusters



Number of clusters

C_k: Total within-clusters sum of squares

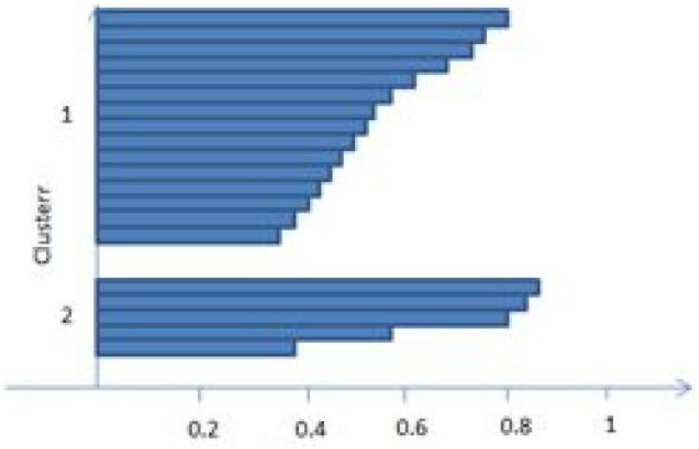
Silhoutte Coefficient

- Can be used to study the separation distance between the resulting clusters
- A measure how close each point in one cluster is to points in the neighboring clusters → can be assessed visually in silhoutte plots
- a(i) average distance between i and all observations within the same cluster
- b(i) be the smallest average distance of i to all points in any other cluster (excluding the cluster that it is member of)

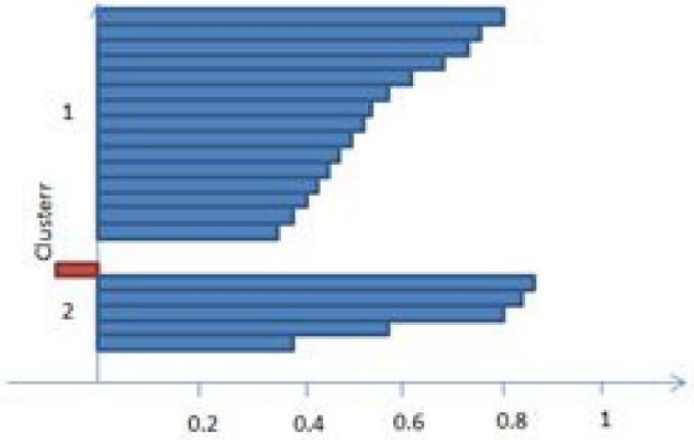
$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

$$s(i) = \begin{cases} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{cases}$$

Silhoutte Plot: example



Silhoutte Coefficient

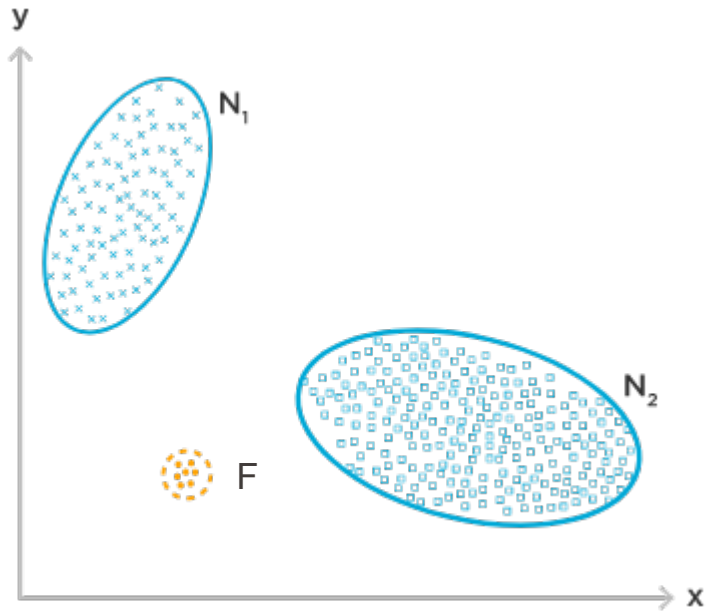


Silhoutte Coefficient

Clustering for anomaly/fault detection

- Assumption that similar data points tend to cluster together in groups, as determined by their proximity to local centroids.
- Data instances that fall outside of these groups are considered as anomalies

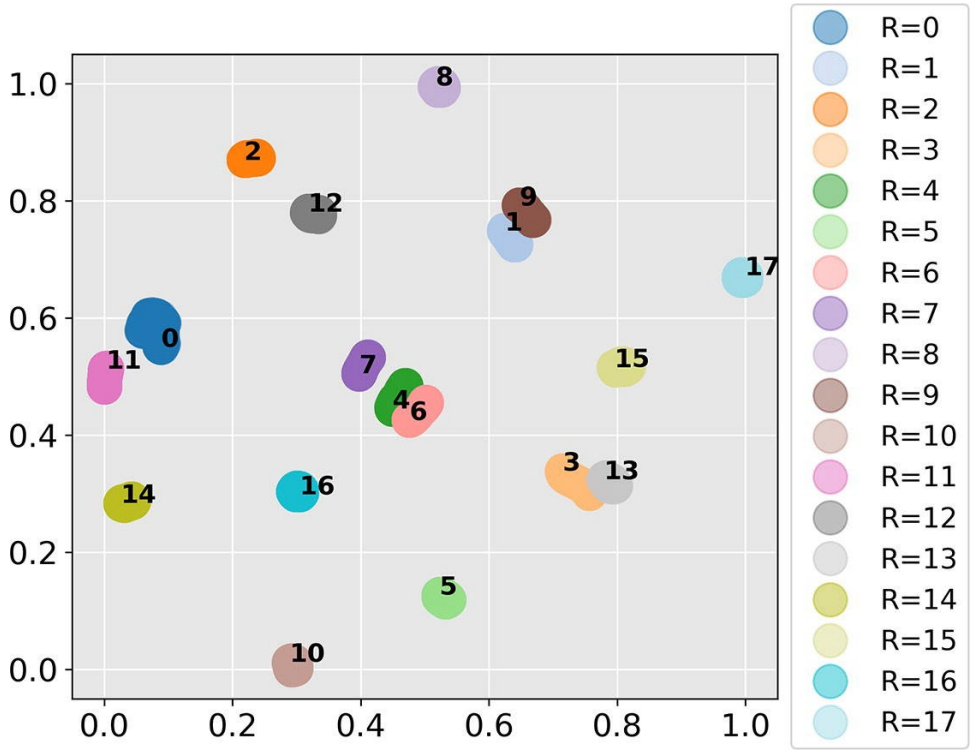
Clustering for fault detection



Clustering for fault dignostics

- Segmentation of different fault types in an unsupervised way
- Only mapping between which cluster belongs to which fault type is missing

Clustering for fault diagnostics



Arias Chao, M., Adey, B. T., & Fink, O. (2021). Implicit supervision for fault detection and segmentation of emerging fault types with Deep Variational Autoencoders. *Neurocomputing*, *454*, 324-338.

Clustering in Fault Detection

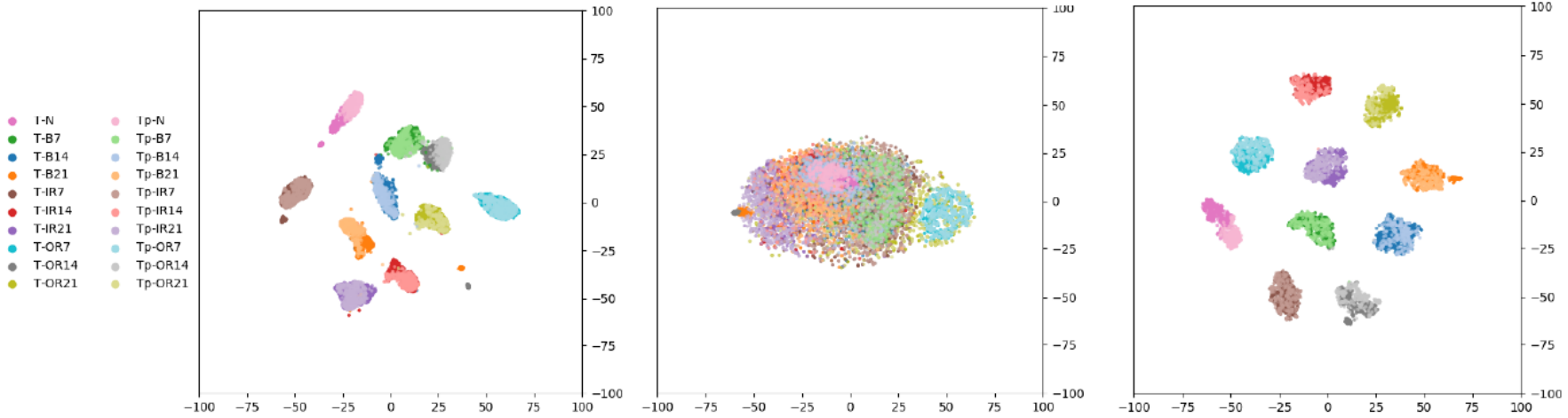
Model Training and Clustering

- **Train Clustering Model:** Apply the chosen clustering algorithm to the preprocessed data to identify distinct groups representing normal and potentially faulty states.
- **Determine Cluster Labels:** Typically, the largest cluster represents normal operation, while smaller clusters may indicate anomalies or faults.

Fault Detection and Diagnosis

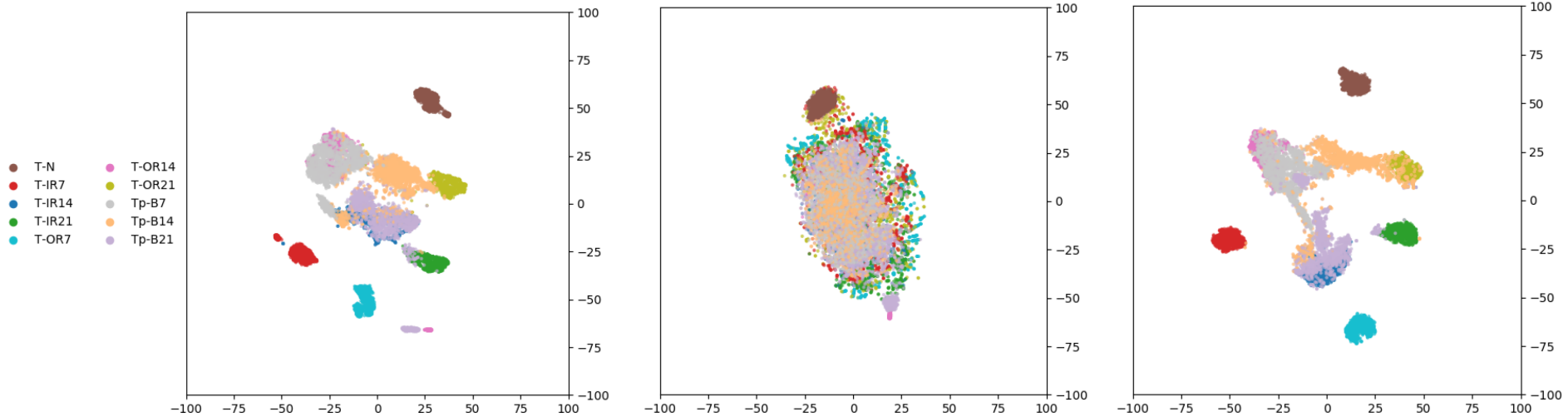
- **Monitor Incoming Data:** Continuously collect new data points and assign them to existing clusters using the trained model.
- **Detect Faults:** Data points that do not fit well into any cluster (e.g., assigned to a "noise" cluster in DBSCAN) or deviate significantly from normal clusters are flagged as potential faults.
- **Diagnose Fault Types:** Analyze the characteristics of the anomalous clusters to identify specific fault types and their underlying causes.

Separability of fault types in the feature space Bearing case study (CWRU) → 10 classes (9 faulty + 1 healthy)



Rombach, K., Michau, G., & Fink, O. (2021). Contrastive learning for fault detection and diagnostics in the context of changing operating conditions and novel fault types. *Sensors*, *21*(10), 3550.

Detectability of new fault types (not used for training)

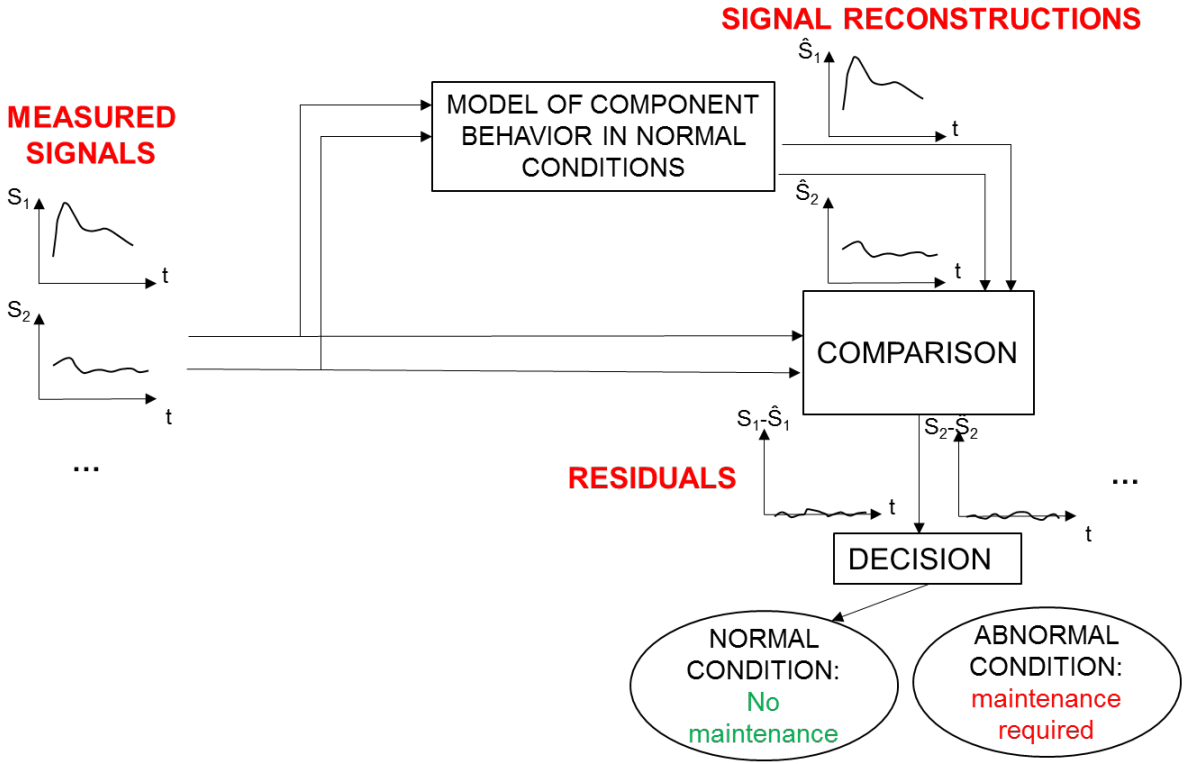


(a) CLE y_{true} (b) AE y_{true} (c) TE y_{true}

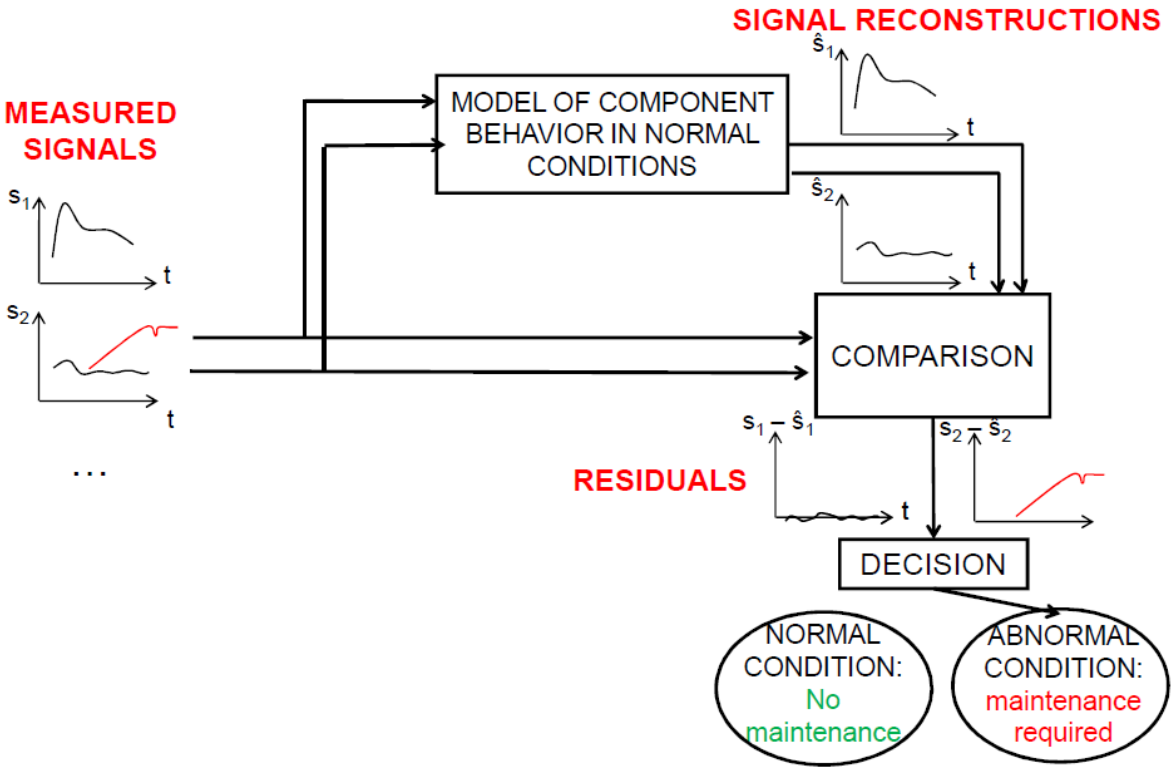
Rombach, K., Michau, G., & Fink, O. (2021). Contrastive learning for fault detection and diagnostics in the context of changing operating conditions and novel fault types. *Sensors*, *21*(10), 3550.

Signal reconstruction / Residual-based approaches

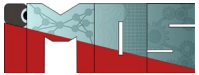
Fault detection with residual based approaches



Fault detection with residual based approaches

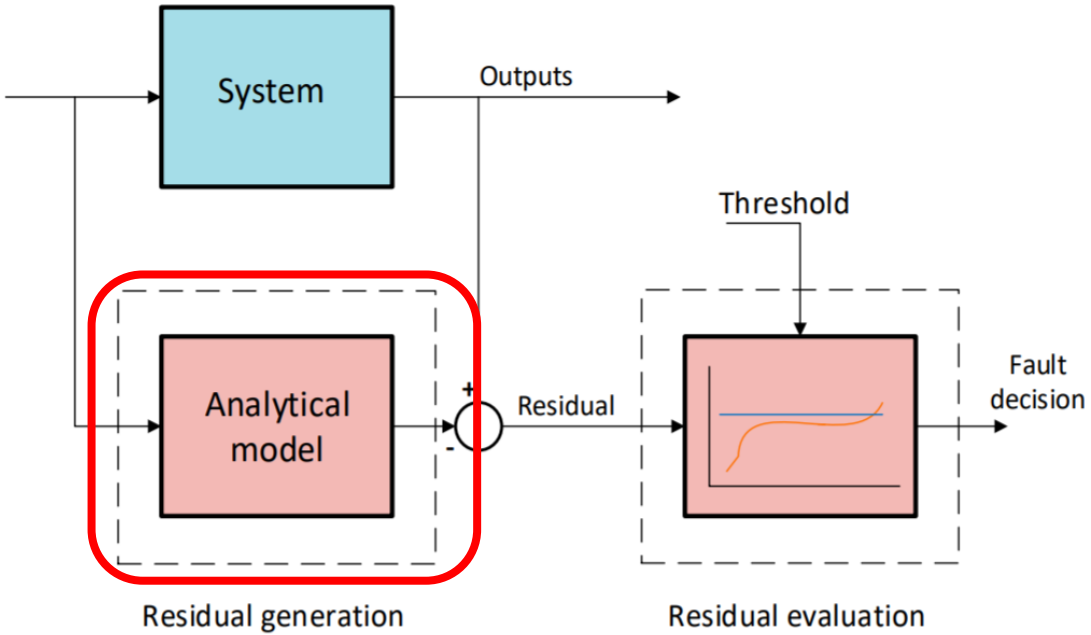


Fundamental Concepts of Residual-Based Fault Detection

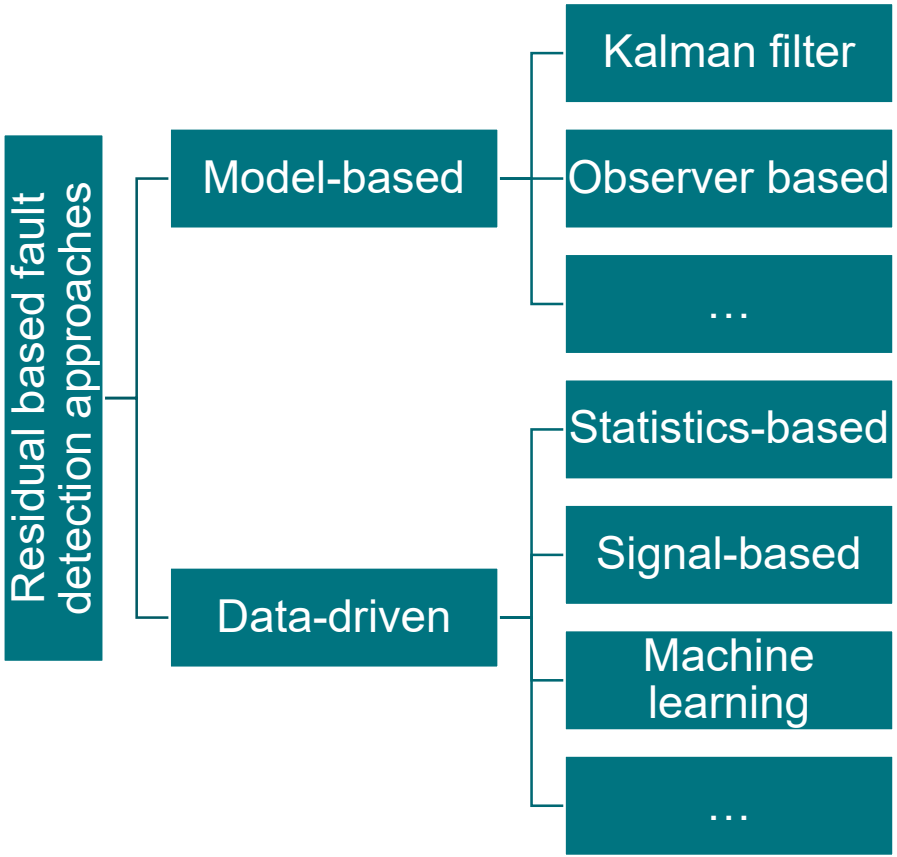


- **System Modeling**
  - At the core of residual-based fault detection is an accurate model of the system under normal operating conditions.
  - **Analytical Models:** Derived from first principles and mathematical equations representing the system's physical laws.
  - **Data-Driven Models:** Developed using historical data through techniques like machine learning, statistical analysis, or system identification methods.
- **Residual Generation**
  - Residuals are calculated by comparing the actual system outputs with the outputs predicted by the model. Mathematically, it can be expressed as:
  - **Residual=Observed Output−Predicted Output**
  - Under normal conditions, residuals should ideally be zero or within a predefined acceptable range. Significant deviations from this range suggest potential faults.
- **Threshold Setting**
  - To determine what constitutes an abnormal residual, thresholds are established.
  - **Static Thresholds:** Fixed values based on historical data or safety margins.
  - **Adaptive Thresholds:** Dynamic values that adjust based on operating conditions, environmental factors, or system variability.

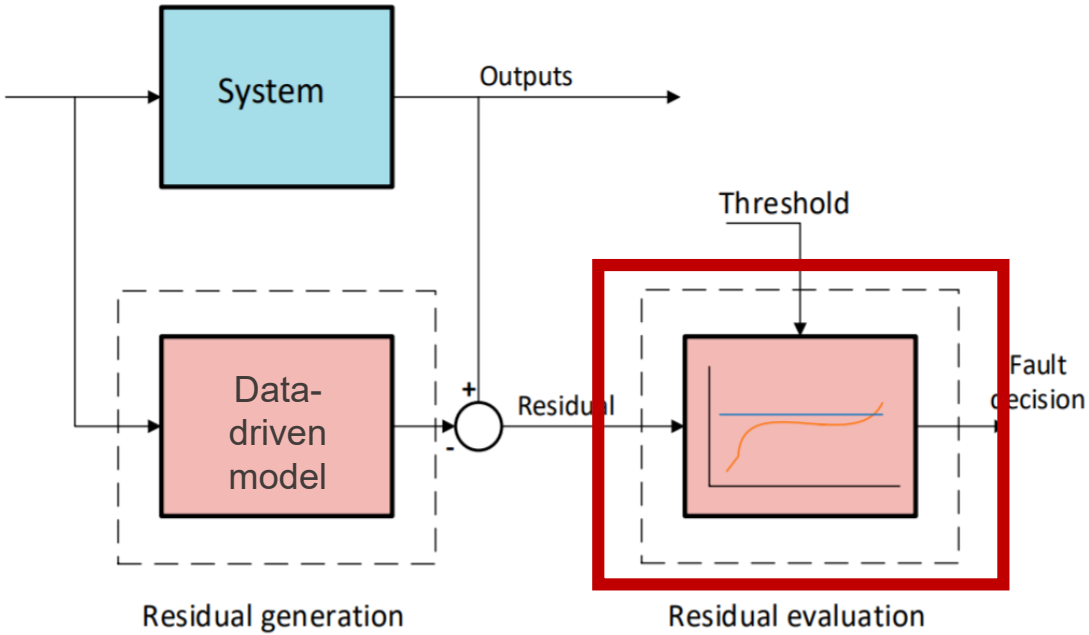
Basic idea of residual based methods



Different approaches to residual-based methods



Basic idea of residual based methods



Thresholds

- Determine the thresholds based on the validation dataset (+ add additional margin)
- Two types of thresholds: for all the signals + for single signals → fault isolation
- Perform statistical tests on the distributions of the residuals

Fault Detection Logic

- The detection logic involves monitoring residuals and comparing them against the set thresholds to decide whether a fault has occurred. This can include:
  - **Simple Thresholding:** Triggering an alarm if the residual exceeds the threshold.
  - **Statistical Methods:** Using statistical tests to assess the significance of residual deviations.
  - **Pattern Recognition:** Identifying specific patterns or trends in residuals that correlate with certain fault types.

Residual-Based Fault Detection

Advantages

- **Simplicity:** Conceptually straightforward and easy to implement with a well-defined residual.
- **Generality:** Applicable to a wide range of systems and fault types.
- **Real-Time Capability:** Enables continuous monitoring and timely fault detection.
- **Scalability:** Can be extended to complex and large-scale systems by decomposing them into manageable subsystems.

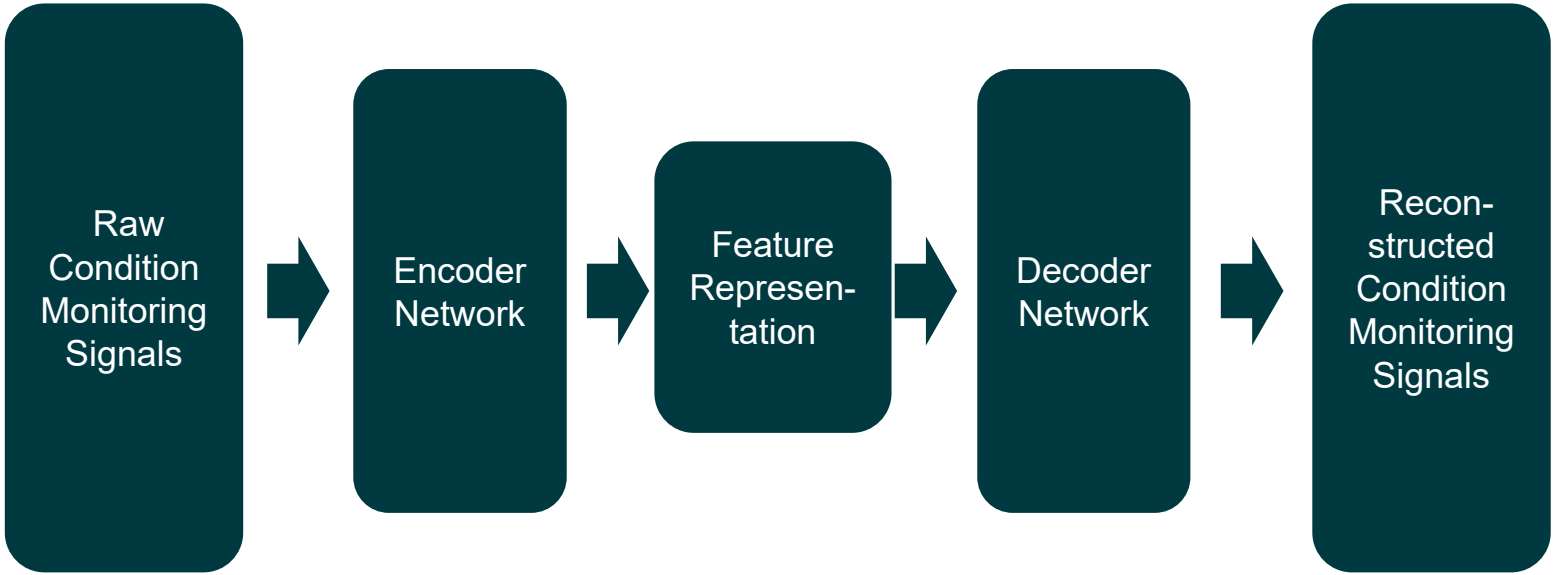
Challenges and Limitations

- **Model Accuracy:** The effectiveness heavily depends on the accuracy of the system model. Inaccurate models can lead to false alarms or missed detections.
- **Noise Sensitivity:** High levels of measurement noise can obscure residual signals, making fault detection more difficult.
- **Threshold Determination:** Setting appropriate thresholds is critical and can be challenging, especially in systems with variable operating conditions.
- **Complex Faults:** Simultaneous or multiple faults may be difficult to detect and isolate using residual-based methods alone.

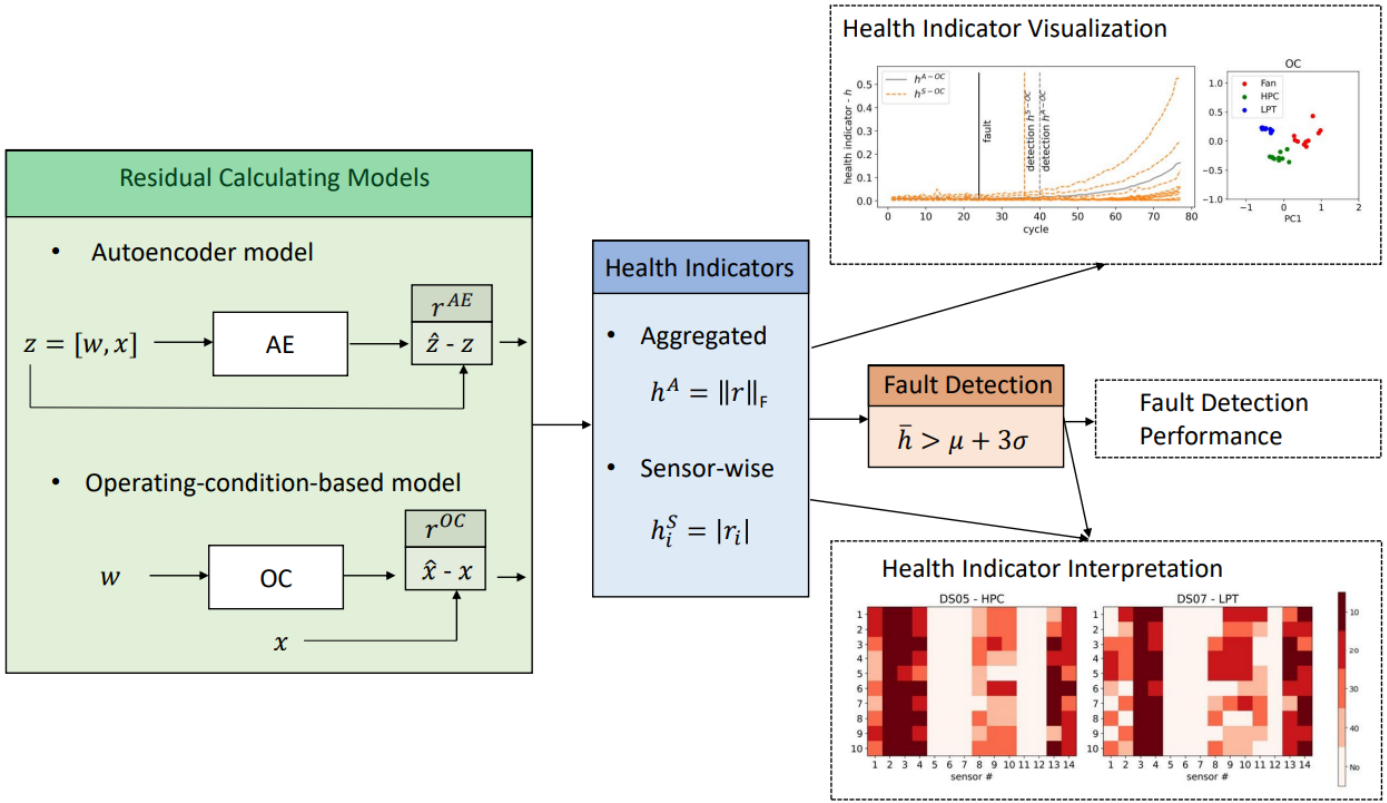
Different types of residual-based approaches

- Signal reconstruction (reconstruct the signal at the current point in time (t)) → Autoencoder model
- Forecasting (predict the measurements at t+1)
- Input (operating conditions + control) – Output (signal measurements) mappings → operating conditions models

Learning features from raw condition monitoring data



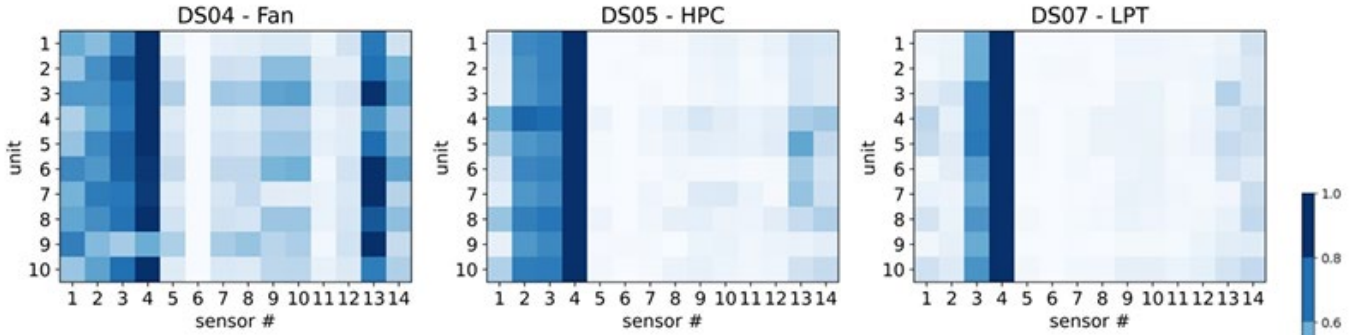
Residual-based fault detection example



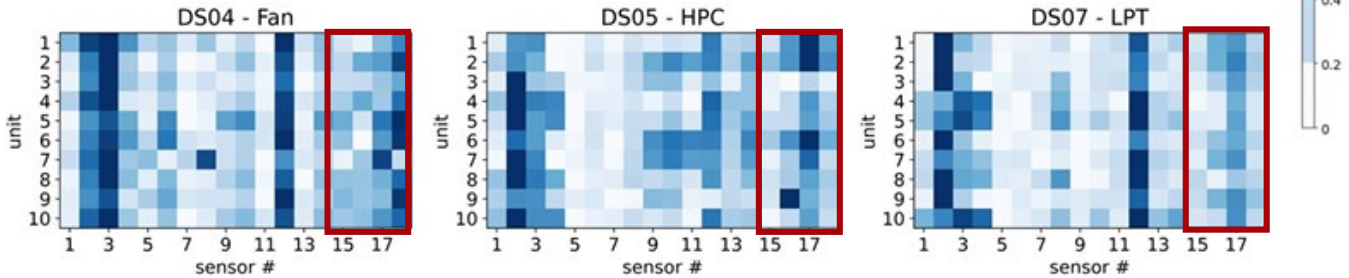
Hsu, C.C., Frusque, G. and Fink, O., 2023. A Comparison of Residual-based Methods on Fault Detection, PHM Society Conference

Residual-based fault detection example

Operating-Conditions-based



Signal-Reconstruction-Based



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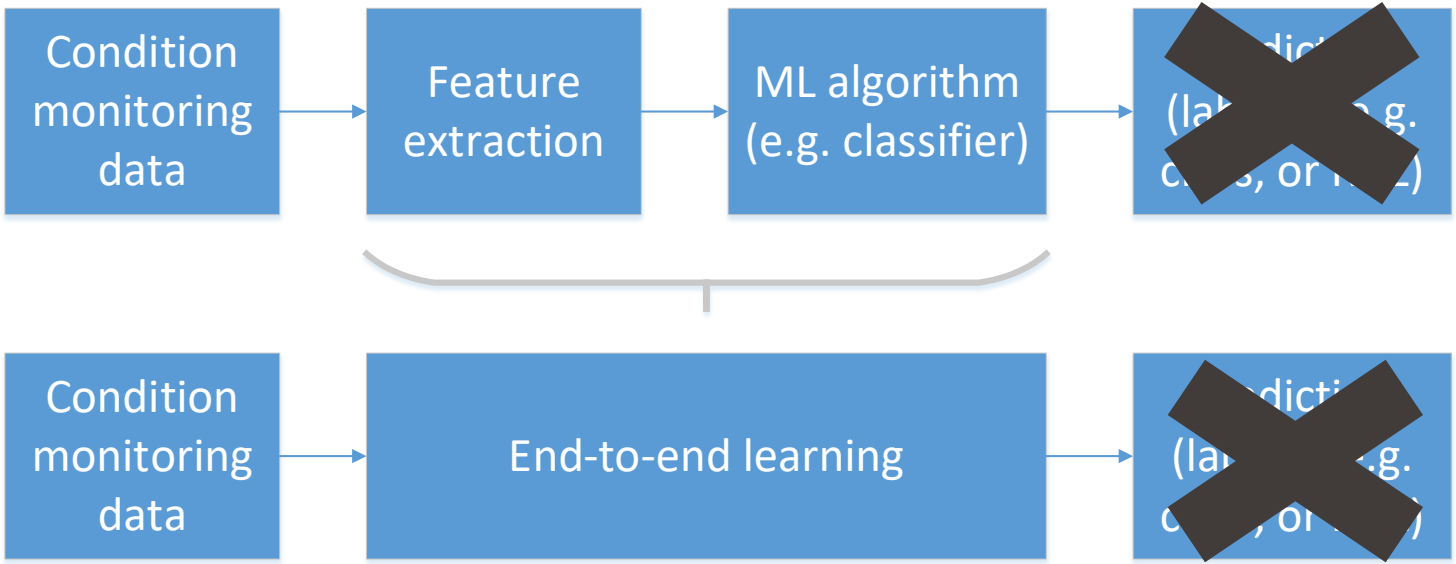
Unsupervised / Self-supervised learning

Learning Architectures



How much information is the machine given during learning?

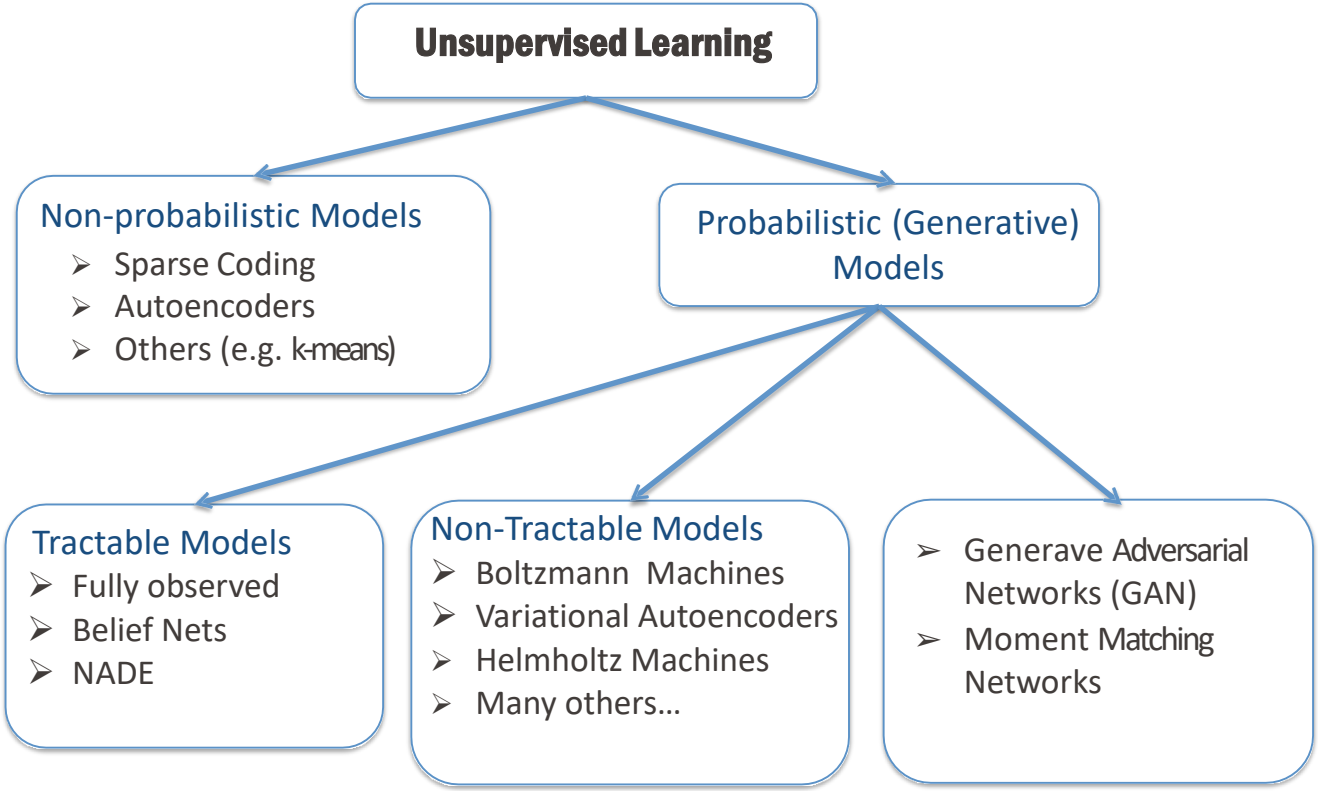
- **"Pure" Reinforcement Learning (cherry)**
  - The machine predicts a scalar reward given once in a while.
  - **A few bits for some samples**
- **Supervised Learning (icing)**
  - The machine predicts a category or a few numbers for each input
  - Predicting human-supplied data
  - **10→10,000 bits per sample**
- **Self-Supervised Learning (cake génoise)**
  - The machine predicts any part of its input for any observed part.
  - Predicts future frames in videos
  - **Millions of bits per sample**

Source: Y. LeCun

Unsupervised (also self-supervised, predictive) Learning

- We have access to {x1, x2, x3, · · ·, xN} but not {y1, y2, y3, · · ·, yN}

- Why would we want to tackle such a task:
  - Extracting interesting information from data
  - Clustering
  - Discovering interesting trend
  - Data compression
  - Learn better representations



Source: R. Salakhutdinov

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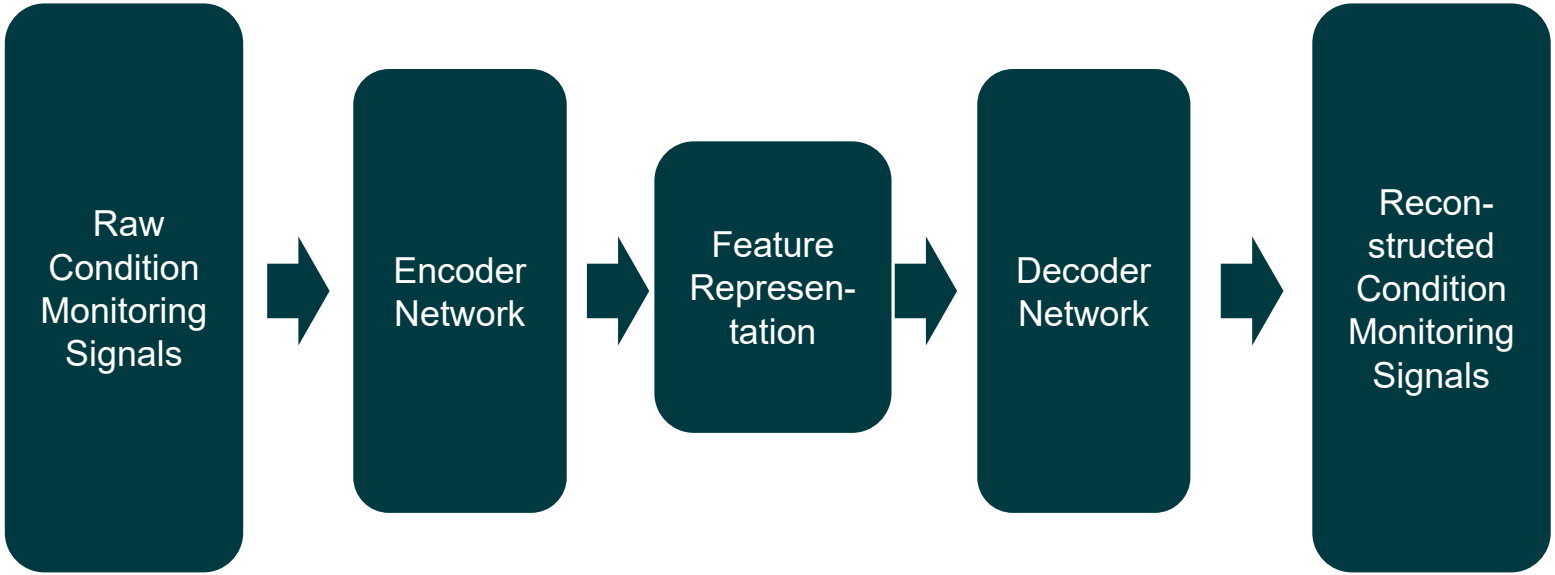
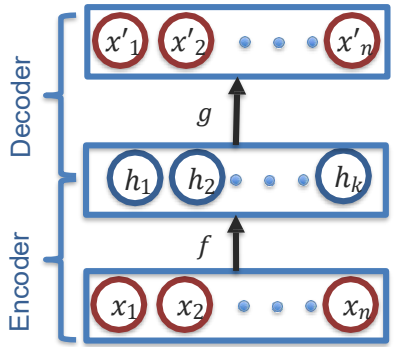


Autoencoders

- Network is trained to output the input (learn identify function).
- Two parts encoder/decoder
  - $x' = g(f(x))$
  - g - decoder
  - f - encoder



Trivial solution unless:
- Constrain number of units in Layer 2 (learn compressed representation), or
- Constrain Layer 2 to be **sparse**

Basic principles of an autoencoder

If the input is $x \in \mathbb{R}^n$ an autoencoder will produce a $h \in \mathbb{R}^d$ where $d < n$, which is designed to contain most of the important features of $\mathbf{x}$ to reconstruct it.

Autoencoder performs the following steps:

- **Encoder**: Perform a dimensionality reduction step on the data, $\mathbf{x} \in \mathbb{R}^n$ to obtain features $\mathbf{h} \in \mathbb{R}^d$.
- **Decoder**: Map the features $\mathbf{h} \in \mathbb{R}^d$ to closely reproduce the input, $\hat{\mathbf{x}} \in \mathbb{R}^n$.

Thus, the autoencoder implements the following problem:

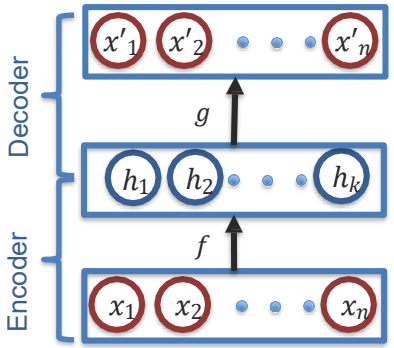
Let $\mathbf{x} \in \mathbb{R}^n$, $f(\cdot) : \mathbb{R}^n \to \mathbb{R}^d$ and $g(\cdot) : \mathbb{R}^d \to \mathbb{R}^n$. Let

$$\hat{\mathbf{x}} = g(f(\mathbf{x}))$$

Define a loss function, $\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}})$, and minimize $\mathcal{L}$ with respect to the parameters of $f(\cdot)$ and $g(\cdot)$.

There are different loss functions that you could consider, but a common one is the squared loss:

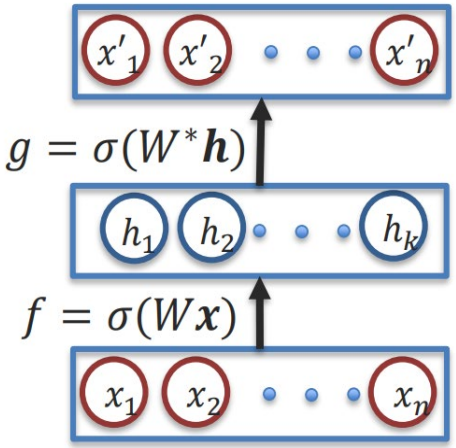
$$\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}) = \|\mathbf{x} - \hat{\mathbf{x}}\|^2$$



Source: J.C. Kao, UCLA

Nonlinear dimensionality reduction

- Mostly follows Neural Network structure
- Activation will depend on type of $\boldsymbol{x}$
- Often we use tied weights to force the sharing of weights in encoder/decoder (in this case a single-layer network)
  - $W^* = W^T$
- In a more general form, f() and g() could be deep neural networks, learning potentially more nonlinear and expressive features h.



Source: J.C. Kao, UCLA

Sparse autoencoders

A sparse autoencoder is one that is regularized to not only minimize the loss, but to also incorporate sparse features. If $\mathbf{h} = f(\mathbf{x})$ and $\hat{\mathbf{x}} = \mathbf{g}(\mathbf{h})$, then the sparse encoder has the following loss:

$$\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}) + \lambda \sum_i |h_i|$$

where h_i is the ith element of $\mathbf{h}$. This is intuitive, as we know L1-regularization introduces sparsity.

Source: J.C. Kao, UCLA

Denoising autoencoders

Say you wanted to obtain an autoencoder that was robust to noise. One could generate noise, ε, and add it to the input $\mathbf{x}$, so that $\tilde{\mathbf{x}} = \mathbf{x} + \varepsilon$. Then, the loss function of the autoencoder would have loss:

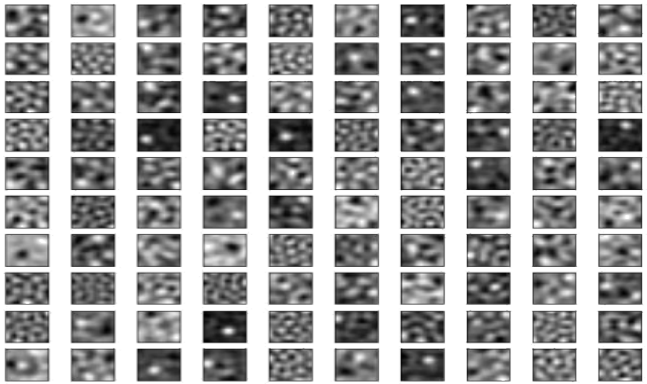
$$\mathcal{L}(\mathbf{x}, g(f(\tilde{\mathbf{x}})))$$

and it would learn to denoise $\tilde{\mathbf{x}}$ to reproduce $\mathbf{x}$. This can cause your autoencoder to be robust to certain types of noise.

Source: J.C. Kao, UCLA

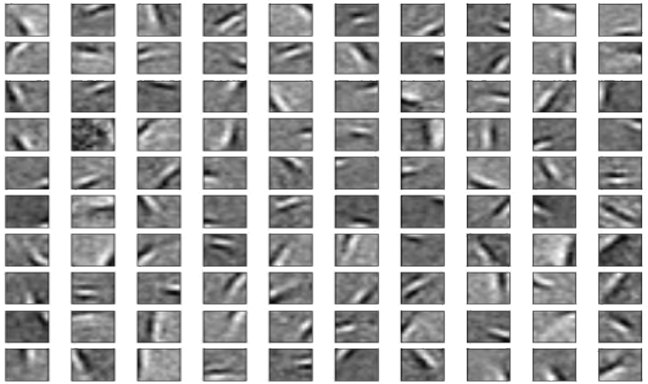
Sparse Vs Denoising (example)

- Filter weights, 12x12 patches



Sparse AE

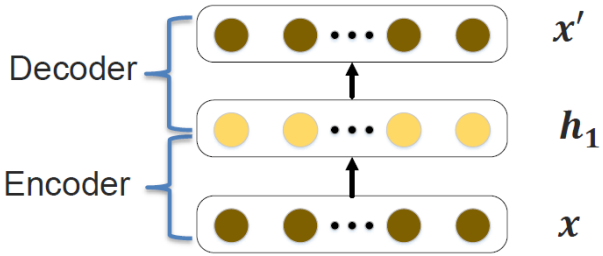
Actually meaningless :)

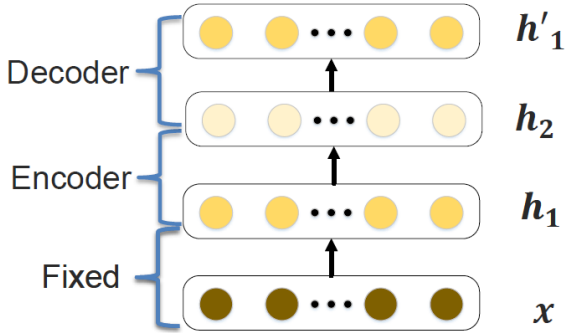


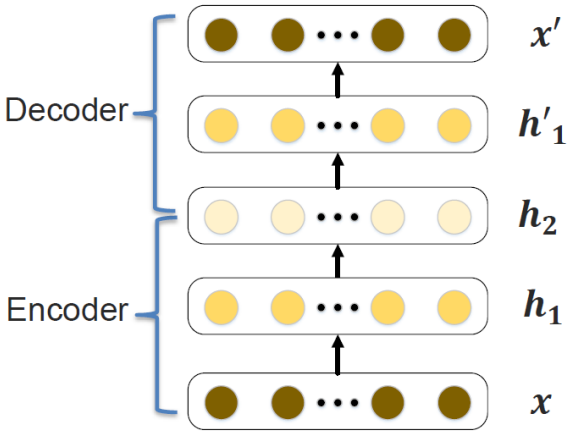
Denoising AE

[Vincent et al. 2010]

Stacked autoencoders



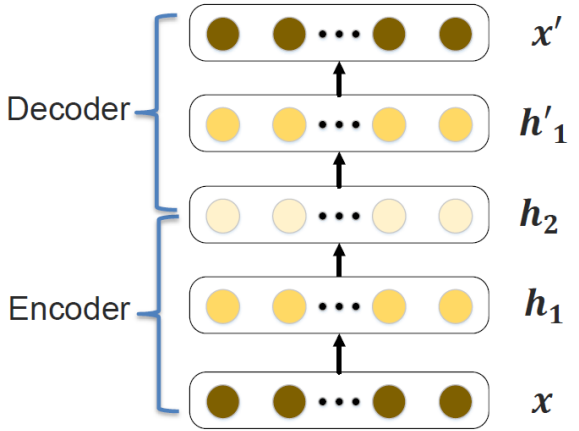




Source: L.P. Morency

Stacked denoising autoencoders

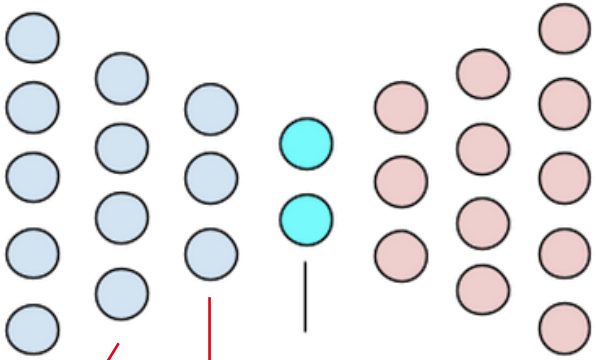
- Can extend this to a denoising model
- Add noise when training each of the layers
- Often with increasing amount of noise per layer
- 0.1 for first, 0.2 for second, 0.3 for third



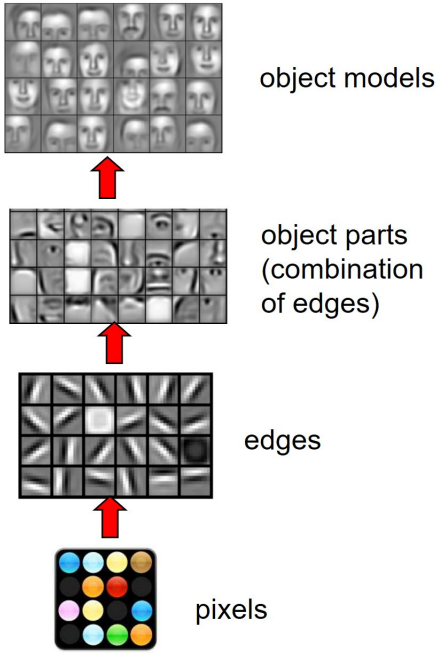
Source: L.P. Morency

Learning features with deep learning algorithms

Input



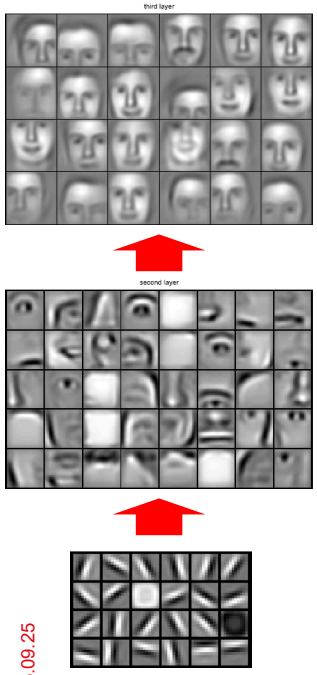
Output



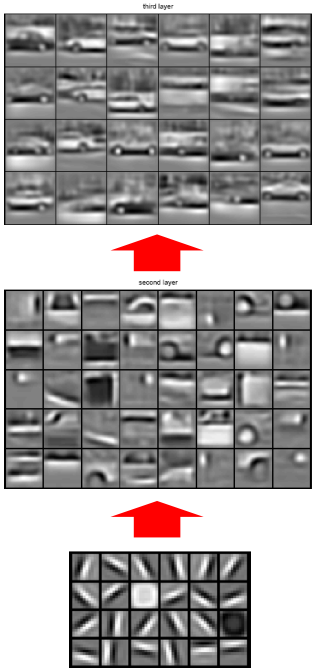
Source: A. NG

Examples of learned object parts from object categories

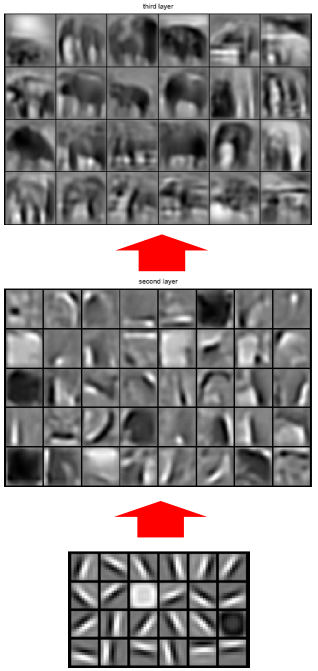
Faces



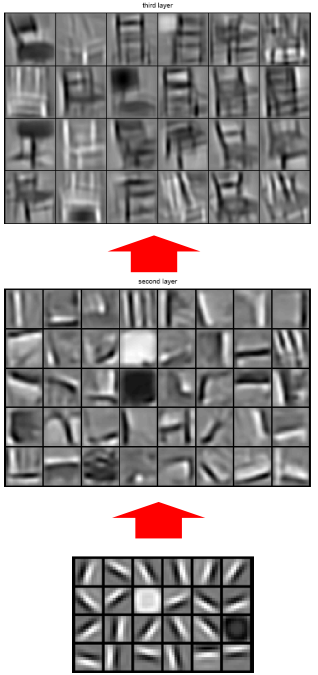
Cars



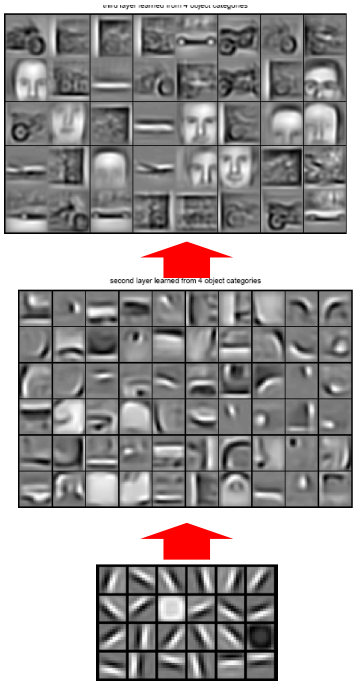
Elephants



Chairs



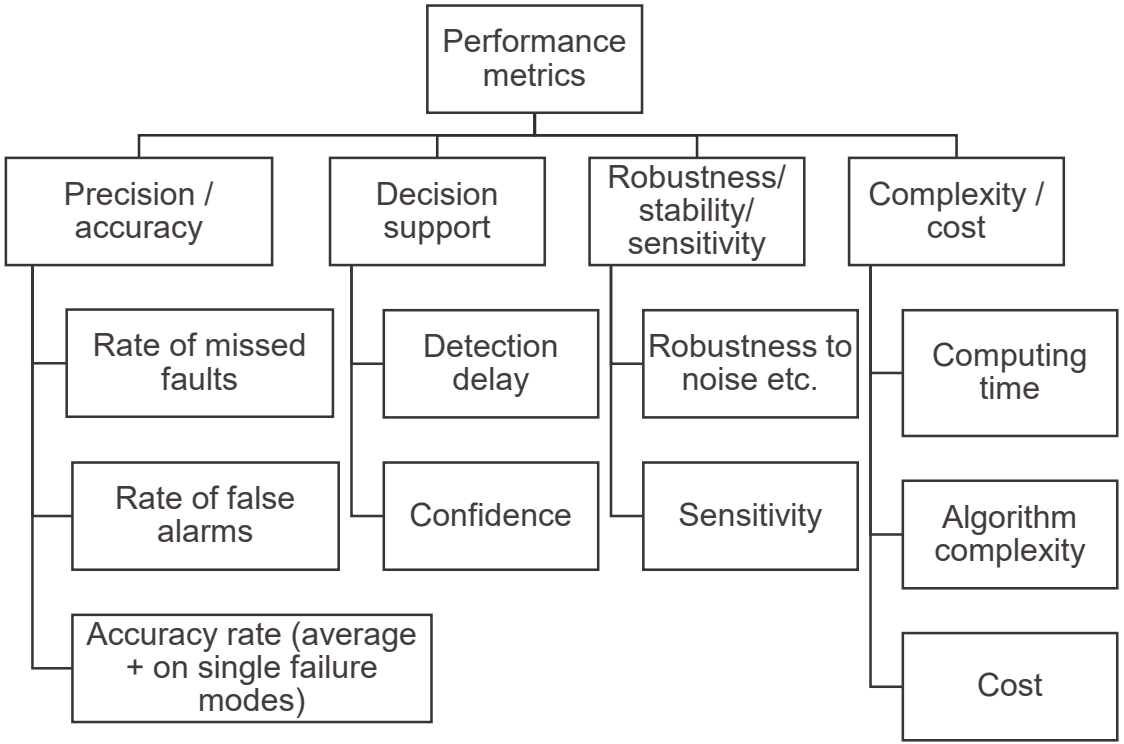
Trained on 4 classes



Source: A. NG

Performance Evaluation

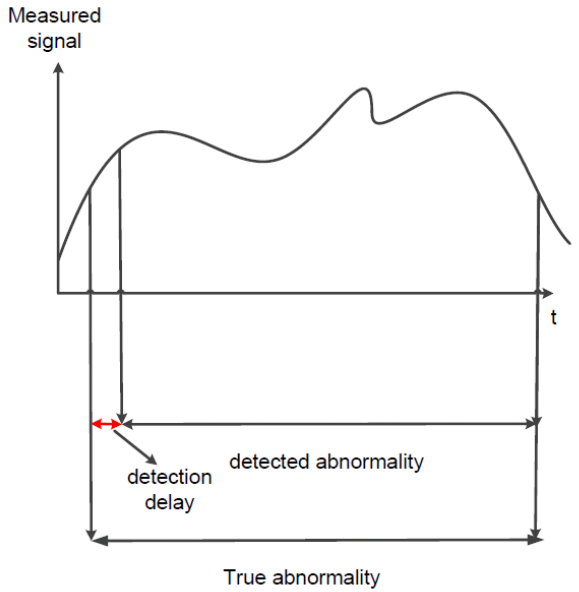
Performance metrics (selected)



Detection delay

- Detection delay:

→ Time span between the initiation and the detection of a fault (failure) event



Confusion matrix: missed alarms/ false alarms

True class → / Predicted class ↓	Fault	No fault
Positive (detected)	TP	FP
Negative (not detected)	FN	TN
	P=TP+FN	N=FP+TN

- Rate of missed alarms:
  FN/(TP+FN)
- Rate of false alarms:
  FP/(FP+TN)

Classification performance

$$Precision = \frac{True\ Positive}{True\ Postitive + False\ Positive}$$

$$Specificity = \frac{True\ Negative}{True\ Negative + False\ Postitive}$$

$$Recall(Sensitivity) = \frac{True\ Positive}{True\ Postitive + False\ Negative}$$

$$Accuracy = \frac{True\ Positive + True\ Negative}{Total}$$

$$F_1 = \frac{2 \cdot (Recall \cdot Precesion)}{Recall + Precesion}$$

$$F_\beta = (1 + \beta^2)\frac{Recall \cdot Precesion}{Recall + \beta^2 Precesion}$$

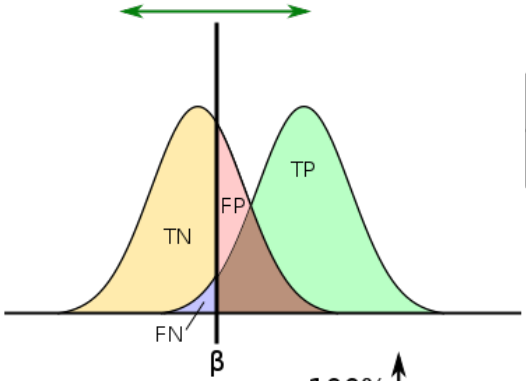
True class → / Predicted class ↓	Fault	No fault
Positive (detected)	TP	FP
Negative (not detected)	FN	TN

Precision

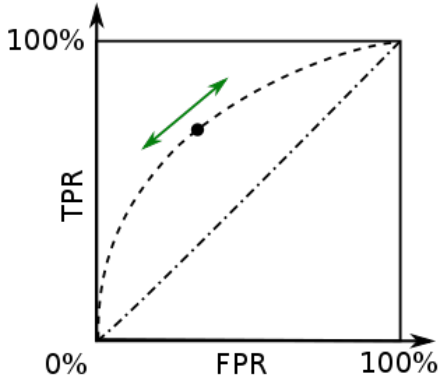
Recall

Specificity

ROC = Receiver Operating Characteristic
AUC = Area under the curve



TP	FP
FN	TN



Source: Wikimedia

Regression Metrics

- **Mean Absolute Error (MAE)**
  - **Definition:** The average of the absolute differences between predicted and actual values.
  - **Formula:**

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |\hat{y}_i - y_i|$$

  - **Use Case:** Provides a straightforward interpretation of average error in the same units as the target variable.

Regression Metrics

- **Mean Squared Error (MSE)**
  - **Definition:** The average of the squared differences between predicted and actual values.
  - **Formula:**

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$$

  - **Use Case:** Penalizes larger errors more than MAE, useful when large errors are particularly undesirable.

Regression Metrics

- **Root Mean Squared Error (RMSE)**
  - **Definition:** The square root of the MSE, bringing the metric back to the original units of the target variable.
  - **Formula:**

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$$

  - **Use Case:** Easier to interpret than MSE, while still penalizing larger errors.

Regression Metrics

- **R-squared (Coefficient of Determination)**
  - **Definition:** Measures the proportion of variance in the dependent variable that is predictable from the independent variables.
  - **Formula:**

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

  - **Use Case:** Indicates the goodness of fit of the model; values closer to 1 signify a better fit.

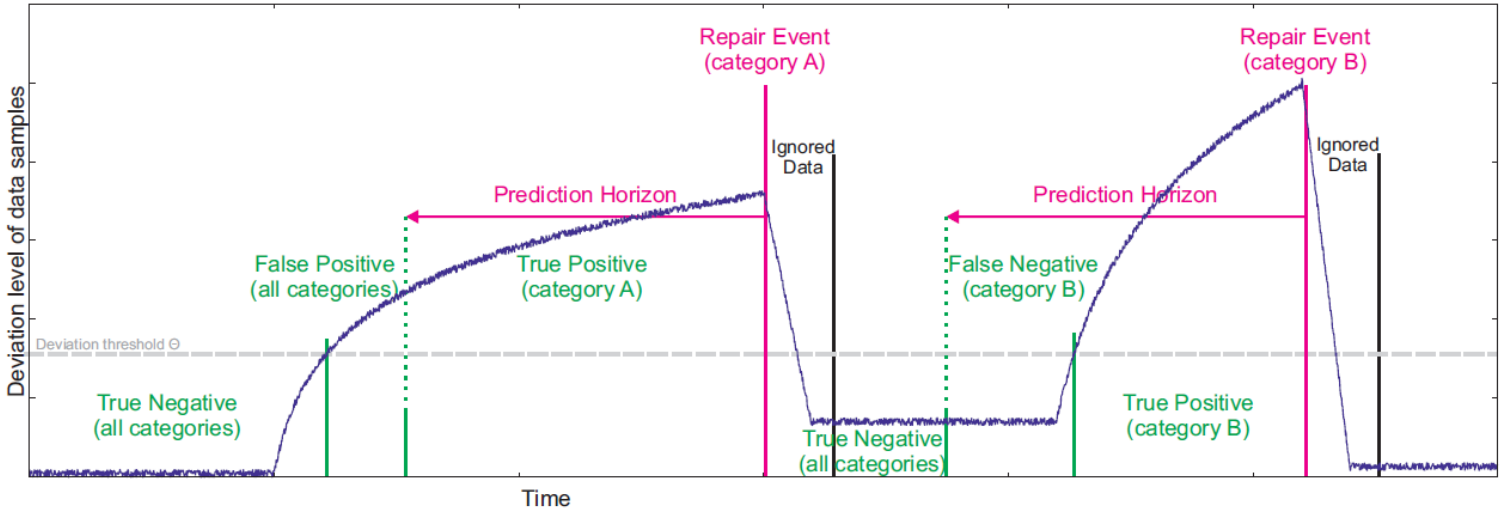
Clustering Metrics

- **Silhouette Score**
  - **Definition:** Measures how similar an object is to its own cluster compared to other clusters.
  - **Range:** -1 to 1, where higher values indicate better clustering.
  - **Use Case:** Evaluates the consistency within clusters of data.

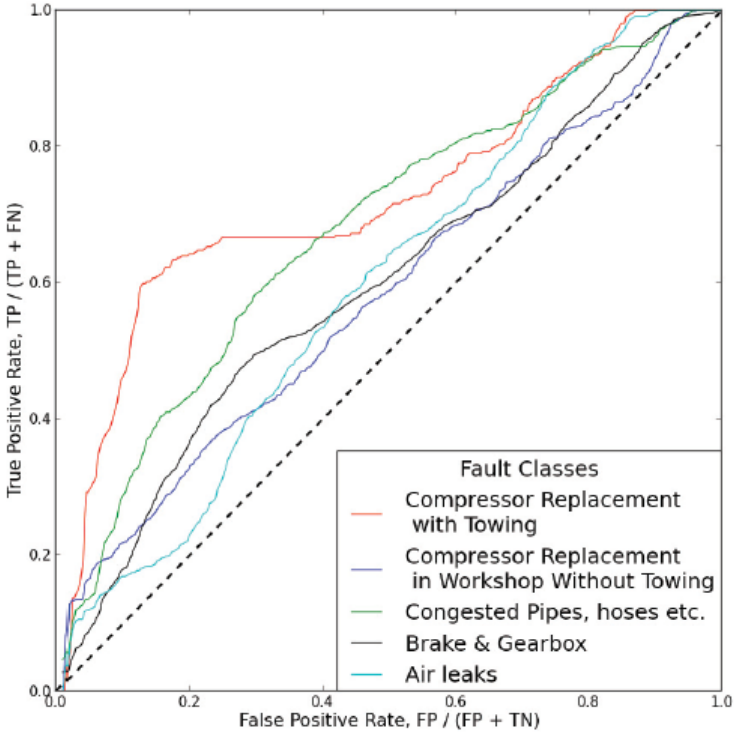
Choosing the Right Metric

- **Data Characteristics:**
  - **Balanced vs. Imbalanced Classes:** Metrics like precision, recall, F1 score, and ROC AUC are more informative for imbalanced datasets.
  - **Presence of Noise and Outliers:** Robust metrics like MAE are less sensitive to outliers compared to MSE.
- **Business Objectives:**
  - **Cost of Errors:** If false positives are more costly, prioritize precision; if false negatives are more costly, prioritize recall.
  - **Interpretability:** Choose metrics that stakeholders can easily understand and relate to business outcomes.

Example from a publication



Example of a ROC curve



One-Class SVM /

Support Vector Data Description (SVDD)

One-class SVM

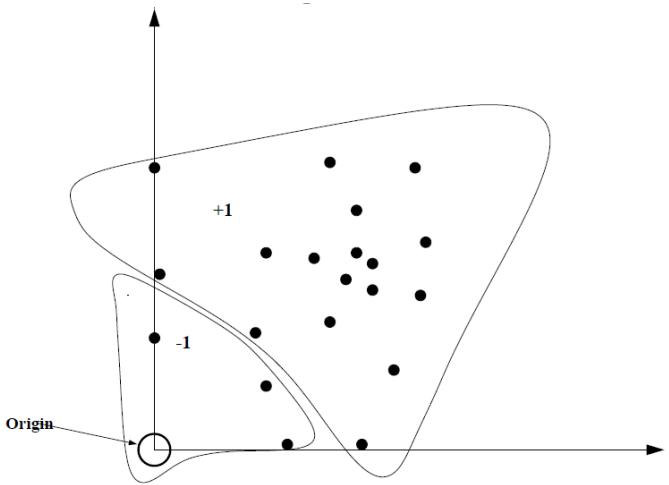
- Suppose that a dataset has a probability distribution *P* in the feature space.
- Find a “simple” subset *S* of the feature space such that the probability that a test point from *P* lies outside *S* is bounded by some a priori specified value $v \in (0, 1)$
- The solution for this problem is obtained by estimating a function *f* which is positive on *S* and negative on the complement $\bar{S}$.

$$f(x) = \begin{cases} +1 & \text{if } x \in S \\ -1 & \text{if } x \in \overline{S} \end{cases}$$

Source: Manevitz, 2001

One-class SVM

- The algorithm can be summarized as mapping the data into a feature space *H* using an appropriate kernel function, and then trying to separate the mapped vectors from the origin with maximum margin



Source: Manevitz, 2001

One-class SVM

$$\min_{w,\,\xi_i,\,\rho} \frac{1}{2}\|w\|^2 + \frac{1}{\nu n}\sum_{i=1}^{n}\xi_i - \rho$$

subject to:

$$(w \cdot \phi(x_i)) \geq \rho - \xi_i \qquad \text{for all } i = 1, \ldots, n$$

$$\xi_i \geq 0 \qquad \text{for all } i = 1, \ldots, n$$

Source: Manevitz, 2001

ν-parameter

- In this formula it is the parameter ν that characterizes the solution;
- it sets an upper bound on the fraction of outliers (training examples regarded out-of-class)
- it is a lower bound on the number of training examples used as Support Vector

Source: Manevitz, 2001

Decision function

If *w* and *ρ* solve this problem, then the decision function

$$f(x) = \operatorname{sgn}((w \cdot \phi(x_i)) - \rho) = \operatorname{sgn}(\sum_{i=1}^{n} \alpha_i K(x, x_i) - \rho)$$

will be positive for most examples x_i contained in the training set.

Source: Manevitz, 2001

Support Vector Data Description (SVDD)

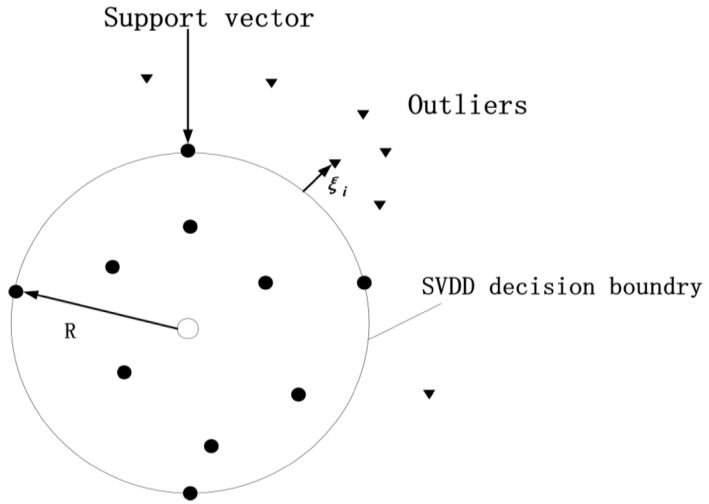
- Obtains a spherical boundary, in feature space, around the data.
- The volume of this hypersphere is minimized→ minimizes the effect of incorporating outliers in the solution

$$\min_{R,\,\mathbf{a}} R^2 + C\sum_{i=1}^{n}\xi_i$$

subject to:

$$\|x_i - \mathbf{a}\|^2 \leq R^2 + \xi_i \qquad \text{for all } i = 1,\ldots,n$$

$$\xi_i \geq 0 \qquad \text{for all } i = 1,\ldots,n$$



Source: Tax & Duin

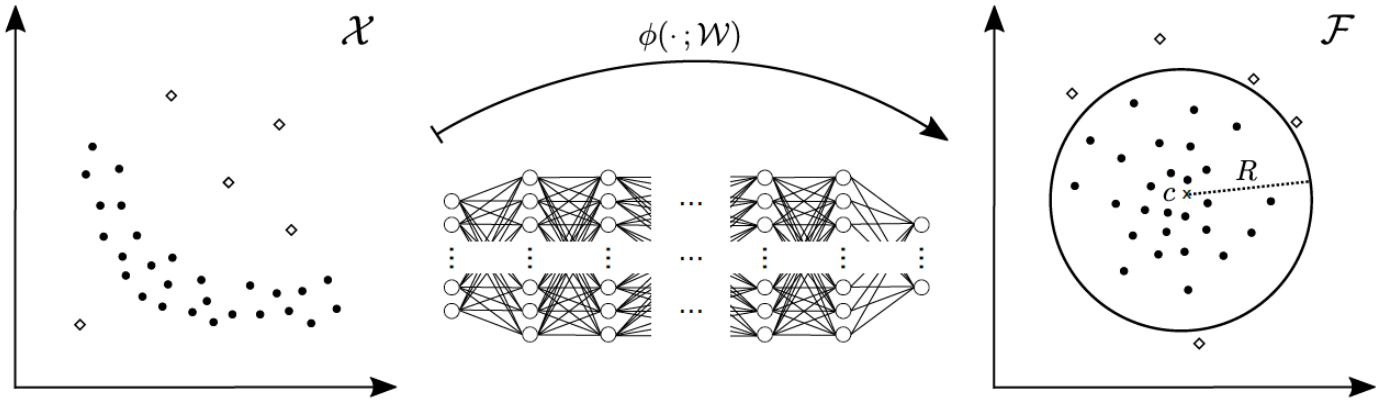
Support Vector Data Description (SVDD)

- After solving this by introducing Lagrange multipliers α_i, a new data point z can be tested to be in or out of class.
- It is considered in-class when the distance to the center is smaller than or equal to the radius, by using the Gaussian kernel as a distance function over two data points:

$$\|z - \mathbf{x}\|^2 = \sum_{i=1}^{n} \alpha_i \exp\left(\frac{-\|z - x_i\|^2}{\sigma^2}\right) \geq -R^2/2 + C_R$$

Source: Tax & Duin

Deep SVDD



Soft-boundary Deep SVDD objective

$$\min_{R,\mathcal{W}} \quad R^2 + \frac{1}{\nu n}\sum_{i=1} \max\{0, \|\phi(\boldsymbol{x}_i;\mathcal{W}) - \boldsymbol{c}\|^2 - R^2\} + \frac{\lambda}{2}\sum_{\ell=1}^{L} \|\boldsymbol{W}^\ell\|_F^2.$$

One-Class Deep SVDD objective

$$\min_{\mathcal{W}} \quad \frac{1}{n}\sum_{i=1}^{n} \|\phi(\boldsymbol{x}_i;\mathcal{W}) - \boldsymbol{c}\|^2 + \frac{\lambda}{2}\sum_{\ell=1}^{L} \|\boldsymbol{W}^\ell\|_F^2$$

Ruff, Lukas, Robert Vandermeulen, Nico Goernitz, Lucas Deecke, Shoaib Ahmed Siddiqui, Alexander Binder, Emmanuel Müller, and Marius Kloft. "Deep one-class classification." In *International conference on machine learning*, pp. 4393-4402. PMLR, 2018.

Deep SVDD

- **Foundation: Support Vector Data Description (SVDD)**
  - **Purpose:** SVDD is primarily used for one-class classification, aiming to identify whether new data points belong to a predefined class or are anomalies.
  - **Mechanism:** It constructs the smallest possible hypersphere in the feature space that encapsulates the majority of the data points from the target class.
  - **Limitations:** Traditional SVDD operates in a fixed, often low-dimensional feature space, which can be insufficient for capturing complex data patterns.
- **Integration with Deep Learning**
  - **Deep Feature Learning:** Deep SVDD leverages deep neural networks to automatically learn rich, high-dimensional feature representations from raw input data.
  - **End-to-End Training:** Unlike traditional SVDD, Deep SVDD trains the feature extractor (neural network) and the data description simultaneously, enabling the model to capture intricate data structures.
- **Objective Function**
  - **Sphere Minimization:** Similar to SVDD, the primary objective is to minimize the volume of the hypersphere that contains the data.
  - **Regularization Term:** Deep SVDD incorporates regularization to prevent the network from mapping all inputs to a trivial point (collapse), ensuring meaningful feature learning.
  - **Loss Function:** The loss typically combines the distance of data points from the center of the hypersphere with the regularization term, optimizing both the network weights and the sphere parameters.
- **Representation Learning**
  - **Layer-wise Feature Extraction:** Deep SVDD uses multiple layers in the neural network to extract hierarchical features, allowing the model to understand data at various levels of abstraction.
  - **Non-Linear Mappings:** The deep architecture facilitates non-linear transformations of the input data, making it possible to capture complex patterns that linear methods like traditional SVDD cannot.
- **Advantages Over Traditional SVDD**
  - **Enhanced Feature Representation:** By learning deep features, Deep SVDD can model more complex data distributions, improving anomaly detection accuracy.
  - **Scalability:** Deep SVDD can handle large and high-dimensional datasets more effectively due to the scalability of neural networks.
  - **Flexibility:** The deep architecture allows for integration with various types of data (e.g., images, text, time-series) by customizing the neural network structure accordingly.

Isolation Forest

Isolation Forest – overview

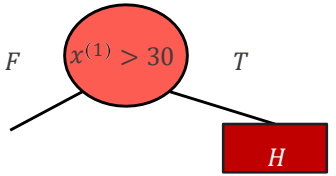
- **Aim:** provide a ranking that reflects the degree of "anomaly" for each data point
  - Sort data points according to their path lengths or anomaly scores
  - Outliers are the points with the biggest anomaly scores
- **Isolation Tree (iTree)**: binary tree where each node in the tree has exactly zero or two daughter nodes
- **Isolation Forest (iForest) algorithm**: Unsupervised Machine Learning algorithm inspired by random forests
  - Unsupervised: observations in the dataset are unlabeled
  - No need to profile normal instances and to calculate point-based distances
  - Builds an ensemble of random trees based on a mechanism called "isolation", an iterative (random) partitioning process to separate outliers from normal points
  - Uses the observation that **outliers are more likely to be isolated with fewer steps**, compared to normal points

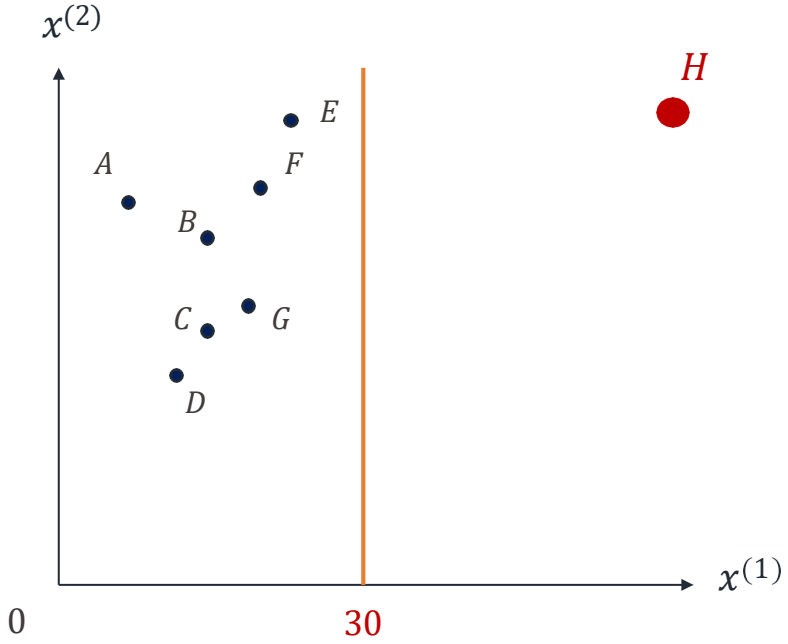
- *Liu, F. T., Ting, K. M., and Zhou, Z.-H. (2008). Isolation forest. In 2008 Eighth IEEE International Conference on Data Mining, pages 413-422. IEEE.*

Source: Alexandre Boumezoued

Isolation Forest – example of iTree

- Example of an Isolation Tree, two-dimensional case ($d = 2$)
- Point H (outlier) is isolated with only 1 step
- More steps are needed to isolate the other points





Source: Alexandre Boumezoued

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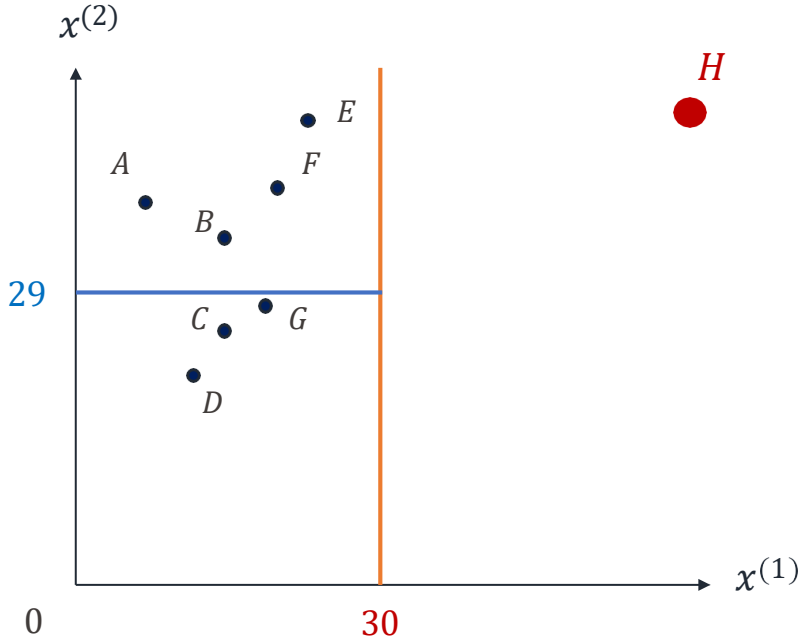

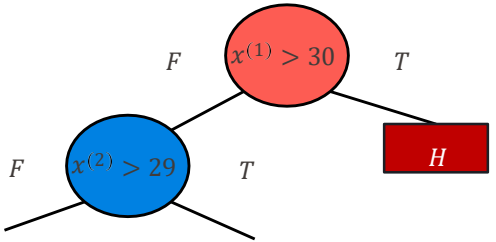

Source: Alexandre Boumezoued

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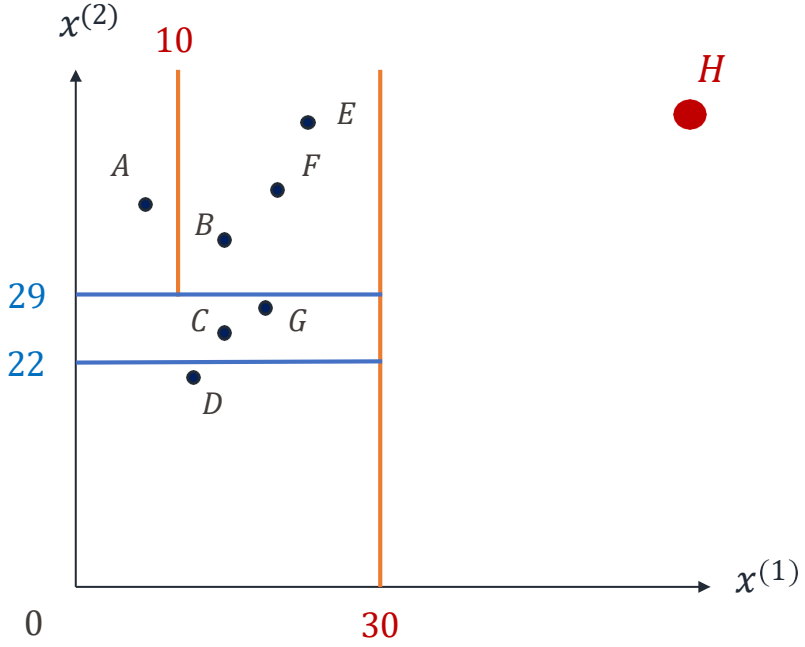

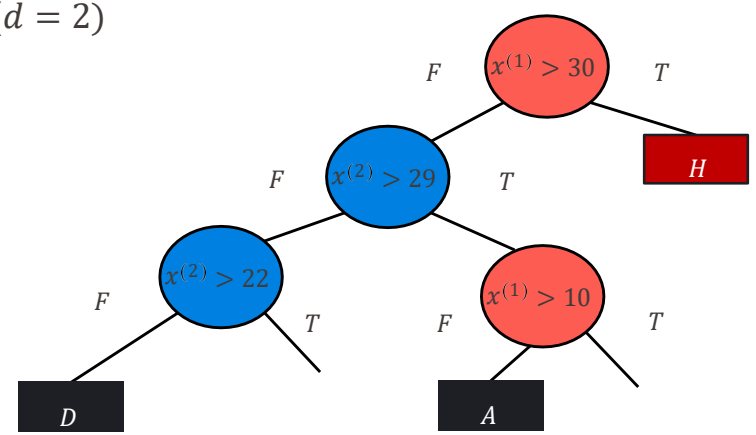

Source: Alexandre Boumezoued

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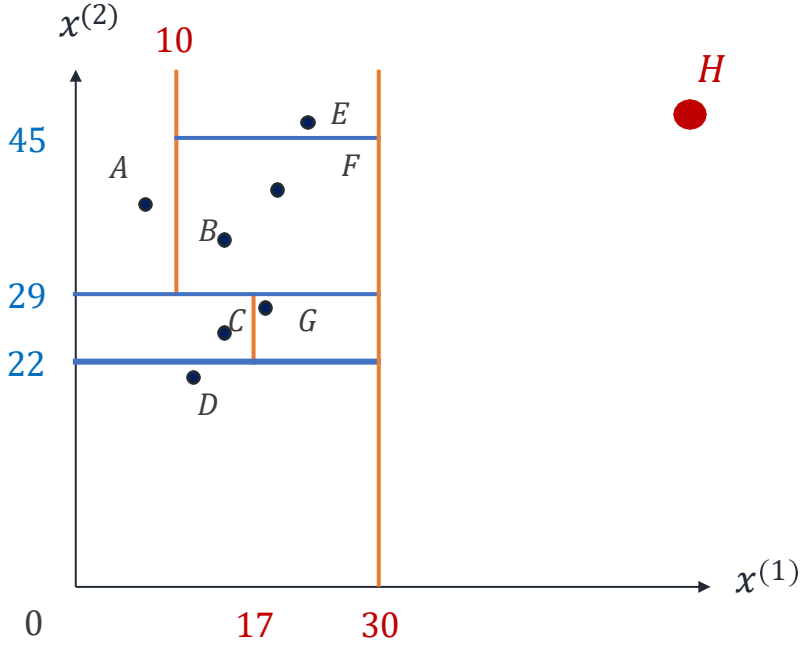

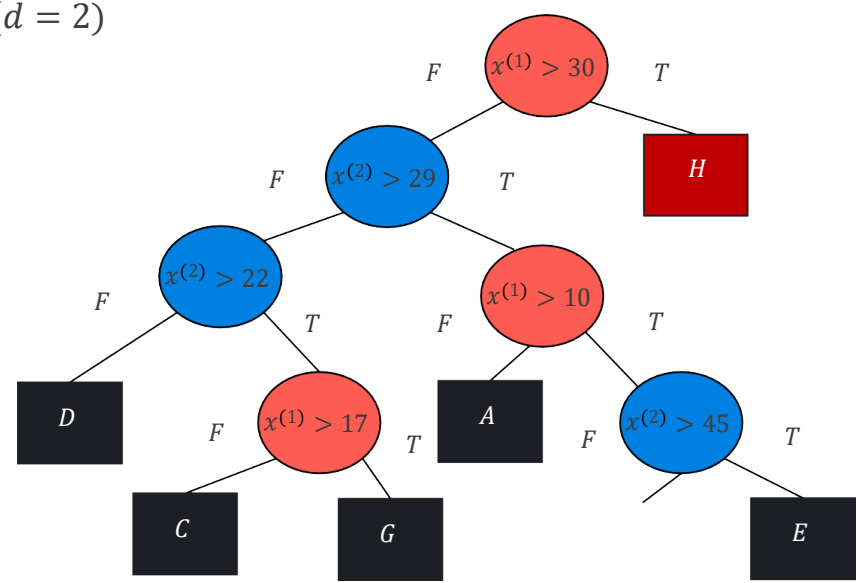

Source: Alexandre Boumezoued

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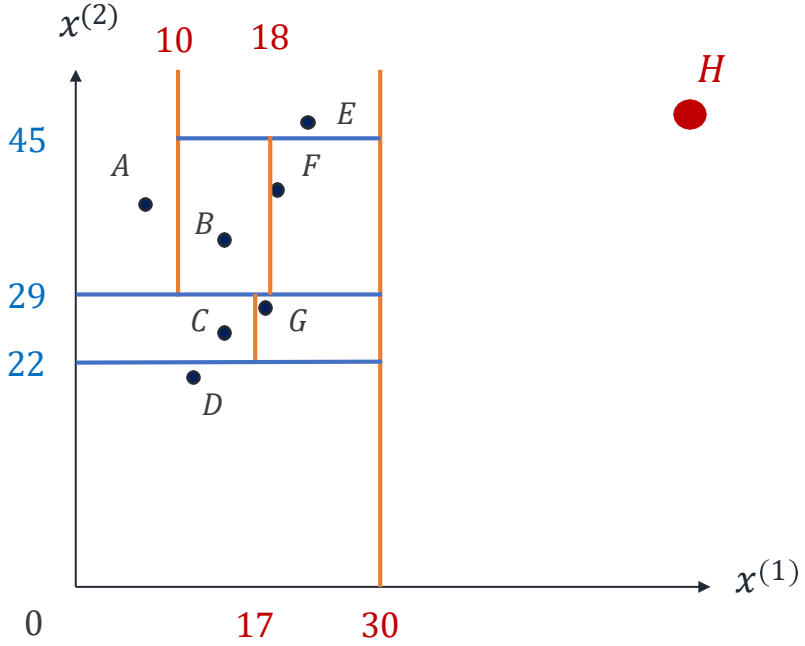
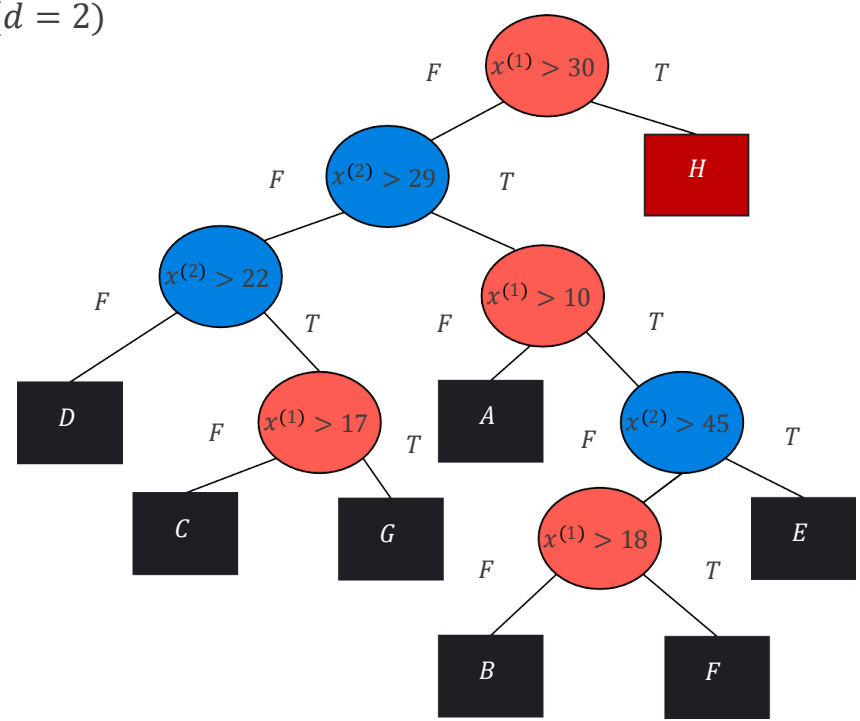
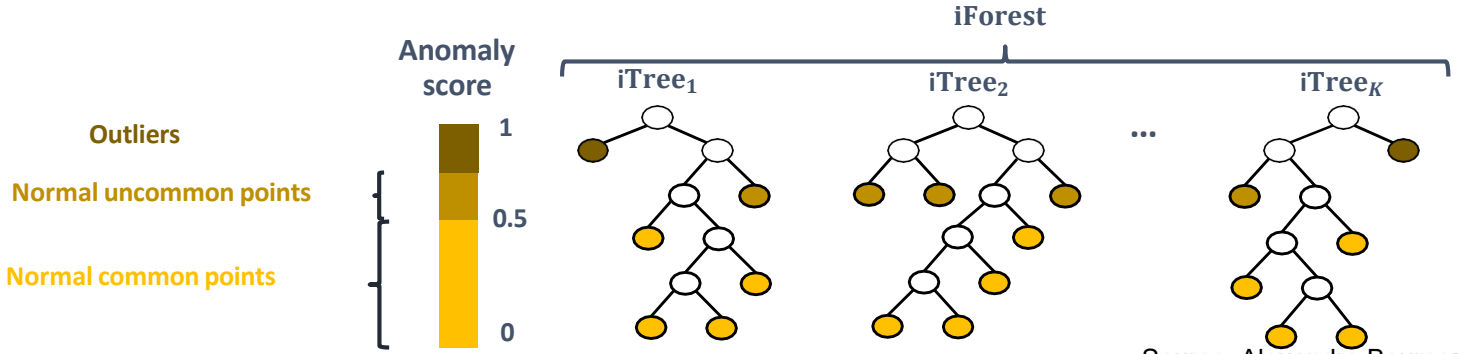




Source: Alexandre Boumezoued

Isolation Forest – from iTree to iForest

- **Ensemble method:** generates multiple iTrees → iForest
  - Path length of an observation obtained as the sum of:
    - total number of splits needed to isolate it
    - adjustment term to add if observation terminates at an external node. (Accounts for an unbuilt subtree beyond some tree height limit ℓ → saves computational time)
  - Compute the **average path lengths** $\overline{h(X_i)}$ for each observation X_i
- **Calculation of the anomaly scores**
  - Normalization by the average (universal) path length L in a binary tree
  - Anomaly score: $s(X_i) = 2^{-\frac{\overline{h(X_i)}}{L}} \in [0,1]$ ⇒ small average path length = high anomaly score



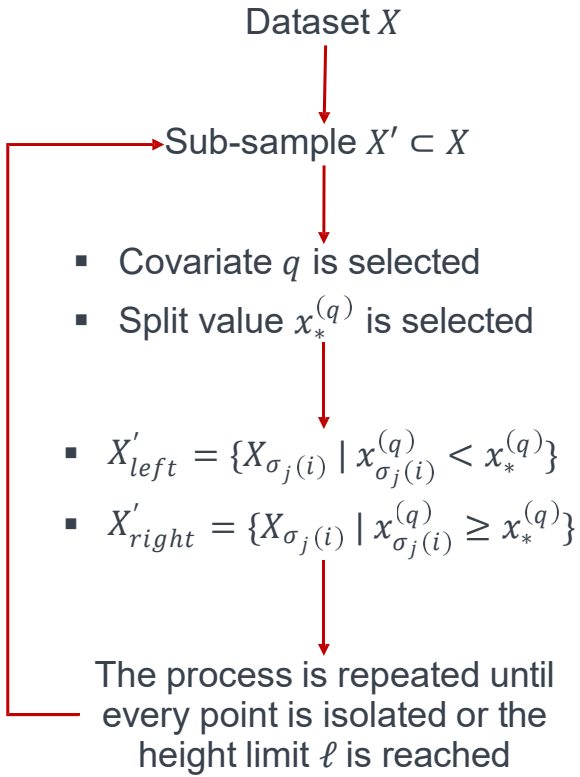
Source: Alexandre Boumezoued

Isolation Forest – details

- **Dataset**: $X = (X_1, \dots, X_n)$, with $X_i = \left(x_i^{(1)}, \dots, x_i^{(d)}\right) \in \mathbb{R}^d$ where:
  - n is the number of instances
  - d is the number of covariates

- **Sub-sampling**: An iTree j is obtained by selecting a random subset $X' \subset X$, where $|X'| = \psi < n$, $X' = \left(X_{\sigma_j(1)}, \dots, X_{\sigma_j(\psi)}\right)$, and $\sigma_j : [\![1, \psi]\!] \to [\![1, n]\!]$ is a (random) injective function.

- X' is then divided recursively by **randomly selecting a covariate** $q \in \{1, \dots, d\}$ and a **split value** $x_*^{(q)} \in [\min_{1 \le i \le \psi} x_{\sigma_j(i)}^{(q)}, \max_{1 \le i \le \psi} x_{\sigma_j(i)}^{(q)}]$ until:
  - Either the tree reaches the height limit ℓ, which is approximately the average tree height
  - Or $|X'| = 1$, i.e. there is only one unique point remaining



Source: Alexandre Boumezoued

Isolation Forest – about swamping and masking

- Swamping & masking are standard issues in outlier detection problems
  - **Swamping**: wrong identification of normal instances as outliers in the case where many variables are non informative on the “outlier” nature (the split based on these variables is not appropriate)
  - **Masking**: when too many outliers coexist in the dataset, the splitting rules are not efficient to isolate data points since many iterations are needed
- Both problems are consequences of too many data for the purpose of outlier detection
- Solution of iForest algorithm: **Sub-sampling**
  - Controls data size, which helps to better isolate examples of outliers
  - Each iTree can be specialized, each sub-sample including a different set of outliers
- It has been shown that iForest's outlier detection ability is superior when sub-sampling is used

Source: Alexandre Boumezoued

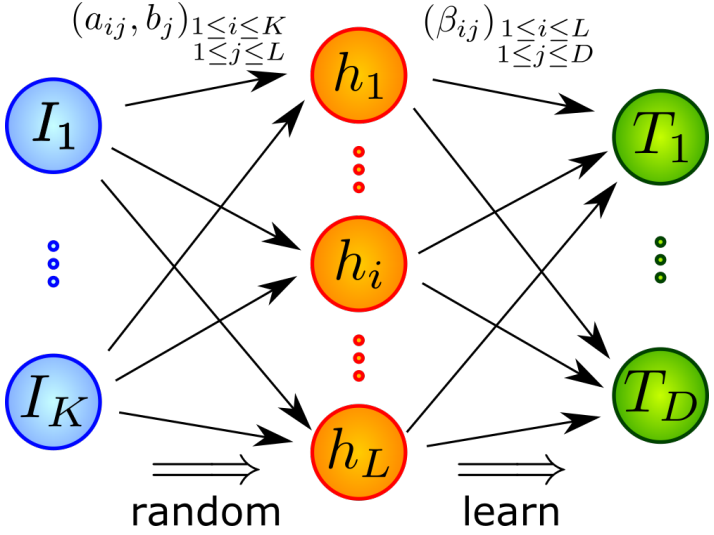
Isolation Forest – pros and challenges

- **Pros**
  - Unsupervised method: does not require labels of outliers provided by expert judgements
  - No model needed (the aim is not to model normal instances)
  - Provides a hierarchy by assigning an anomaly score to each observation
  - Does not require examples of outliers in the training set
  - Requires relatively small samples from large datasets to derive an outlier detection function
  - The algorithm can be trained once and reused without computational cost
  - Achieves a linear time complexity with low memory requirement
    - by using sub-sampling
    - by avoiding building trees after reaching a height limit ℓ
  - Overcomes the problem of swamping/masking by using sub-sampling
- **Challenges**
  - Requires working on the data to provide appropriate format of the covariates
  - Tuning parameters need to be set
  - To avoid the black-box syndrome, it benefits from a pre-selection of covariates in line with the problem to be tackled

Source: Alexandre Boumezoued

Example

Single Layer Feedforward Neural Networks



$$Y = g(\boldsymbol{A}, X, B) \cdot \boldsymbol{\beta}$$

$$\|g(\boldsymbol{A} \cdot X^{\text{Train}} + B) \cdot \hat{\boldsymbol{\beta}} - T\|_u^{\sigma_1} < \epsilon$$

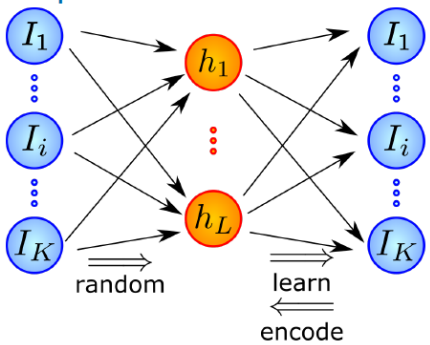
$$\|\boldsymbol{H} \cdot \hat{\boldsymbol{\beta}} - T\|_u^{\sigma_1} < \epsilon$$

$$\mathbf{H} = \begin{bmatrix} g(\mathbf{a}_1, b_1, \mathbf{x}_1) & \cdots & g(\mathbf{a}_L, b_L, \mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ g(\mathbf{a}_1, b_1, \mathbf{x}_{N_T}) & \cdots & g(\mathbf{a}_L, b_L, \mathbf{x}_{N_T}) \end{bmatrix}$$

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\text{Argmin}} \|\boldsymbol{H}\boldsymbol{\beta} - T\|_u^{\sigma_1} + C\|\boldsymbol{\beta}\|_v^{\sigma_2}$$

Single Layer Feedforward Neural Networks: Sparse Autoencoder

Sparse Auto-Encoder:



$$\underset{\beta}{\text{Argmin}}\, \lambda \|\beta\|_1 + \|\boldsymbol{H}\beta - X\|_2^2$$

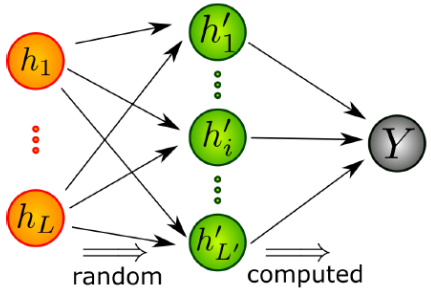
Residual

$$\text{Res} = \|X - X\beta_1{}^\top \beta_1\|_2^2$$

β is solved by FISTA (Fast Iterative Shrinkage-Thresholding Algorithm)

Single Layer Feedforward Neural Networks: one-class classifier

Regularised One-class classifier



$$\underset{\beta}{\text{Argmin}}\, \lambda \|\beta\|_2 + \|\boldsymbol{H}\beta - 1\|_2^2$$

$$\boldsymbol{\beta} = \left(C \cdot \mathbb{I} + \boldsymbol{H}^\top \boldsymbol{H}\right)^{-1} \boldsymbol{H}^\top T$$

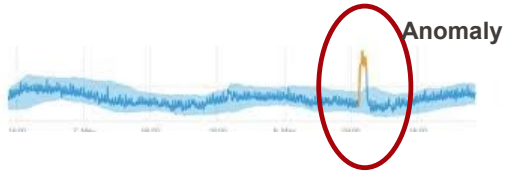
Residual

Distance to 1 (training)

$$d(Y_i, 1) = |Y_i - 1|$$

https://github.com/MichauGabriel/HELM

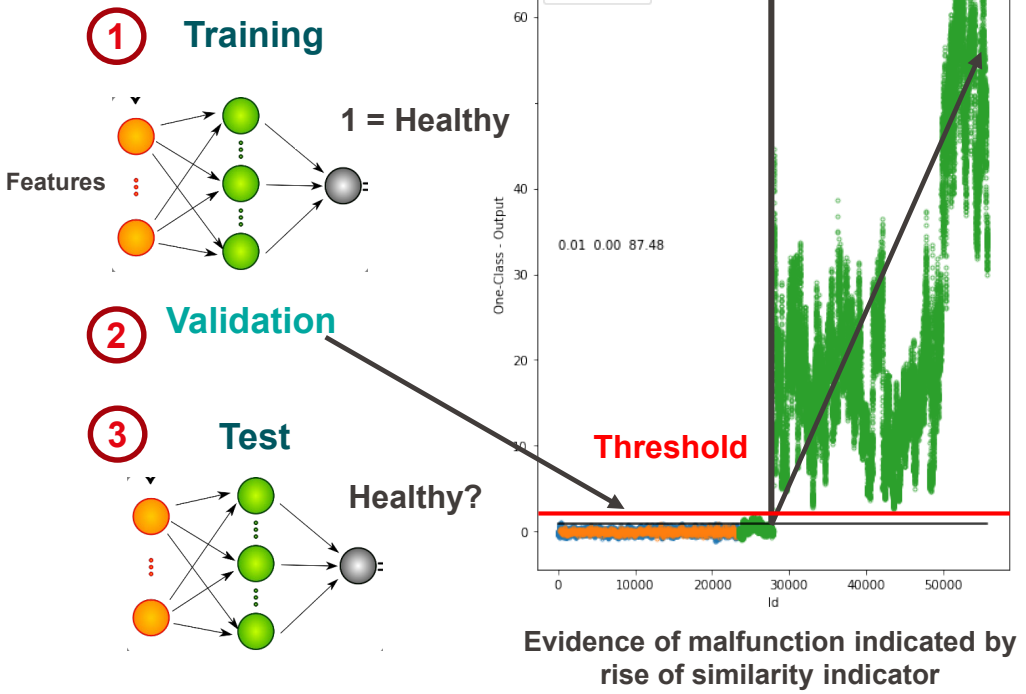
Machine Learning – One Class for Failure Detection



- Neural network learns healthy data
  - ➢ i.e training with healthy data
- Detection threshold defined with validation set

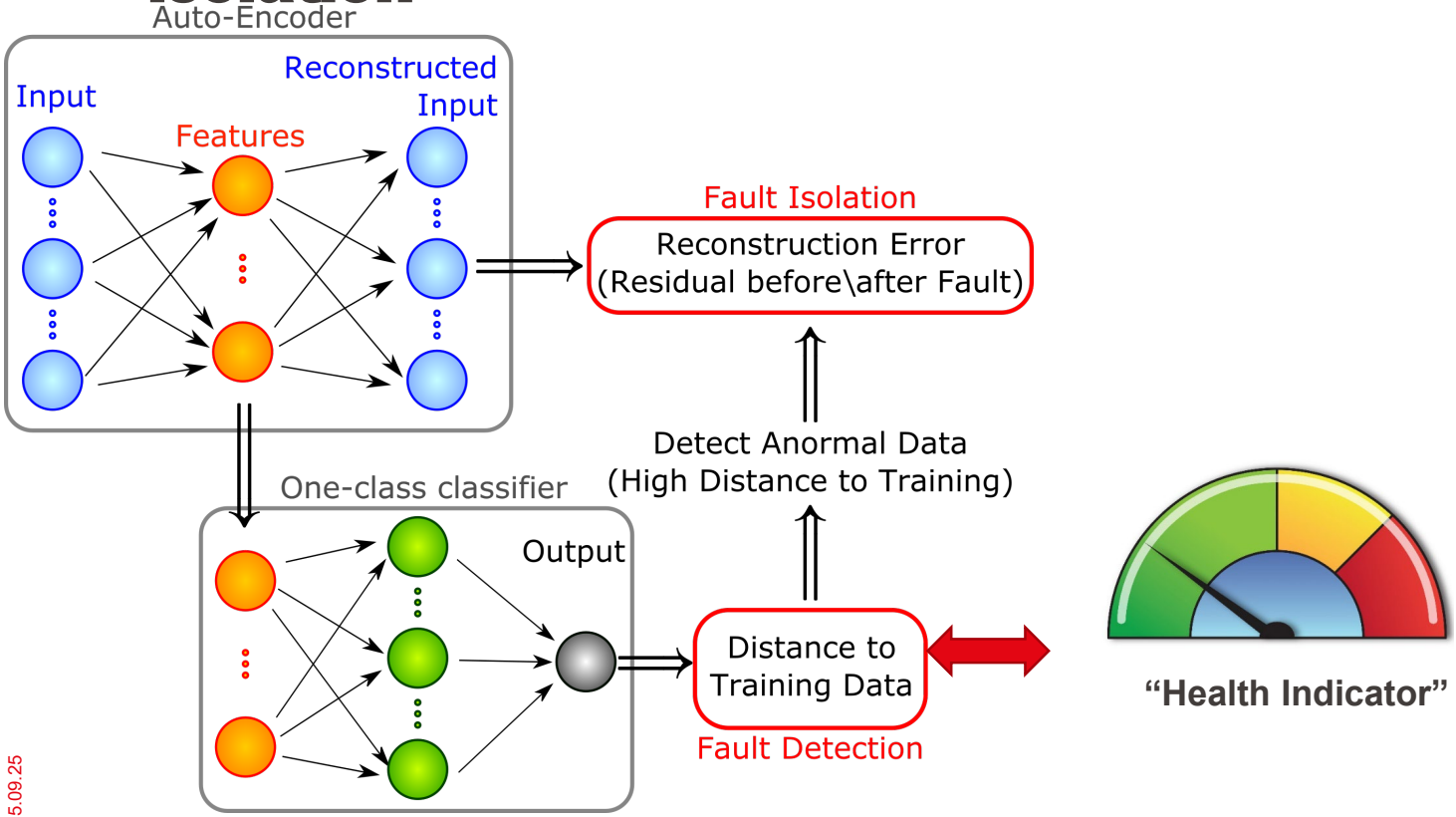
$$Thrd = \gamma \cdot percentile_p(|1 - Y^{Val}|)$$

- Neural network computes similarity index
  - ➢ i.e during testing



Evidence of malfunction indicated by rise of similarity indicator

Analysing the reconstruction residuals for fault isolation



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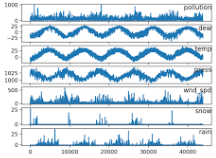
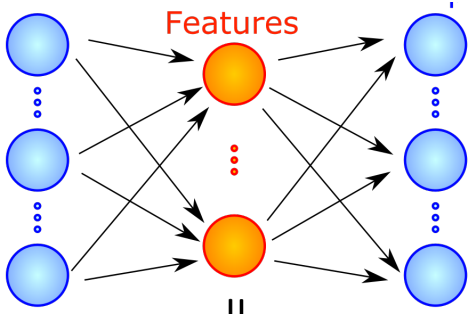
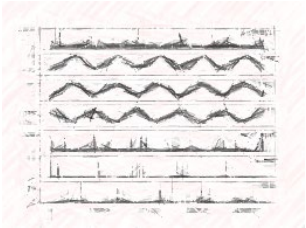
Decoder for Failure Isolation

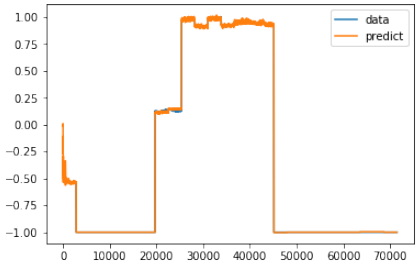
Input (x)



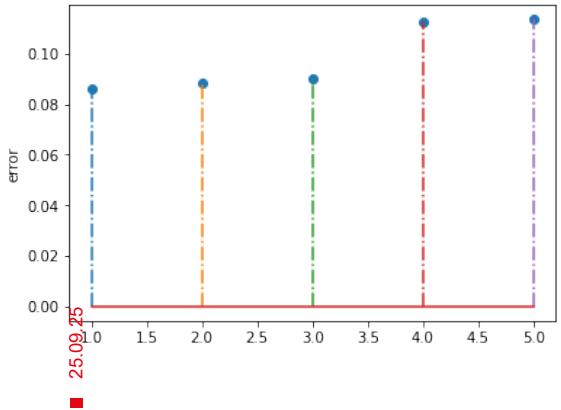


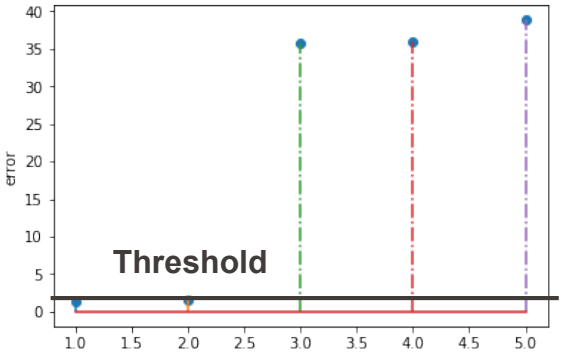
Reconstructed Input ($\bar{x}$)





Residual = $x - \bar{x}$





1 Training

Residual = $\mathrm{abs}(x_i - \bar{x}_i) \sim 0$

2 Validation

Residual threshold defined with healthy data

3 Test

If $\mathrm{abs}(x_i - \bar{x}_i) \gg 0$ then signal i faulty

Generator Health Monitoring

320 monitoring sensors:

- Partial discharge
- Rotor shaft voltage
- Rotor flux
- Stator end winding vibration
- Stator Water Temperature

275 days of recorded operation,

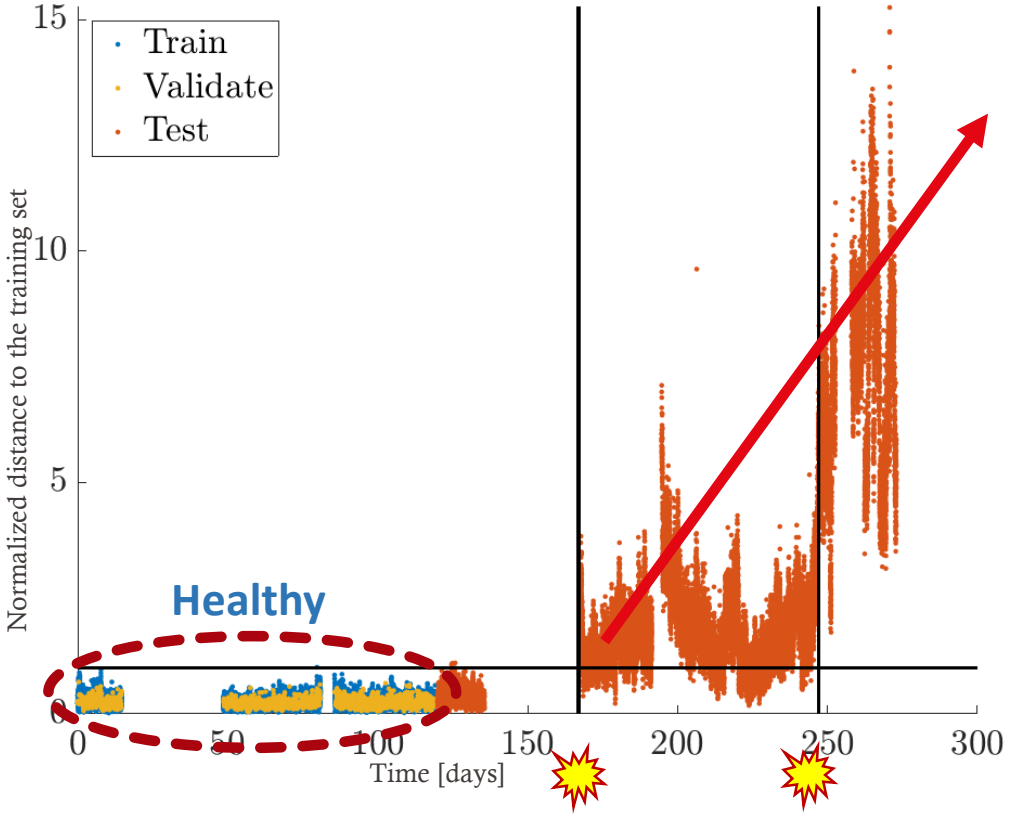
60 000 observations

1 fault

Can only use Healthy data for training!

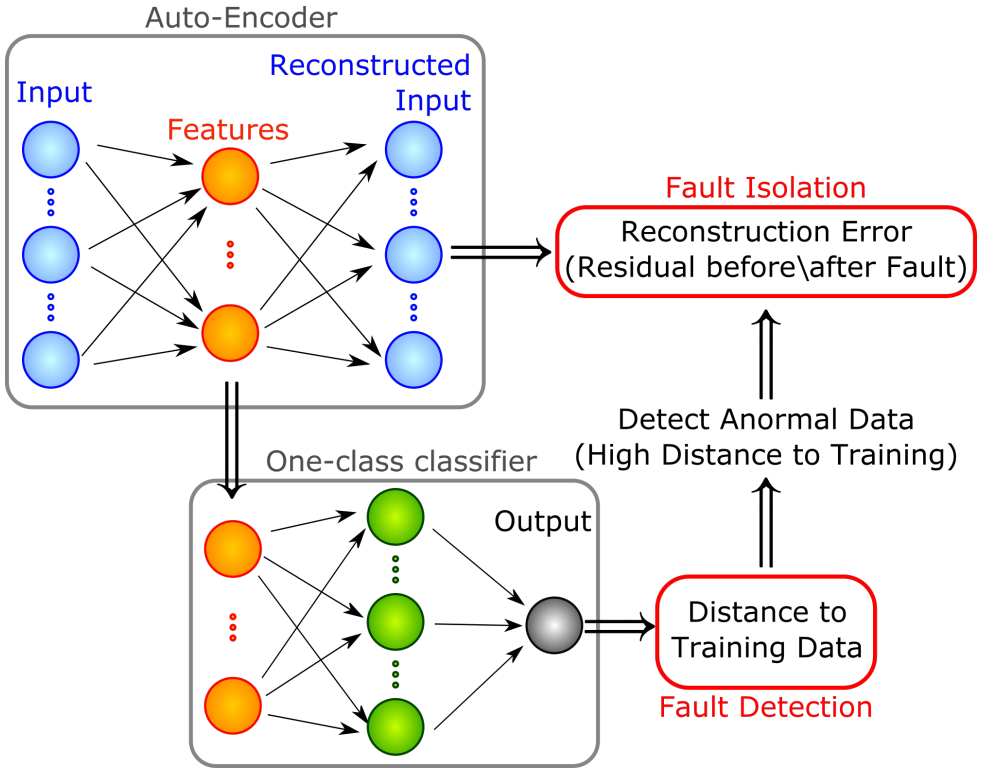
Michau, G., T. Palmé, and O. Fink (2017): Deep Feature Learning Network for Fault Detection and Isolation, Annual conference of the PHM society, October 2017

Generator Health Monitoring

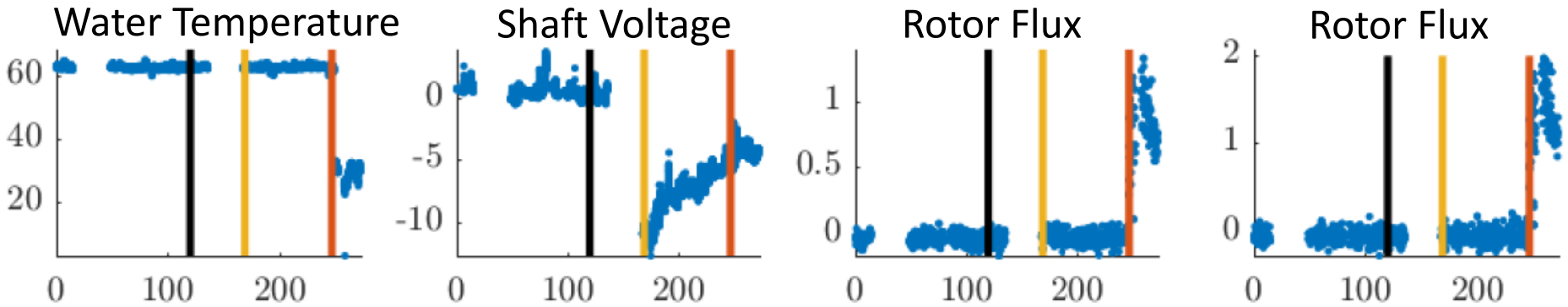


Abnormal behavior 100 days before!

Combined Architecture



Integrated fault diagnostics: Generator case study



Integrated!

At no additional cost!

Michau, G., T. Palmé, and O. Fink (2017): Deep Feature Learning Network for Fault Detection and Isolation, Annual conference of the PHM society, October 2017