WWTP diagnosis based on robust principal component analysis

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Outline

1. Principle of the Principal component analysis
2. Robust PCA
3. Fault detection and isolation
4. Application to hydraulic part of a wastewater treatment plant
Data matrix $X \in \mathbb{R}^{N \times n}$ in a normal process operation
Principle of the Principal component analysis

- Data matrix $X \in \mathbb{R}^{N \times n}$ in a normal process operation

**PCA**

Maximization of the variance projections $T = XP$

- $T \in \mathbb{R}^{N \times n}$: principal component matrix
- $P \in \mathbb{R}^{n \times n}$: projection matrix
Principal of the Principal component analysis

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### Decomposition in eigenvalues/eigenvectors of the covariance matrix

\[
\Sigma = \frac{1}{N-1} X^T X = P \Lambda P^T \quad \text{with} \quad PP^T = P^T P = I_n
\]

\[
\Sigma = \begin{bmatrix}
P_{\ell} & P_{n-\ell}
\end{bmatrix}
\begin{bmatrix}
\Lambda_{\ell} & 0 \\
0 & \Lambda_{n-\ell}
\end{bmatrix}
\begin{bmatrix}
P_{\ell}^T \\
P_{n-\ell}^T
\end{bmatrix}
\]
Principle of the Principal component analysis

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\Sigma = \begin{bmatrix} P_l & P_{n-l} \end{bmatrix} \begin{bmatrix} \Lambda_l & 0 \\ 0 & \Lambda_{n-l} \end{bmatrix} \begin{bmatrix} P_l^T \\ P_{n-l}^T \end{bmatrix}
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Principle of the Principal component analysis

Decomposition
Principle of the Principal component analysis

Decomposition

Principal part

\[ \hat{X} = X \, C_\ell \]
with

\[ C_\ell = P_\ell \, P_\ell^T \]
Principle of the Principal component analysis

Decomposition

Principal part
\[ \hat{X} = X C_\ell \]
with \( C_\ell = P_\ell P_\ell^T \)

Residual part
\[ E = X - \hat{X} \]
\[ = X (I_n - C_\ell) \]
\[ = X P_{n-\ell} P_{n-\ell}^T \]
Principle of the Principal component analysis

Decomposition

Principal part
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Determination of the number of principal components \( \ell \)
PCA weakness

Sensitive to outliers

Outliers: Data different from the normal operating conditions (faulty data, data obtained during shutdown or startup periods or data issued from different operating mode)

Robust PCA with respect to outliers

→ Outliers detection and isolation
Outliers

- $n = 2$ variables ($x_1, x_2$)
- $X = [x_1 \ x_2]$
- $\ell = 1$
Outliers

- $n = 2$ variables ($x_1, x_2$)
- $X = \begin{bmatrix} x_1 & x_2 \end{bmatrix}$
- $\ell = 1$
- Outliers 1: green observation
- Outliers 2: red observation
Robust PCA

Residual $r(k)$

$$r(k) = \|P_{n-\ell}^T (x(k) - \mu)\|^2$$

with $x(k)$ an observation

$\mu$ the mean of the data $X$

$P_{n-\ell}$ is the eigenvector matrix of the robust covariance matrix corresponding to its $n-\ell$ smallest eigenvalues

PCA minimise the following criterion:

$$\frac{1}{N} \sum_{k=1}^{N} (r(k))$$

with the constraint $P_{n-\ell}^T P_{n-\ell} = I_{n-\ell}$. 
Robust PCA

Residual $r(k)$

$$r(k) = ||P_{n-\ell}^T (x(k) - \mu)||^2$$

with $x(k)$ an observation

$\mu$ the mean of the data $X$

$P_{n-\ell}$ is the eigenvector matrix of the robust covariance matrix corresponding to its $n-\ell$ smallest eigenvalues

The general scale-M estimator minimizes the following objective function with the constraint $P_{n-\ell}^T P_{n-\ell} = I_{n-\ell}$:

$$\frac{1}{N} \sum_{k=1}^{N} \rho \left( \frac{r(k)}{\hat{\sigma}} \right)$$

with the function $\rho$ as the objective function, $\hat{\sigma}$ the robust scale of the residual $r(k)$ calculated by minimising the following criterion:

$$\frac{1}{N} \sum_{k=1}^{N} \rho \left( \frac{r(k)}{\hat{\sigma}} \right) = \delta$$
Initialization with a robust covariance matrix

Robust covariance matrix

\[ V = \frac{\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} w(i,j)(x(i) - x(j))(x(i) - x(j))^T}{\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} w(i,j)} \]

where the weights \( w(i,j) \) themselves are defined by:

\[ w(i,j) = \exp \left( -\frac{\beta}{2} (x(i) - x(j))^T \Sigma^{-1} (x(i) - x(j)) \right) \]

with \( \beta \) turning parameter

For \( \beta = 0 \), \( V = 2 \Sigma \)
Robust PCA

Only robust to outliers with a projection onto the residual space

scale M-estimator

The scale M-estimator maximizes the following criterion with the constraint $P_\ell^T P_\ell = I_\ell$:

$$\frac{1}{N} \sum_{k=1}^{N} \rho \left( \frac{\|P_\ell^T (x(k) - \mu)\|^2}{\hat{\sigma}} \right)$$

with $\hat{\sigma}$ the robust scale of the residual $r$ and $\rho$ the objective function.
### The reconstruction $\hat{x}_R$

Minimizing the influence of fault

$$\hat{x}_R(k) = x(k) - \Xi_R f_R$$

with $x(k)$: an observation
- $f_R$: the fault magnitude (unknown)
- $\Xi_R$: matrix of reconstruction directions
Fault detection and isolation

The reconstruction $\hat{x}_R$

Minimizing the influence of fault

$$\hat{x}_R(k) = x(k) - \Xi_R f_R$$

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- $f_R$: the fault magnitude (unknown)
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For example, to reconstruct 2 variables ($R = 2, 4$) among 5 variables

$$\Xi_R = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}^T$$
Fault detection and isolation

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Estimation of the fault magnitude $\hat{f}_R$:

$$\hat{f}_R = \arg \min_{f_R} \{ D_R(k) \}$$

with $D_R(k) = \hat{x}_R(k)^T P \Lambda^{-1} P^T \hat{x}_R(k)$
The reconstruction vector $\hat{x}_R(k)$ of the vector $x(k)$ is given by:

$$\hat{x}_R(k) = (I - \Xi_R(\Xi_R^T P \Lambda^{-1} P^T \Xi_R)^{-1} \Xi_R^T P \Lambda^{-1} P^T) x(k)$$
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Condition of reconstruction:

Existence of $(\Xi_R^T \Lambda^{-1} P^T \Xi_R)^{-1} \Rightarrow$ matrix $\Xi_R^T \Lambda^{-1} P^T \Xi_R$ of full rank
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To reconstruct a fault, it must be at least projected onto the principal space ($r \leq \ell$) or onto the principal space ($r \leq n - \ell$). This implies that the number of reconstructed variables $r$ must respect the following inequality:

$$r \leq \max(n - \ell, \ell)$$

with $r$ : Number of reconstructed variables  
$\ell$ : Number of principal components  
$n$ : Number of variables
Fault detection and isolation

The reconstruction vector $\hat{x}_R(k)$ of the vector $x(k)$ is given by:

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$$r \leq \max(n - \ell, \ell)$$

with $r$ : Number of reconstructed variables
$\ell$ : Number of principal components
$n$ : Number of variables

The number of maximum reconstruction:

$$\max(n - \ell, \ell) - 1 \sum_{r=1}^{\max(n - \ell, \ell)} \binom{n}{r}$$

with $\binom{n}{r}$ denotes the combination of $r$ from $n$. 
Fault detection indicator $D_R$

$$D_R(k) = \hat{x}_R(k)^T P \Lambda^{-1} P^T \hat{x}_R(k)$$
### Fault detection indicator $D_R$

$$D_R(k) = \hat{x}_R(k)^T P \Lambda^{-1} P^T \hat{x}_R(k)$$

### Fault detection

A fault is detected, if:

$$D_R(k) > \gamma^2_\alpha$$

with $\gamma^2_\alpha$ the detection threshold of indicator $D_R$,
Fault detection and isolation

Fault detection indicator $D_R$

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Fault detection

A fault is detected, if:

$$D_R(k) > \gamma_2^2$$

with $\gamma_2^2$ the detection threshold of indicator $D_R$.

Fault isolation

For the faulty observations, the faulty variables $\hat{R}$ are determined as follows:

$$\hat{R} = \arg \min_{R \in \mathcal{S}} D_R(k) < \gamma_2^2$$

with $\gamma_2^2$ the detection threshold of indicator $D_R$ and $\mathcal{S}$ all combinations of possible reconstruction directions.
Fault detection and isolation

Reduction of the number of reconstruction

Determination of the colinear direction projection

A global indicator $K$ is built:

$$K(R_1, R_2) = \max\{d(R_1, R_2), \tilde{d}(R_1, R_2)\}$$

with $R_1$ and $R_2$ correspond to sets of variable reconstruction and $d(R_1, R_2)$ distance between two sub-spaces onto principal space and $\tilde{d}(R_1, R_2)$ distance between two sub-spaces onto residual space

$$d(R_1, R_2) = ||\tilde{\Xi}_R_1 (\tilde{\Xi}_R_1^T \tilde{\Xi}_R_1)^{-1} \tilde{\Xi}_R_1^T - \tilde{\Xi}_R_2 (\tilde{\Xi}_R_2^T \tilde{\Xi}_R_2)^{-1} \tilde{\Xi}_R_2^T||_2$$

$$\tilde{d}(R_1, R_2) = ||\tilde{\Xi}_R_1 (\tilde{\Xi}_R_1^T \tilde{\Xi}_R_1)^{-1} \tilde{\Xi}_R_1^T - \tilde{\Xi}_R_2 (\tilde{\Xi}_R_2^T \tilde{\Xi}_R_2)^{-1} \tilde{\Xi}_R_2^T||_2$$

with $\tilde{\Xi}_R_1 = \Lambda_n^{1/2} P_{n-\ell}^T \Xi_{R_1}, \tilde{\Xi}_{R_1} = \Lambda_{n-\ell}^{1/2} P_{n-\ell}^T \Xi_{R_1}$.

For example, to reconstruct 2 variables ($R_1 = 2, 4$) among 5 variables

$$\Xi_{R_1} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}^T$$
Fault detection and isolation
Algorithm for the determination of the detectable and isolable faults

- $r = 1$
- Calculate for all available directions ($R_1 \in \mathcal{I}$ and $R_2 \in \mathcal{I}$) the indicator $K(R_1, R_2)$.
  - If $K(R_1, R_2)$ is equal to zero:
    - Only a set of variables potentially faulty may be determined, i.e. the faulty variables are associated to the indices $R_1$ or $R_2$ or $R_1$ and $R_2$. Thus, it is only required to determine one direction, for example $R_1$.
  - If $K(R_1, R_2)$ is closed to zero:
    - Magnitude of the fault has to be important to ensure fault isolation.
  - Else the fault are isolable
- $r = r + 1$
- While $r < \max(\ell, n - \ell)$ do to the step 2
Construction of the data matrix

Dynamic process: Temporal lag
Non linear process: Transformed variables

\[
x(k) = \begin{bmatrix} H1(k) & H2(k) & H3(k) & Q5(k) & H6(k) \\
\tanh((Q5(k-1) - 550)/150) & H1(k-1) & H6(k-1) & C4(k) \end{bmatrix}^T
\]

The data matrix \( X \) is constituted of \( N \) observations of the vector \( x(k) \).
Construction of the model

4 principal components are determined
Application to hydraulic part of a wastewater treatment plant

Analysis of the reconstruction directions

The maximum number of reconstructions is then equal to 255 \( \max(n - \ell, \ell) - 1 = 4 \)

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
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<tbody>
<tr>
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<tr>
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<tr>
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<td>0.97</td>
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</tr>
</tbody>
</table>

Indicator \( K \) for \( r = 1 \)

The number of useful reconstruction can be reduced to 202
Fault detection

Figure: Fault detection with Mahalanobis distance
Fault isolation

<table>
<thead>
<tr>
<th>Fault index</th>
<th>Reconstruction direction under the detection threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>16, 17</td>
<td>$D_1$</td>
</tr>
<tr>
<td>3, 10, 11, 14, 15, 19, 20, 21</td>
<td>$D_3$</td>
</tr>
<tr>
<td>7, 12</td>
<td>$D_{1,6}$</td>
</tr>
<tr>
<td>6, 8, 13, 18, 22</td>
<td>$D_{3,9}$</td>
</tr>
<tr>
<td>1, 2, 5</td>
<td>$D_{1,3,4}$</td>
</tr>
<tr>
<td>4</td>
<td>$D_{3,7,9}$</td>
</tr>
<tr>
<td>9</td>
<td>$D_{1,2,3,7}$</td>
</tr>
</tbody>
</table>

Table: Summary of fault isolation

Faults 16 and 17 are under the threshold when the first variable ($H_1(k)$) is reconstructed. 
⇒ variable $H_1(k)$ is faulty
Conclusion

- Robust PCA with respect to outliers
  → directly applicable on data containing potential faults

- use of the principle of reconstruction and projection of the reconstructed data together
  → outliers detection and isolation

- Reduction of the computational load
  → determination of the detectable and isolable faults

- Application to hydraulic part of a wastewater treatment plant