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# Principal Component Pursuit for Pattern Identification in Environmental Health

*Joint Statistical Meetings*

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# Why care about mixtures?

- We are exposed to hundreds (thousands?) of chemicals at any single time point
- Traditionally, epi studies have focused on single-chemical analyses
    - This does not represent reality
- The combination of exposures likely induces different responses

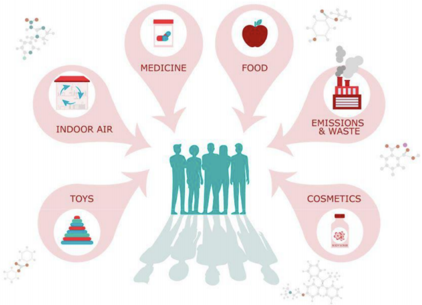
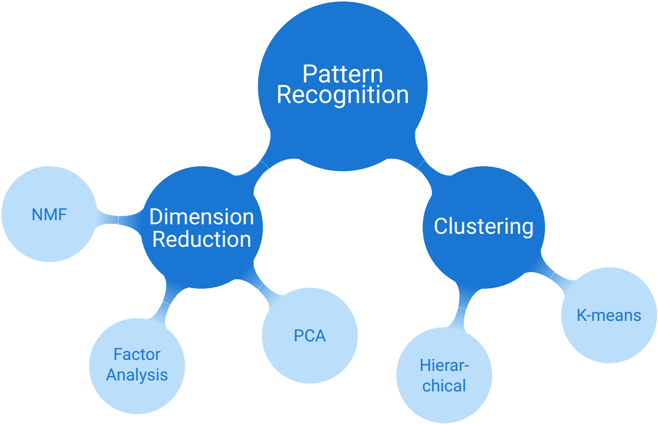



Image: ec.europa.eu via Yanelli Núñez

# Exposure pattern recognition

- Why should we care about identifying exposure patterns to chemicals in a population?
    - Sources
    - Behaviors
- If we link these patterns to (multiple) adverse health outcomes
    - Efficient regulations
    - Targeted interventions

# Some existing pattern recognition methods




*Not an exhaustive list of methods!!

# Problems with existing methods

- Choice of $k$ patterns/components/factors is subjective
- Local minima depend on initialization
- Outliers may affect solution
- Chemical concentrations may be <LOD

$\Longrightarrow$ Proposed solution: **Principal Component Pursuit**

# Principal Component Pursuit

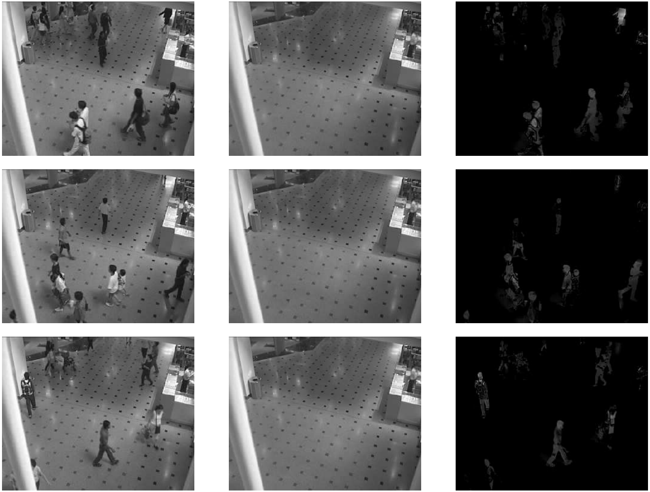
- Robust Principal Component Analysis (PCA)
- Unsupervised dimensionality reduction method adapted from computer vision
- Decomposes design matrix into low rank and sparse
  - Low rank matrix estimates consistent exposure patterns
  - Sparse matrix identifies unique events

$$\min_{L,S} \|L\|_\star + \lambda\|S\|_1 + \frac{\mu}{2}\|L + S - X\|_F^2$$

- Robust to noisy/corrupt data
- Global minimum

# PCP image example

Original | $\widehat{L_0}$ | $\widehat{S_0}$



## PCP extensions

- Non-negativity constraint on low rank matrix
- Novel penalties for values < LOD
  - Observed value < LOD & predicted value > LOD

$$\min_{L,S} \|L\|_\star + \lambda \|S\|_1 + \frac{\mu}{2} \|L + S - LOD\|_F^2 \tag{1}$$

  - Observed value < LOD & predicted value < 0

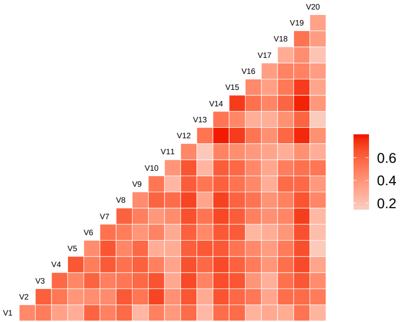
$$\min_{L,S} \|L\|_\star + \lambda \|S\|_1 + \frac{\mu}{2} \|L + S\|_F^2 \tag{2}$$

  - Observed value < LOD & predicted value [0 – LOD]

$$\min_{L,S} \|L\|_\star + \lambda \|S\|_1 \tag{3}$$

# Simulations

- Matrix size
  - 1,000 $\times$ 20
- Low rank structure
  - Uniform distributions
  - Matrix product
  - Rank: 4
- Added noise
  - Gaussian
  - 0.6 $\times$ low rank SD
- Values <LOD
  - 0%–90%




Simulated Correlation Matrix

# Simulations

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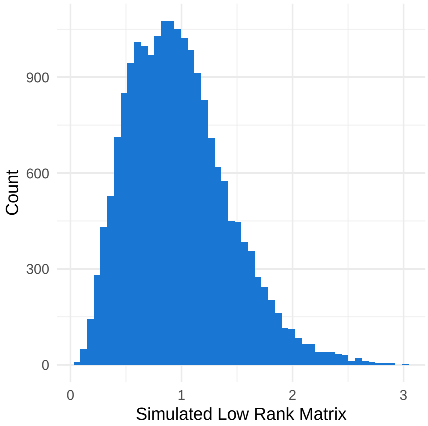
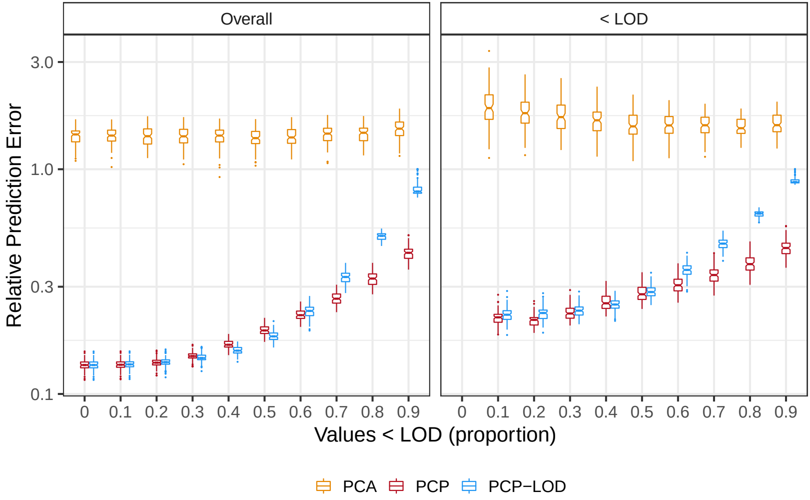
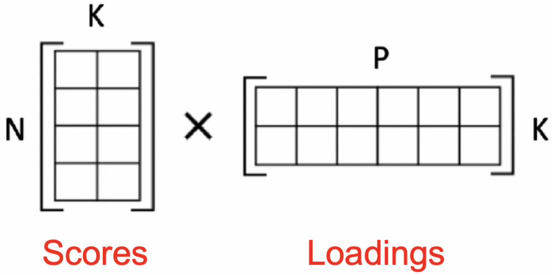


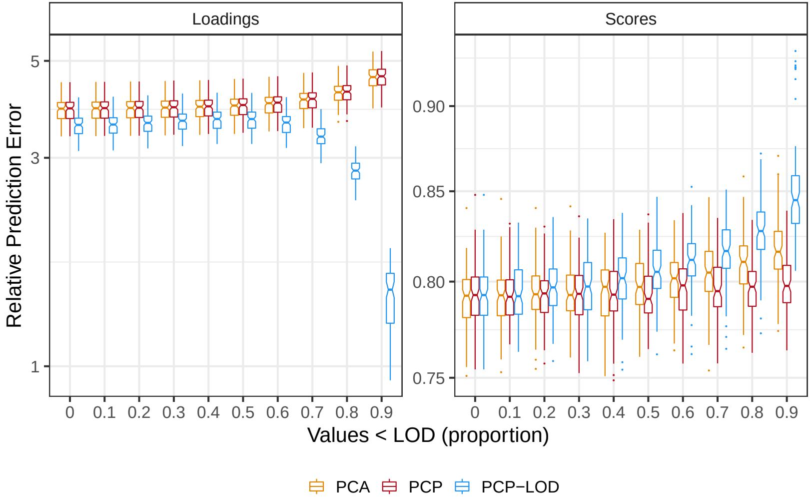
# Relative error overall & <LOD



# Relative error in loadings and scores



# Relative error in loadings and scores



## Results

- PCP-LOD outperforms PCA
- PCP-LOD outperforms PCP imputed with LOD/$\sqrt{2}$ under these conditions:
  - True underlying low-rank structure exists
  - Proportion < LOD is low

# Conclusion

Benefits of PCP:

- Researcher does not need to choose $k$
- Global minimum
- Improved predictive accuracy over PCA
- Information on extreme events not lost / does not influence patterns

Benefits of PCP-LOD:

- Do not need to impute values < LOD
- Outperforms PCP imputed with LOD/$\sqrt{2}$ when LOD is low

# Next steps

Immediate next steps:

- Add penalty for known values <LOD
- Determine optimal $\mu$ parameter value / range
- Apply to real environmental data

Where to take the method:

- What to do with S?
- Non-negative pattern identification in L
- User-friendly R package

# Acknowledgements

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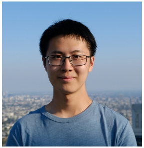
Biostatistics



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