KATHOLIEKE UNIVERSITEIT LEUVEN

Orthogonal grey simultaneous component analysis to distinguish common and distinctive information in coupled data

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Outline

- Introduction
  - Coupled data
  - Research questions
- Method
  - Simultaneous component method
  - Problem
  - Solution: DISCO-GSCA
- Illustration
  - Results
- Conclusion

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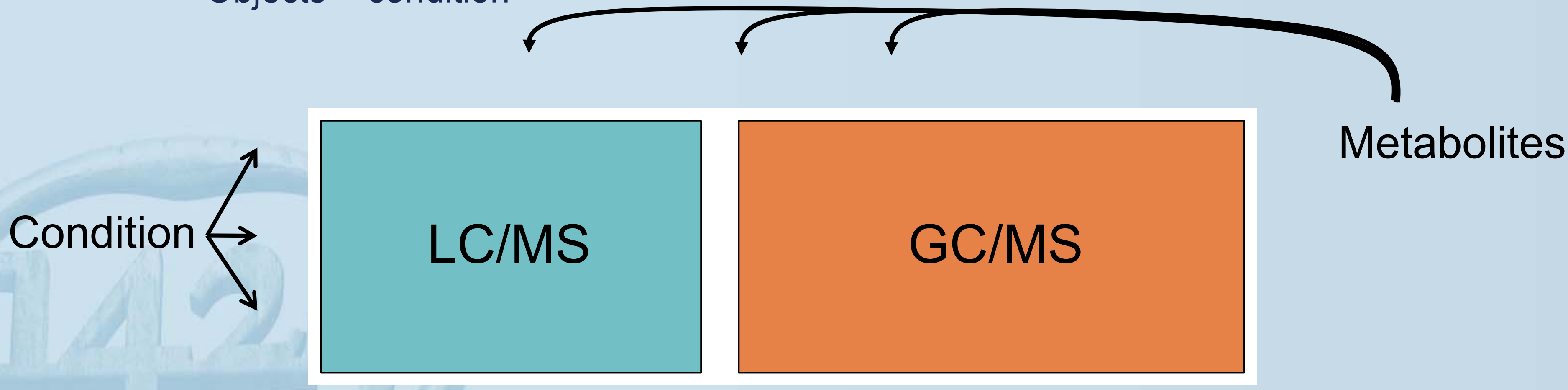
Introduction

- Coupled data: data that consist of different data blocks, which all contain information about the same entities
  - E.g.
    - Data blocks = GC/MS and LC/MS
    - Variables = *E. coli* metabolites
    - Objects = condition



Smilde et al. (2005)

Introduction

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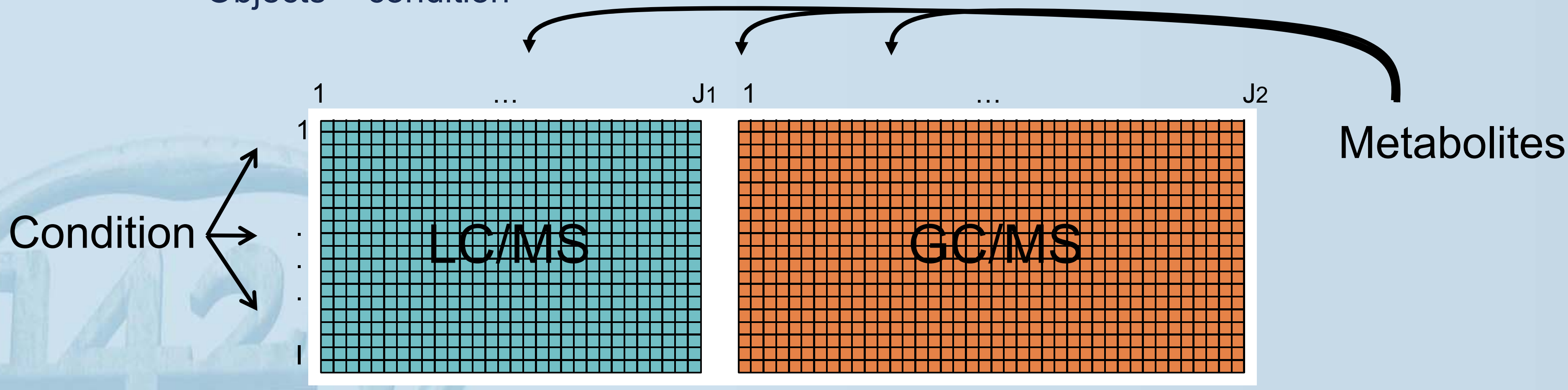

Smilde et al. (2005)

- Finding mechanisms that underly the coupled data
- **RESEARCH QUESTIONS**: which mechanisms are
  - common for both data blocks and
  - distinctive for a single data block?

Which metabolome processes are measured by both separation techniques? Which processes are measured by just one of the two?

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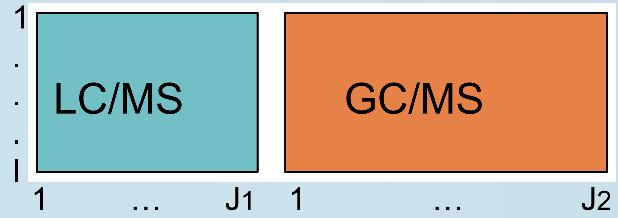
Simultaneous Component Analysis

- Finding underlying mechanisms in
  - ONE data block → Principal Component Analysis (PCA, Jolliffe, 2002)
  - More data blocks → Simultaneous Component Analysis (SCA, Van Deun et al., 2009)

Simultaneous Component Analysis



Simultaneous Component Analysis

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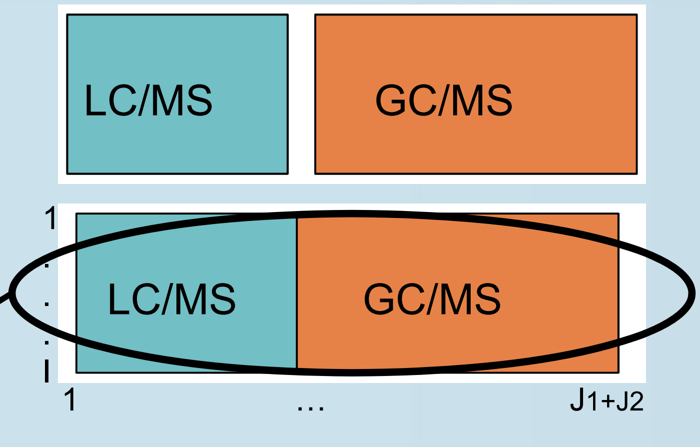
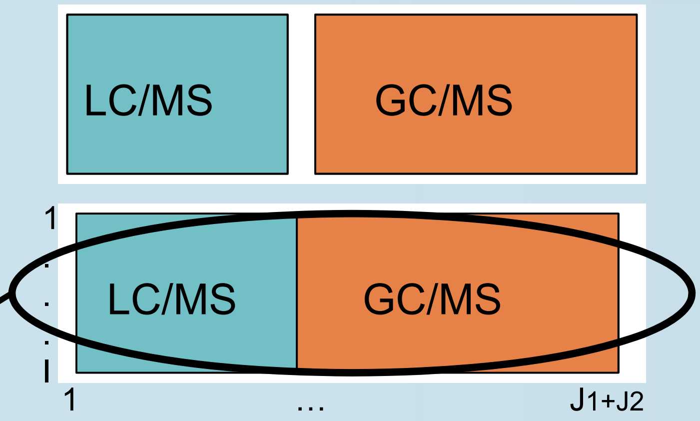


$\mathbf{X}_{conc}$

Simultaneous Component Analysis

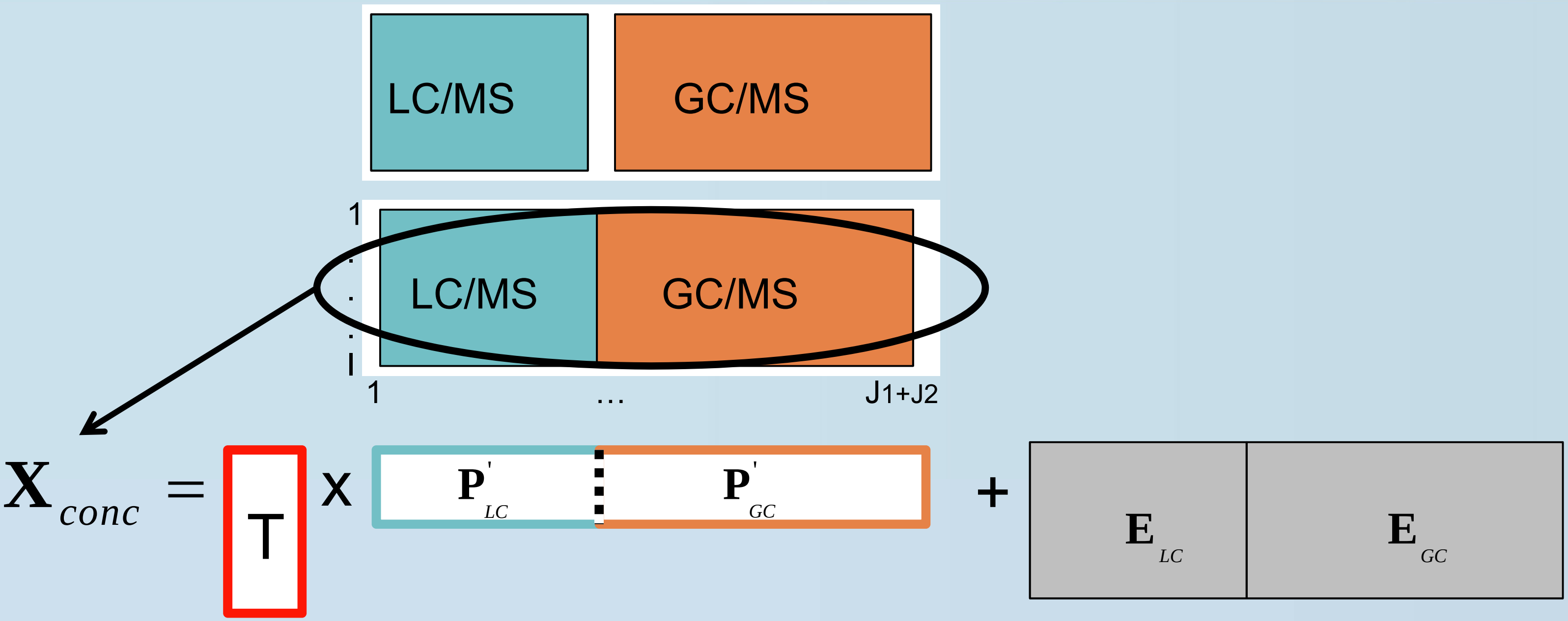


$$\mathbf{X}_{conc} = \mathbf{T} \times \left[\, \mathbf{P}'_{LC} \;\vdots\; \mathbf{P}'_{GC} \,\right] + \left[\, \mathbf{E}_{LC} \;|\; \mathbf{E}_{GC} \,\right]$$

Data = Scores x Loadings P'_{conc} + Error $\mathbf{E}_{conc}$

$I \times (J_1 + J_2)$ $\quad$ $I \times R$ $\quad$ $R \times (J_1 + J_2)$ $\quad$ $I \times (J_1 + J_2)$

Simultaneous Component Analysis



Data	= Scores	x	Loadings P'_{conc}	+	Error $\mathbf{E}_{conc}$
$I \times (J_1 + J_2)$	$I \times R$		$R \times (J_1 + J_2)$		$I \times (J_1 + J_2)$

Objective: $\min_{\mathbf{T},\mathbf{P}_{conc}} \left\| \mathbf{X}_{conc} - \mathbf{T}\mathbf{P}'_{conc} \right\|^2$

- **Distinctive mechanisms**= simultaneous components that underly only one data block
- **Common mechanisms**= simultaneous components that underly both data blocks

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- E.g.,

$$\hat{\mathbf{X}}_{conc} = \mathbf{T}\mathbf{P}'_{conc}$$

$$= \mathbf{T}\left[\mathbf{P}'_{LC} \mid \mathbf{P}'_{GC}\right]$$

$$= \begin{bmatrix} x \\ \vdots \\ x \end{bmatrix} \left[0 \quad \cdots \quad 0 \mid x \quad \cdots \quad x \right]$$

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$$= \mathbf{T}\left[\mathbf{P}'_{LC} \mid \mathbf{P}'_{GC}\right]$$

$$= \begin{bmatrix} x \\ \vdots \\ x \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 & | & x & \cdots & x \end{bmatrix}$$

Distinctive component for GC/MS

- **Distinctive mechanisms**= simultaneous components that underly only one data block
- **Common mechanisms**= simultaneous components that underly both data blocks
- E.g.,

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$$= \begin{bmatrix} x & \cdots & x & | & 0 & \cdots & 0 \\ 0 & \cdots & 0 & | & x & \cdots & x \\ x & \cdots & x & | & x & \cdots & x \end{bmatrix}$$

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Problem

- **Distinctive mechanisms**= simultaneous components that underly only one data block
- **Common mechanisms**= simultaneous components that underly both data blocks
- E.g.,

$$\mathbf{P}^{'}_{conc} = \begin{bmatrix} \mathbf{P}^{'}_{LC} & | & \mathbf{P}^{'}_{GC} \end{bmatrix}$$

$$= \begin{bmatrix} x & \cdots & x & | & 0 & \cdots & 0 \\ 0 & \cdots & 0 & | & x & \cdots & x \\ x & \cdots & x & | & x & \cdots & x \end{bmatrix} \begin{matrix} \text{D1} \\ \text{D2} \\ \text{C} \end{matrix}$$

☹ However… SC method: obtaining such a pattern is outside control…

Problem

- **Distinctive mechanisms**= simultaneous components that underly only one data block
- **Common mechanisms**= simultaneous components that underly both data blocks
- E.g.,

$$\mathbf{P}_{conc}^{target'} = \left[\mathbf{P}_{LC}^{target'} \quad | \quad \mathbf{P}_{GC}^{target'} \right]$$

$$= \begin{bmatrix} x & \cdots & x & | & 0 & \cdots & 0 \\ 0 & \cdots & 0 & | & x & \cdots & x \\ x & \cdots & x & | & x & \cdots & x \end{bmatrix} \begin{matrix} \text{D1} \\ \text{D2} \\ \text{C} \end{matrix}$$

☹ However… SC method: obtaining such a pattern is outside control…

Solution: DISCO-GSCA

- Predecessors:
  - DISCO-SCA (Schouteden et al., 2010)
  - Grey Component Analysis (GCA, Westerhuis et al., 2007)

Solution: DISCO-GSCA

- Impose target structure to a certain power λ

$$\min_{\mathbf{T},\mathbf{P}_{conc}} \left(\left\| \mathbf{X}_{conc} - \mathbf{T}\mathbf{P}_{conc}^{'} \right\|^{2} + \lambda \left\| \mathbf{W} \bullet \left(\mathbf{P}_{conc}^{target} - \mathbf{P}_{conc} \right) \right\|^{2} \right) \qquad \mathbf{T}^{'}\mathbf{T} = \mathbf{I}$$

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$$\left(\begin{bmatrix} x & 0 & x \\ \vdots & \vdots & \vdots \\ x & 0 & x \\ - & - & - \\ 0 & x & x \\ \vdots & \vdots & \vdots \\ 0 & x & x \end{bmatrix} - \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ \vdots & \vdots & \vdots \\ p_{I_1 1} & p_{I_1 2} & p_{I_1 3} \\ - & - & - \\ p_{(I_1+I_2)1} & p_{(I_1+I_2)2} & p_{(I_1+I_2)3} \\ \vdots & \vdots & \vdots \\ p_{(I_1+I_2)1} & p_{(I_1+I_2)2} & p_{(I_1+I_2)3} \end{bmatrix} \right)$$

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Elementwise product

$$\begin{bmatrix} 0 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 1 & 0 \\ - & - & - \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \end{bmatrix} \bullet \left(\begin{bmatrix} x & 0 & x \\ \vdots & \vdots & \vdots \\ x & 0 & x \\ - & - & - \\ 0 & x & x \\ \vdots & \vdots & \vdots \\ 0 & x & x \end{bmatrix} - \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ \vdots & \vdots & \vdots \\ p_{I_1 1} & p_{I_1 2} & p_{I_1 3} \\ - & - & - \\ p_{(I_1+I_2)1} & p_{(I_1+I_2)2} & p_{(I_1+I_2)3} \\ \vdots & \vdots & \vdots \\ p_{(I_1+I_2)1} & p_{(I_1+I_2)2} & p_{(I_1+I_2)3} \end{bmatrix} \right)$$

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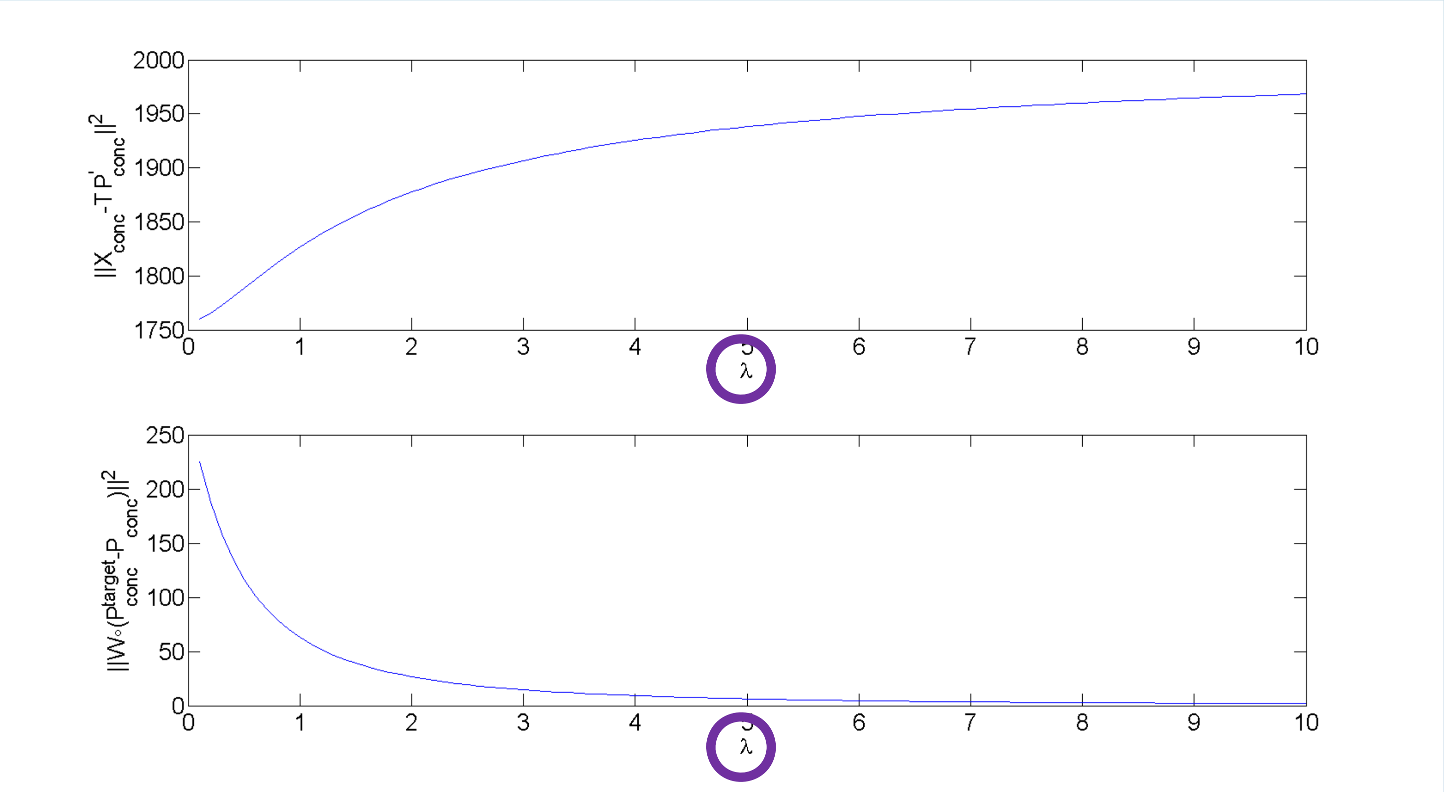
$$\min_{\mathbf{T},\mathbf{P}_{conc}} \left(\left\| \mathbf{X}_{conc} - \mathbf{T}\mathbf{P}'_{conc} \right\|^2 + \lambda \left\| \mathbf{W} \bullet \left(\mathbf{P}^{target}_{conc} - \mathbf{P}_{conc} \right) \right\|^2 \right) \qquad \mathbf{T}'\mathbf{T} = \mathbf{I}$$



Solution: DISCO-GSCA

- Model selection: 3 steps
  - FIRST: Select the number of simultaneous components
    - (SCA, Van Deun et al., 2009)
  - SECOND: characterize these components
    - i.e., how many of them are common/distinctive?
    - (DISCO-SCA, Schouteden et al., 2010)
  - THIRD: define λ
    - L-curve (Hansen, 1992)

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- Data: *E. coli*
- Model:
  - 5 simultaneous components
  - Target:
    - 1 common component
    - 2 distinctive components for GC/MS
    - 2 distinctive components for LC/MS

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GC1 GC2 LC1 LC2 C

$$\begin{bmatrix} \mathbf{P}_{GC}^{Target} \\ - \quad - \quad - \\ \mathbf{P}_{LC}^{Target} \end{bmatrix} = \begin{bmatrix} x & x & 0 & 0 & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & x & 0 & 0 & x \\ - & - & - & - & - \\ 0 & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x & x & x \end{bmatrix}$$

- Data: *E. coli*
- Model:
  - 5 simultaneous components
  - Target:
    - 1 common component
    - 2 distinctive components for GC/MS
    - 2 distinctive components for LC/MS
  - λ=1

$$\begin{bmatrix} \mathbf{P}_{GC}^{Target} \\ - \quad - \quad - \\ \mathbf{P}_{LC}^{Target} \end{bmatrix} = \begin{array}{c} \text{GC1} \quad \text{GC2} \quad \text{LC1} \quad \text{LC2} \quad \text{C} \\ \begin{bmatrix} x & x & 0 & 0 & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & x & 0 & 0 & x \\ - & - & - & - & - \\ 0 & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x & x & x \end{bmatrix} \end{array}$$

Results

% Variance accounted for by DISCO-GSCA (λ=1)

	GC1	GC2	LC1	LC2	C	Total
GC/MS	0.17	0.14	**0.04**	**0.03**	0.12	0.50
LC/MS	**0.03**	**0.03**	0.14	0.31	0.11	0.62
Xconc	0.12	0.10	0.08	0.13	0.12	0.54

Results

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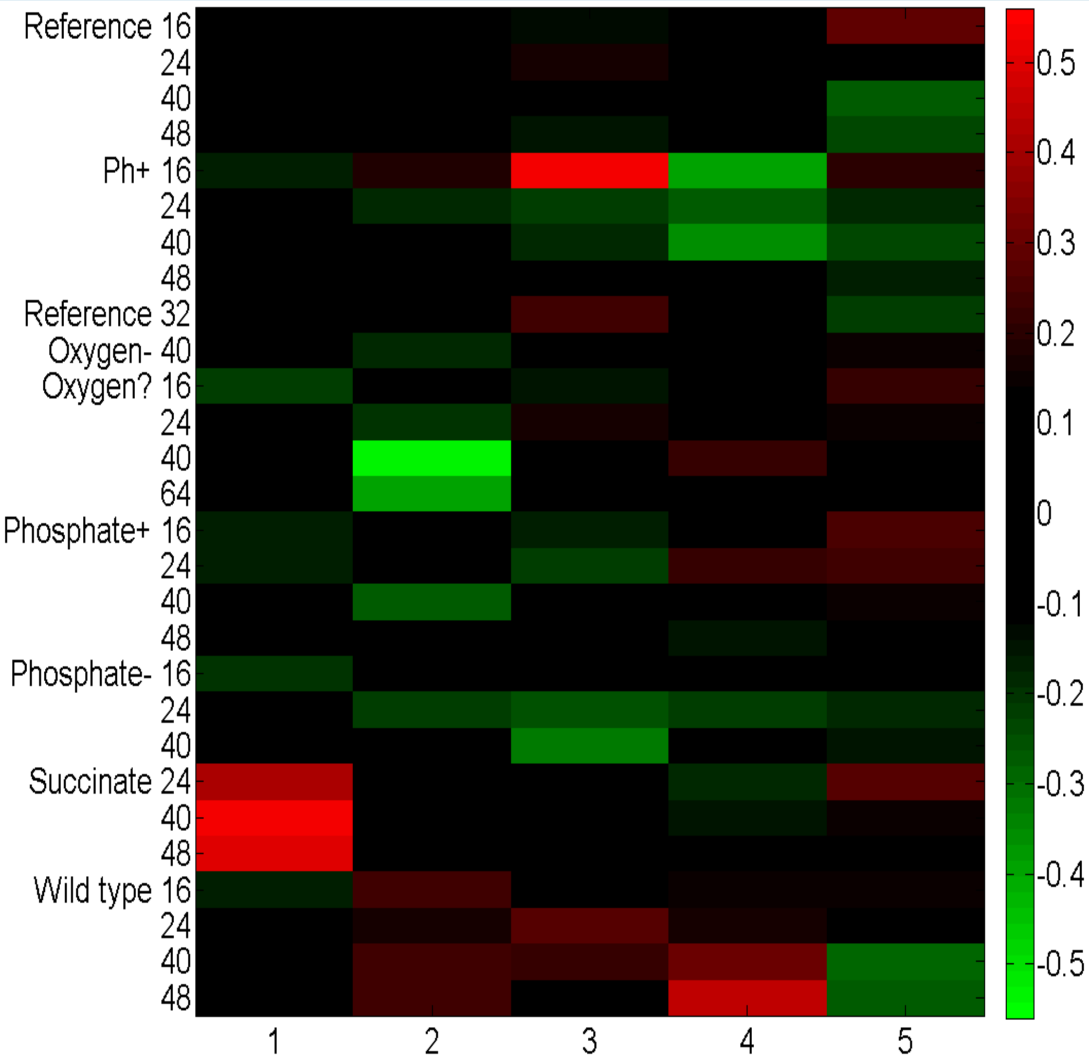
Xconc	0.12	0.10	0.08	0.13	0.12	0.54

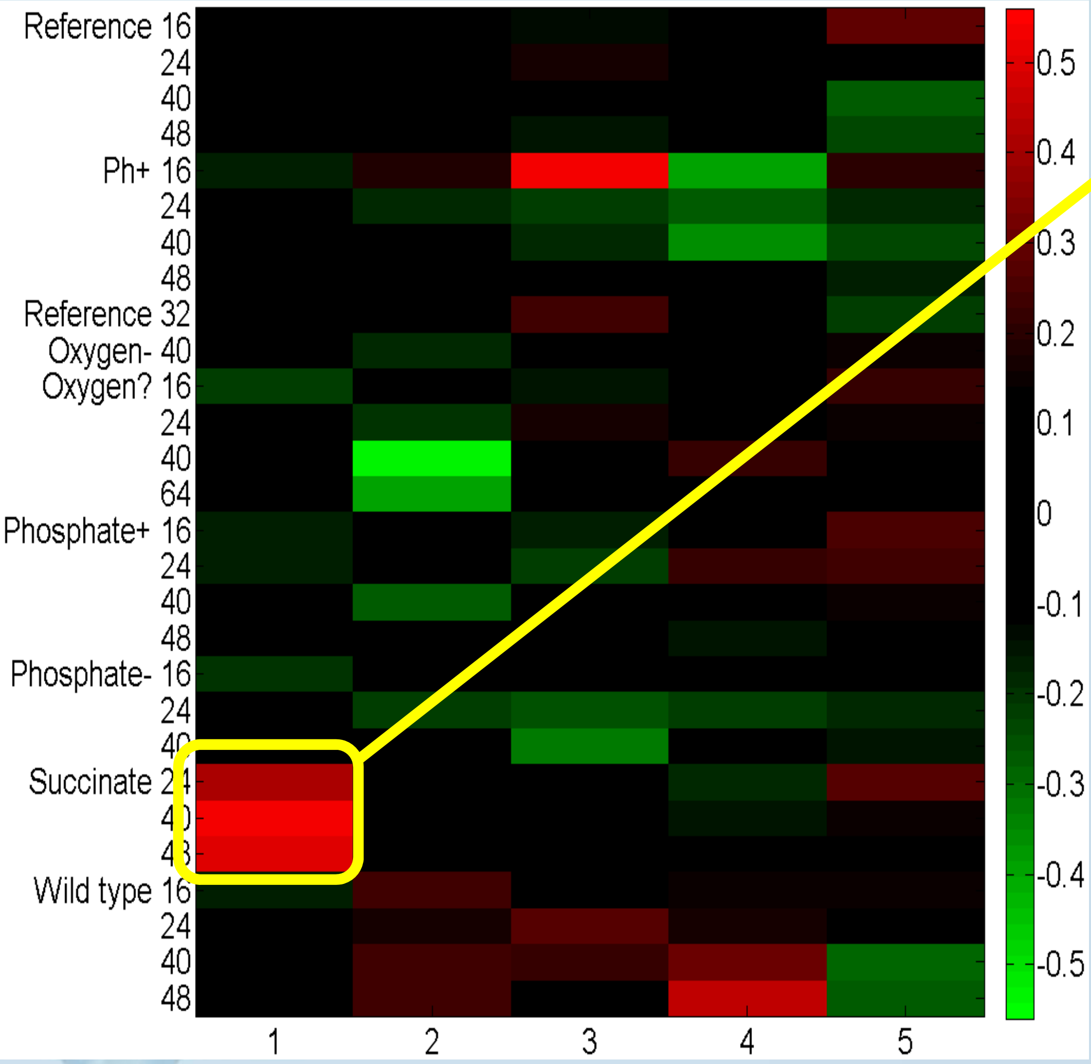
% Variance accounted for by SCA

	GC1	GC2	LC1	LC2	C	Total
GC/MS	0.14	0.13	**0.06**	**0.11**	0.11	0.54
LC/MS	**0.10**	**0.04**	0.12	0.24	0.12	0.62
Xconc	0.12	0.10	0.08	0.15	0.11	0.57

DISCO-GSCA (λ=1)



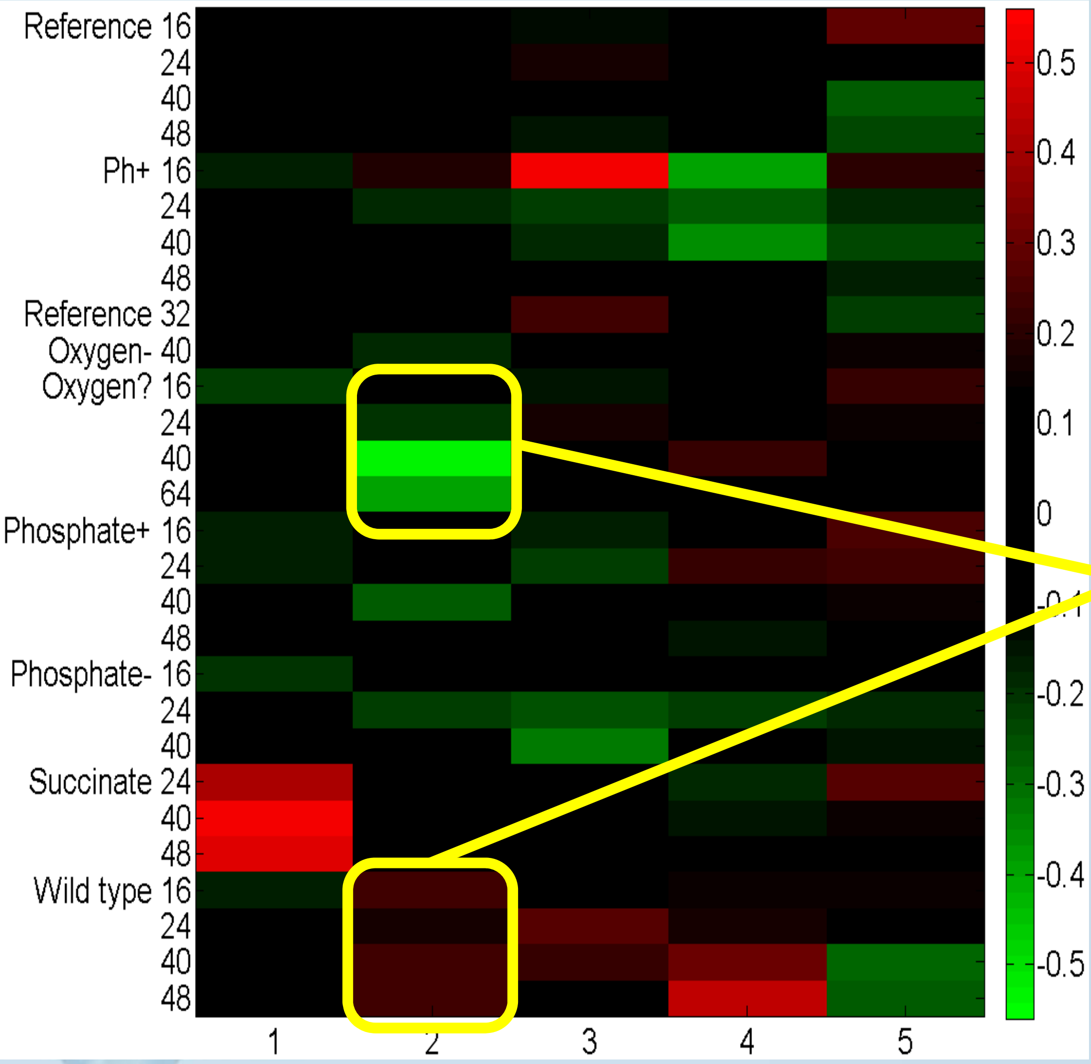
DISCO-GSCA (λ=1)



GC/MS:

1) Processes that are active when the carbon source is succinate instead of glucose

DISCO-GSCA (λ=1)

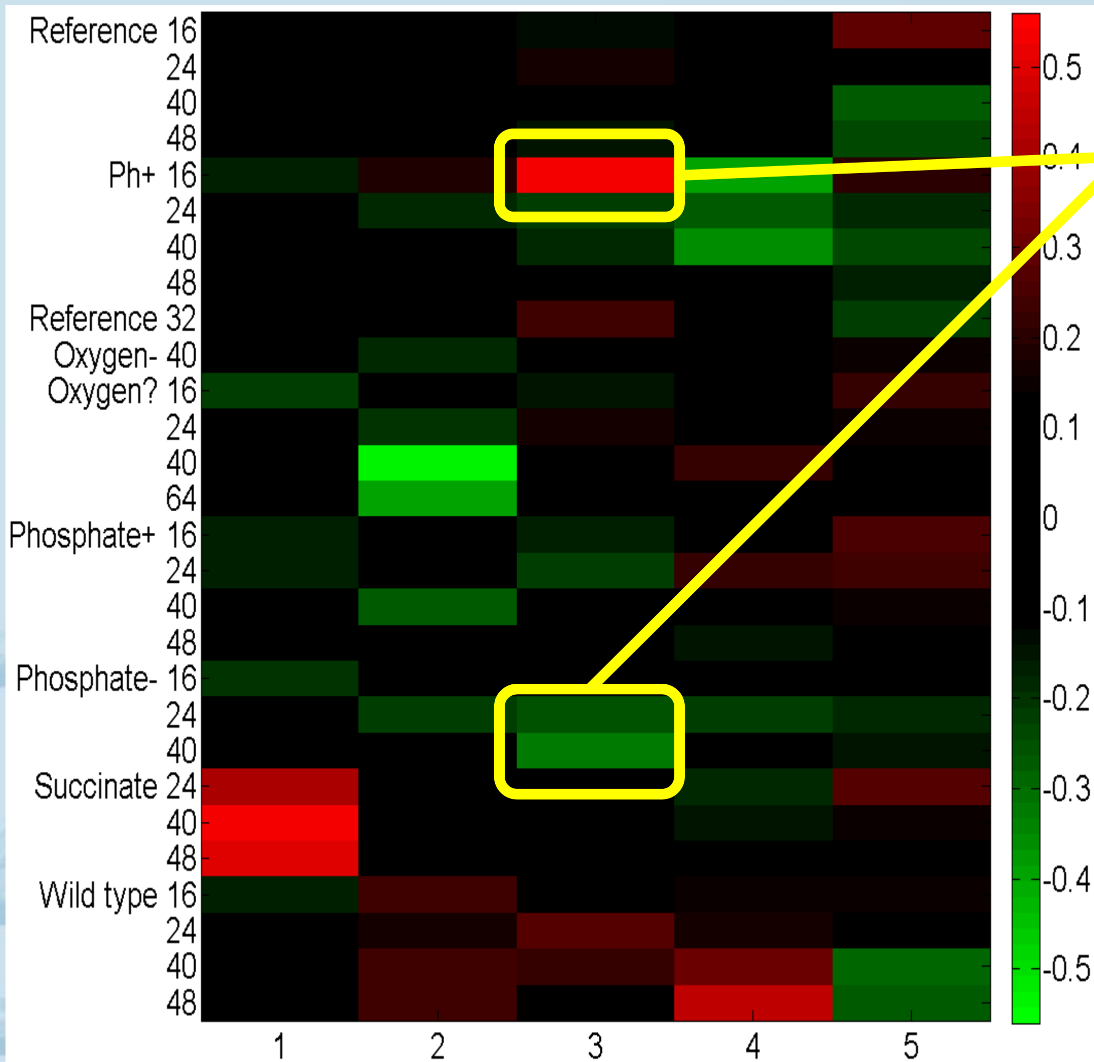


GC/MS:

1) Processes that are active when the carbon source is succinate instead of glucose

2) Processes that are active in the *E. coli* wildtype and when the oxygen tension was not maintained

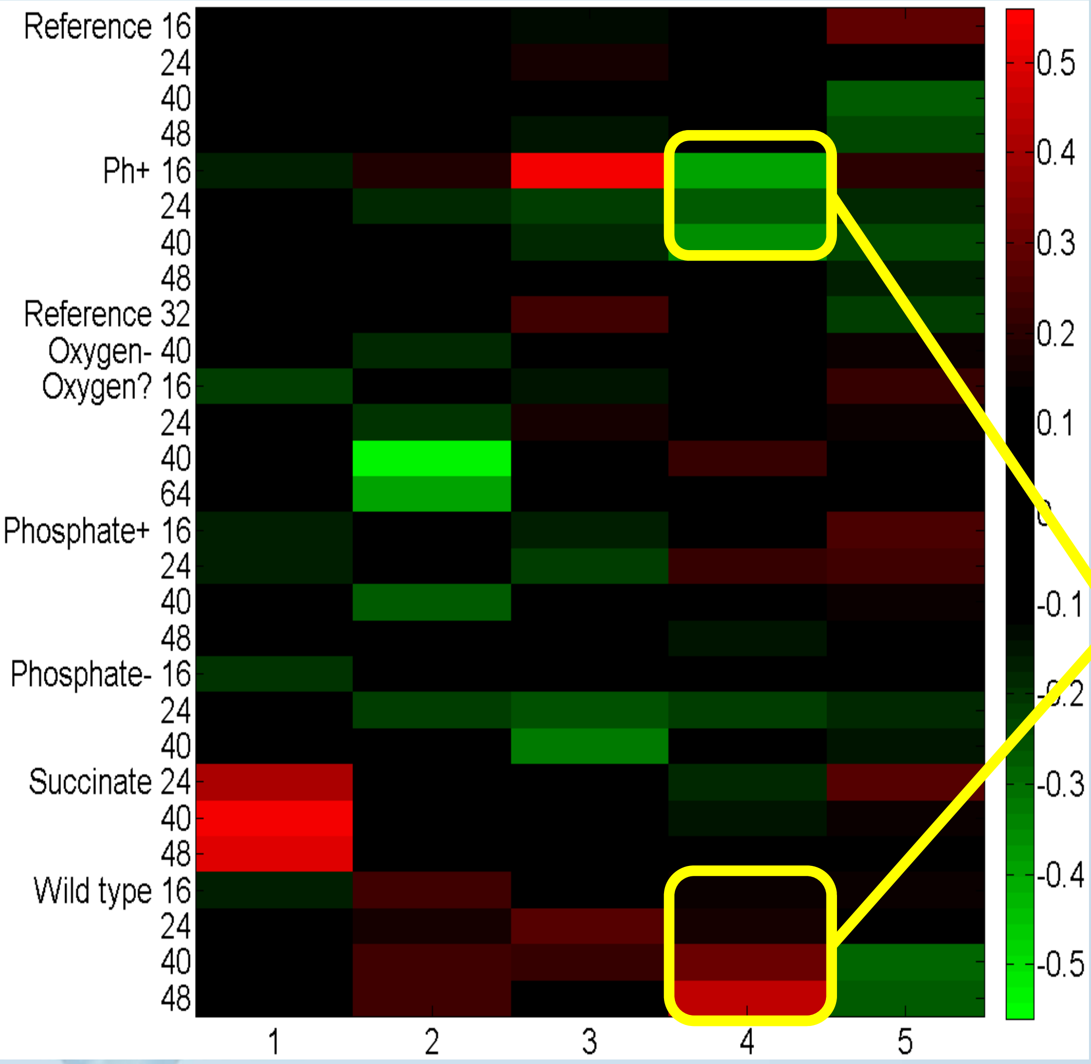
DISCO-GSCA (λ=1)



LC/MS:

1) Processes that are active in pH^+ environments and in low phosphate concentrations

DISCO-GSCA (λ=1)

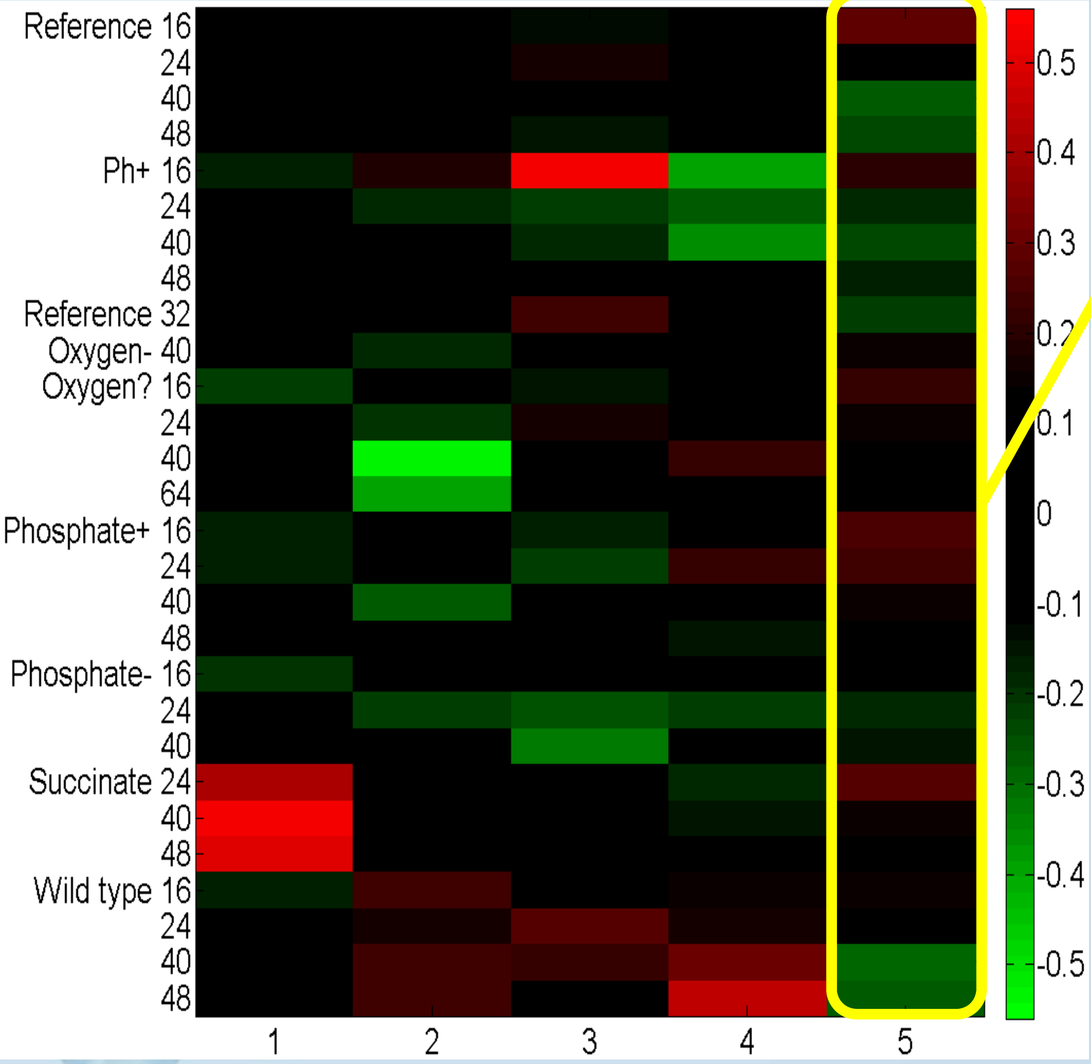


LC/MS:

1) Processes that are active in pH^+ environments and in low phosphate concentrations

2) Processes that are active in the *E. coli* wildtype and in a pH+ environment

DISCO-GSCA (λ=1)



Common: General time-related processes

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Conclusion

- DISCO-GSCA
  - Method to find common & distinctive mechanisms in coupled data
  - Imposes a target matrix to a simultaneous component solution
  - to a user-defined degree (λ)
    - Makes it possible to find an optimal trade-off between obtaining the target structure and a loss of fit

References

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- Van Deun, K., Smilde, A. K., van der Werf, M. J., Kiers, H. A. L., & Van Mechelen, I. (2009). A structured overview of simultaneous component based data integration. *BMC Bioinformatics, 10* (1), 246-261.
- Westerhuis, J. A., Derks, P. P. A., Hoefsloot, H. C. J. and Smilde, A. K. (2007). Grey component analysis. *Journal of chemometrics, 21*, 474-485.

! Thanks For Your Attention !

? Are There Any Questions / Suggestions ?

Extra

- Predecessors of DISCO-GSCA
  - DISCO-SCA (Schouteden et al., 2010)
  - Grey Component Analysis (GCA, Westerhuis et al., 2007)
- Model Selection
  - Step 1: selection of the number of components
  - Step 2: selection of target matrix
  - Step 3: selection of λ

Extra

- **Predecessors of DISCO-GSCA**
  - **DISCO-SCA (Schouteden et al., 2010)**
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DISCO-SCA

- **DISCO-SCA**: rotates the simultaneous components towards target structure

DISCO-SCA

- **DISCO-SCA**: rotates the simultaneous components towards target structure
- Loss function:

$$\min_{\mathbf{B}} \left\| \mathbf{W} \bullet \left(\mathbf{P}_{conc}^{target} - \mathbf{P}_{conc}\mathbf{B} \right) \right\|^2 \qquad \mathbf{BB'} = \mathbf{I}$$

$$\mathbf{T}^{rotated} = \mathbf{TB}$$

$$\mathbf{P}_{conc}^{rotated} = \mathbf{P}_{conc}\mathbf{B}$$

DISCO-SCA

- **DISCO-SCA**: rotates the simultaneous components towards target structure
- Loss function:

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$$\mathbf{T}^{rotated} = \mathbf{TB}$$

$$\mathbf{P}_{conc}^{rotated} = \mathbf{P}_{conc}\mathbf{B}$$

- ☺ Consequences (as compared to SCA):
  - Fit remains

$$\left\| \mathbf{X}_{conc} - \mathbf{T}^{rotated} \mathbf{P}_{conc}^{rotated\,'} \right\|^2 = \left\| \mathbf{X}_{conc} - \mathbf{TBB'P}_{conc}^{'} \right\|^2 = \left\| \mathbf{X}_{conc} - \mathbf{TP}_{conc}^{'} \right\|^2$$

  - Target structure is better obtained

- ☹ consequences
  - Rotation sometimes not powerful enough: the difference between rotated component loadings and a target matrix remains somewhat too large.

- Solution DISCO-GSCA

GCA

- **GCA:** Impose target structure to component solution

$$\min_{\mathbf{T},\mathbf{P}}\left(\left\|\mathbf{X}-\mathbf{TP}'\right\|^2+\lambda\left\|\mathbf{W}\bullet\left(\mathbf{P}^{target}-\mathbf{P}\right)\right\|^2\right)$$

- Needed:
  - Extension towards coupled data
  - Common and distinctive target structure
  - Restriction orthogonal components <-> correlation between components that should not share any information.
- Solution: DISCO-GSCA

Extra

- Predecessors of DISCO-GSCA
  - DISCO-SCA (Schouteden et al., 2010)
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- Predecessors of DISCO-GSCA
  - DISCO-SCA (Schouteden et al., 2010)
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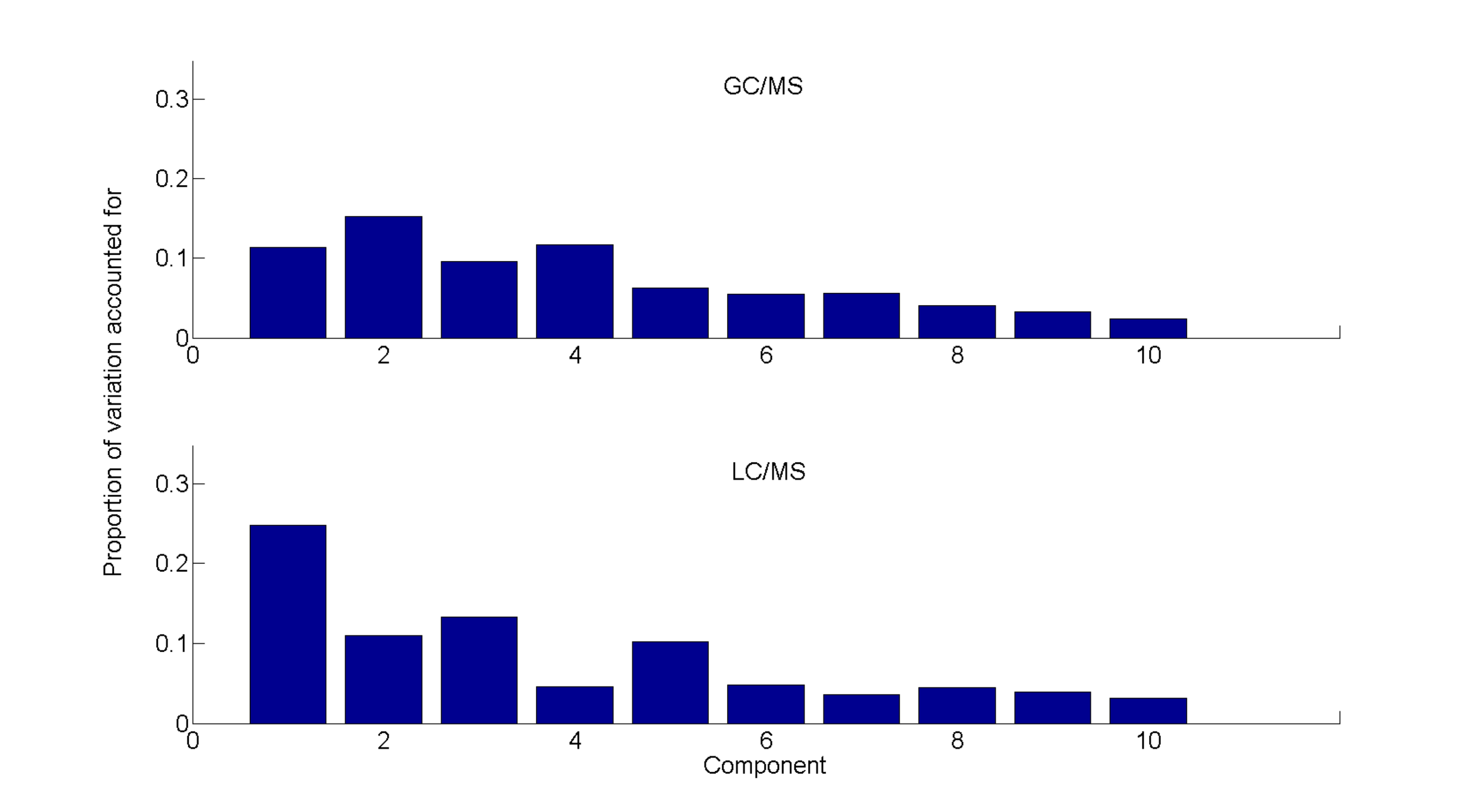
- **Model Selection**
  - **Step 1: selection of the number of components**
  - **Step 2: selection of target matrix**
  - **Step 3: selection of λ**

Model Selection

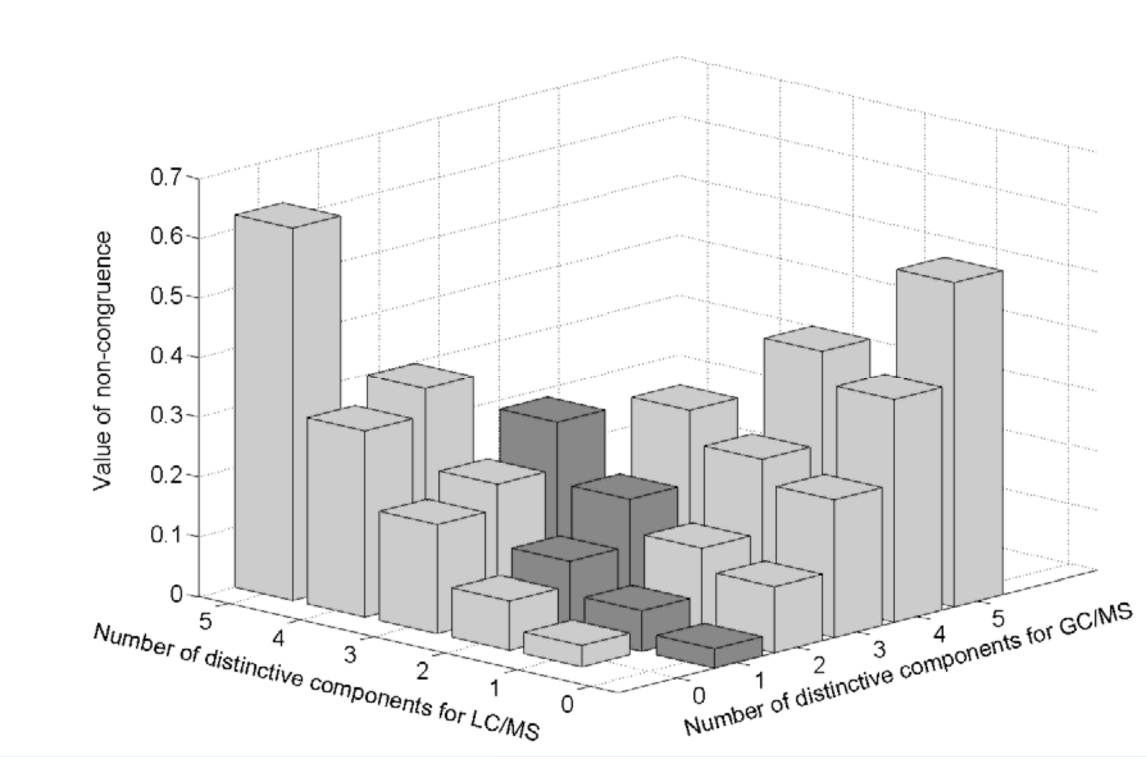
- Data = *E. coli* data set

- Model selection: 3 steps
  - FIRST: select the number of simultaneous components
    - (SCA, Van Deun et al., 2009)
  - SECOND: characterize these components (i.e., select target)
    - (DISCO-SCA, Schouteden et al., 2010)
  - THIRD: define λ
    - (Hansen, 1992)

- STEP 1: define the number of simultaneous components
  - Simultaneous component scree-plot (Van Deun et al., 2009)



- STEP 2: characterization of the components (Schouteden et al., 2010)
  - (Non-)congruence criterion FOR EACH POSSIBLE TARGET-MATRIX
    - = sum of the percentages of variance accounted for by the **rotated** distinctive components in the 'wrong' data blocks
  - Taken the number of distinctive components into account



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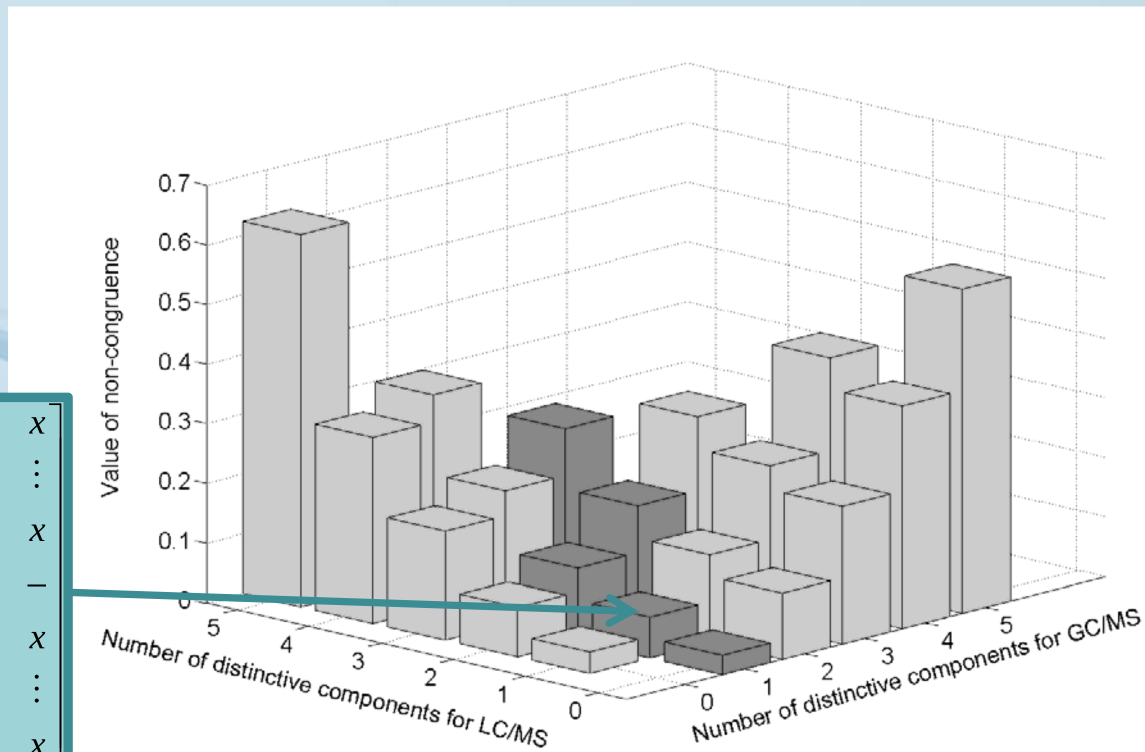

$$\mathbf{P}^{target}_{conc} = \begin{bmatrix} x & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & 0 & x & x & x \\ - & - & - & - & - \\ 0 & x & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & x & x & x & x \end{bmatrix}$$

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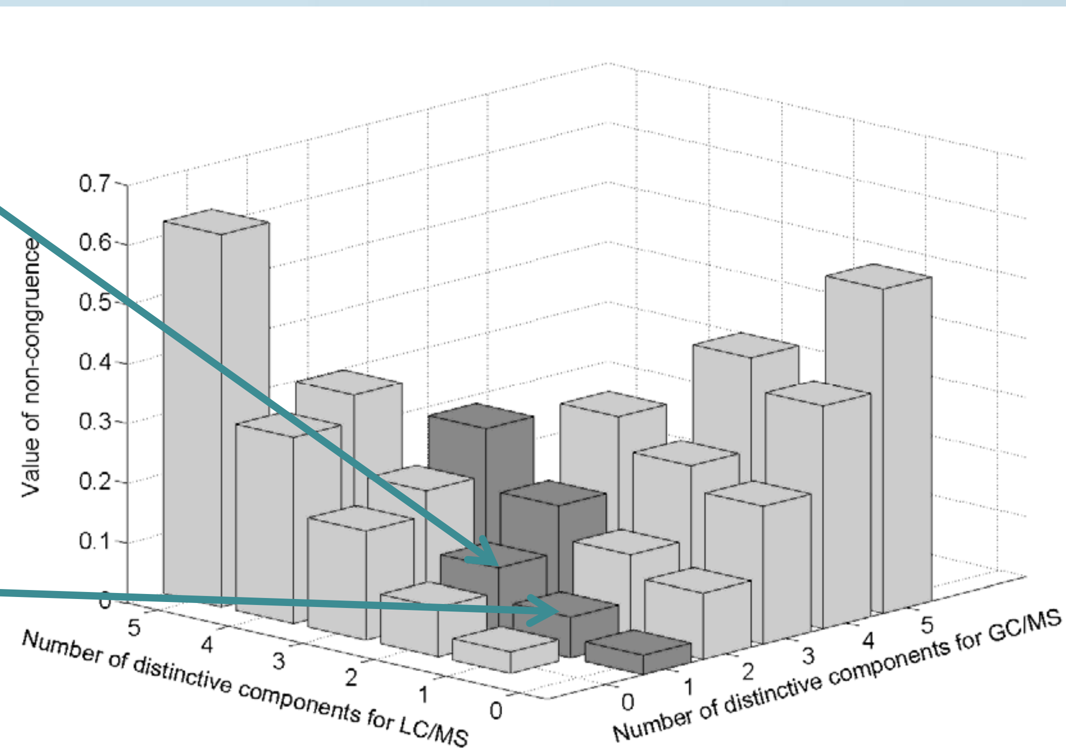
  - Taken the number of distinctive components into account

$$\mathbf{P}_{conc}^{target} = \begin{bmatrix} x & x & 0 & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & x & 0 & x & x \\ - & - & - & - & - \\ 0 & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x & x & x \end{bmatrix}$$

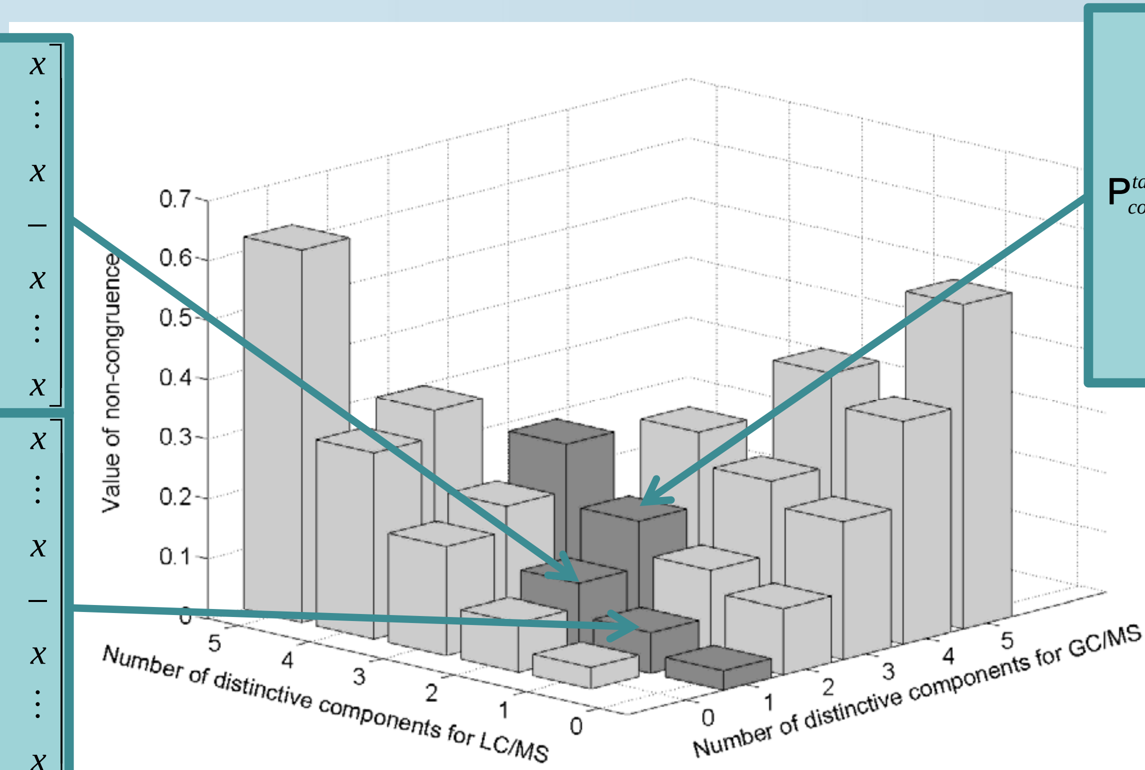
$$\mathbf{P}_{conc}^{target} = \begin{bmatrix} x & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & 0 & x & x & x \\ - & - & - & - & - \\ 0 & x & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & x & x & x & x \end{bmatrix}$$



- STEP 2: characterization of the components (Schouteden et al., 2010)
  - (Non-)congruence criterion FOR EACH POSSIBLE TARGET-MATRIX
    - = sum of the percentages of variance accounted for by the (rotated) distinctive components in the ‘wrong’ data blocks
  - Taken the number of distinctive components into account

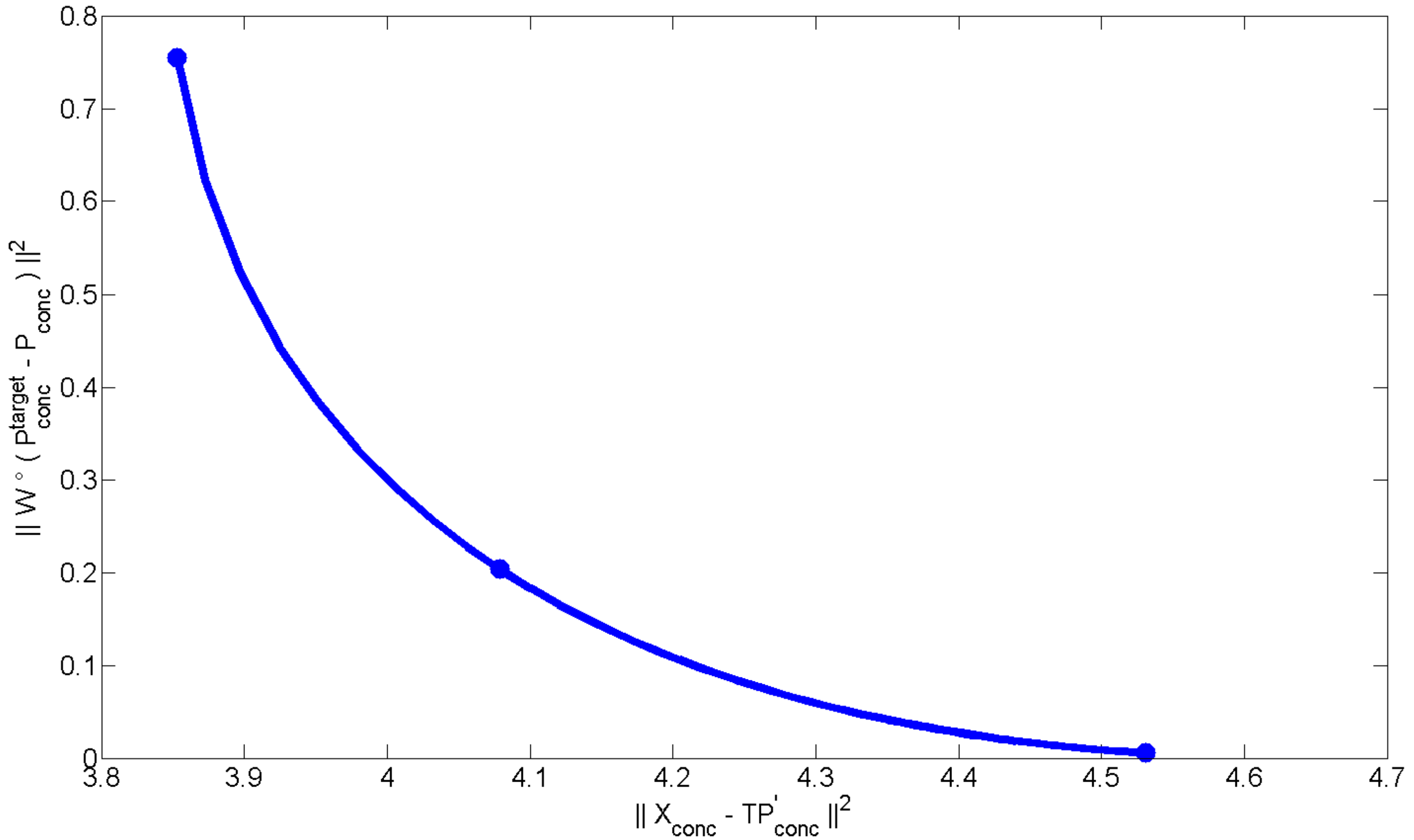
$$\mathbf{P}^{target}_{conc} = \begin{bmatrix} x & x & 0 & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & x & 0 & x & x \\ - & - & - & - & - \\ 0 & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x & x & x \end{bmatrix}$$

$$\mathbf{P}^{target}_{conc} = \begin{bmatrix} x & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & 0 & x & x & x \\ - & - & - & - & - \\ 0 & x & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & x & x & x & x \end{bmatrix}$$



$$\mathbf{P}^{target}_{conc} = \begin{bmatrix} x & x & 0 & 0 & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x & x & 0 & 0 & x \\ - & - & - & - & - \\ 0 & 0 & x & x & x \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & x & x & x \end{bmatrix}$$

STEP 3: define λ with L-curve (Hansen, 1992)



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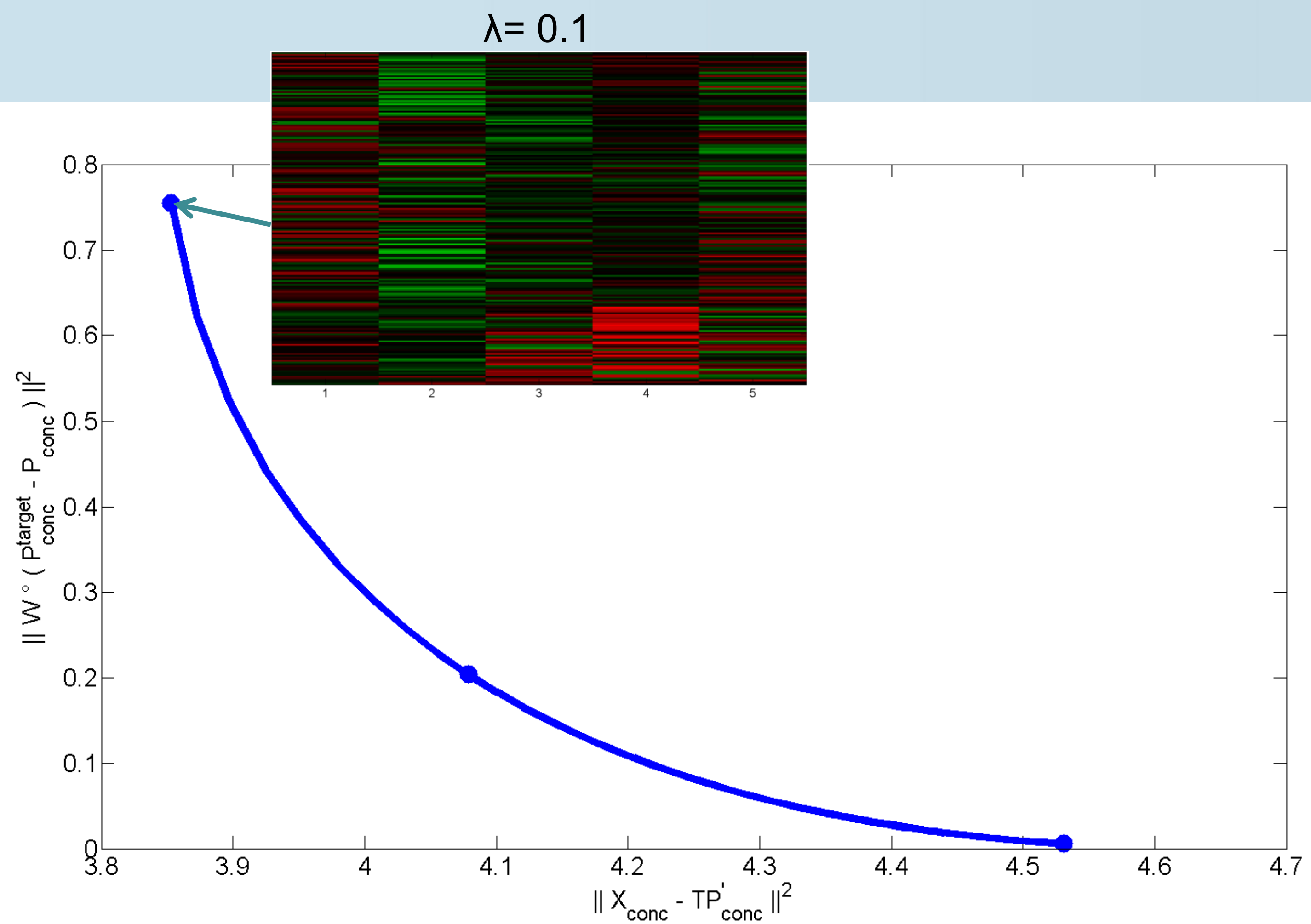

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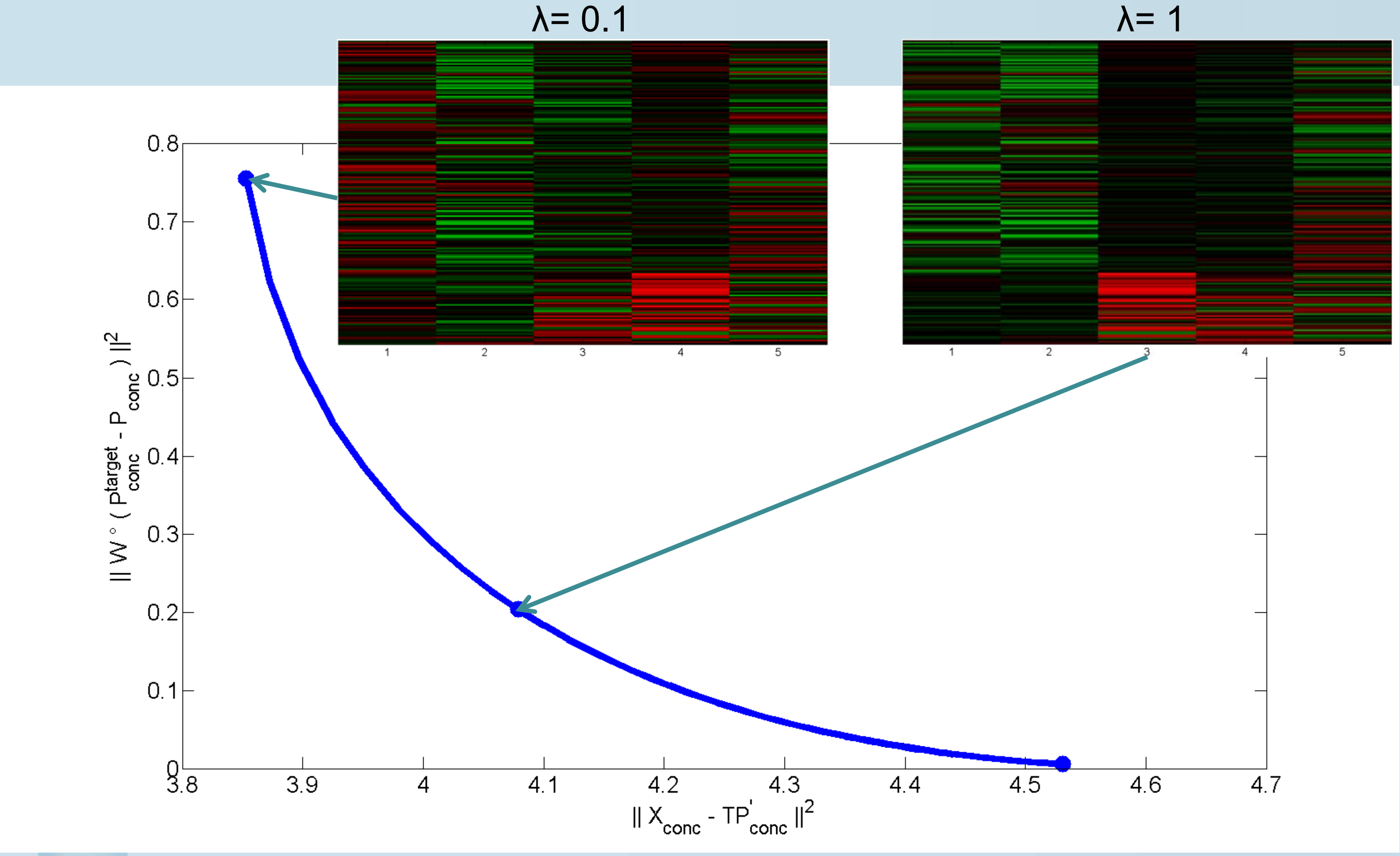

STEP 3: define λ with L-curve (Hansen, 1992)