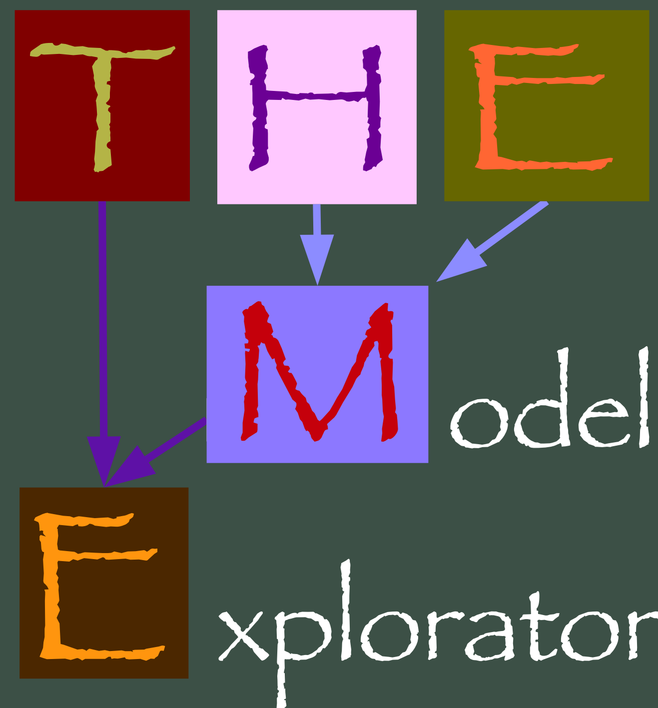
A component-based
Multidimensional Path Modelling technique: THEME
(with a user-friendly R-package)

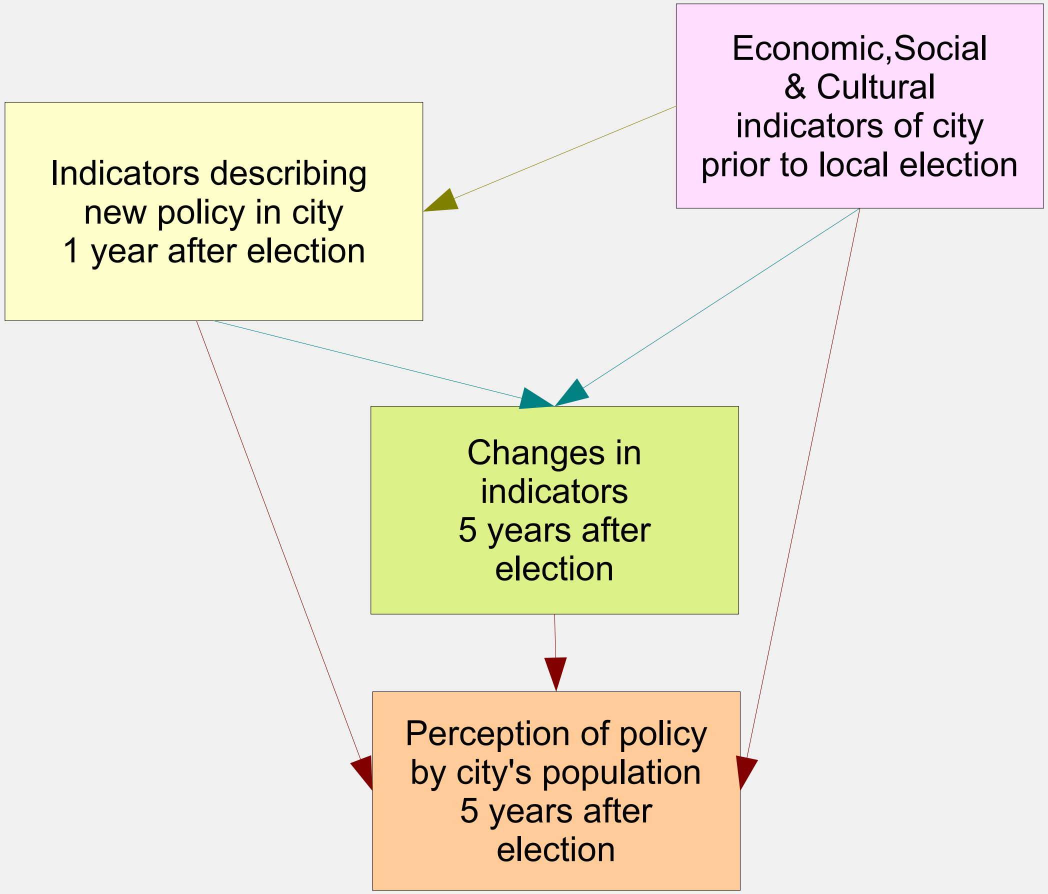


X. Bry *IMAG, Univ. Montpellier*
T. Verron *ITG - SEITA, Centre de recherche*

Data and Problem:

1. Conceptual model of a situation = Thematic Model

Example: *n* cities described through indicators:



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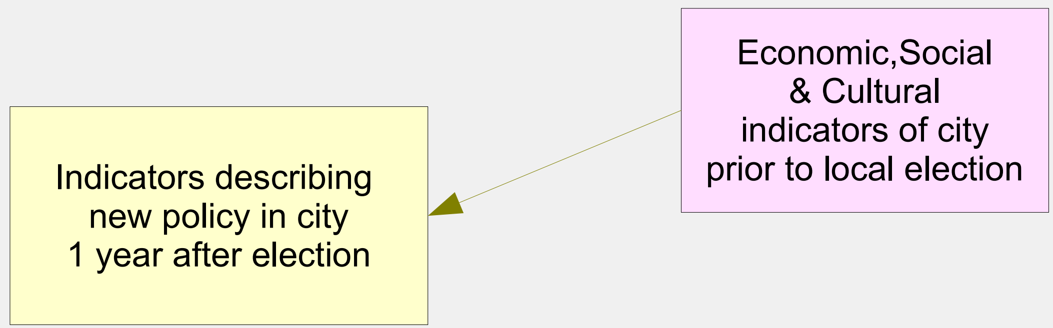
Example: *n* cities described through indicators:

Thematic equation 1



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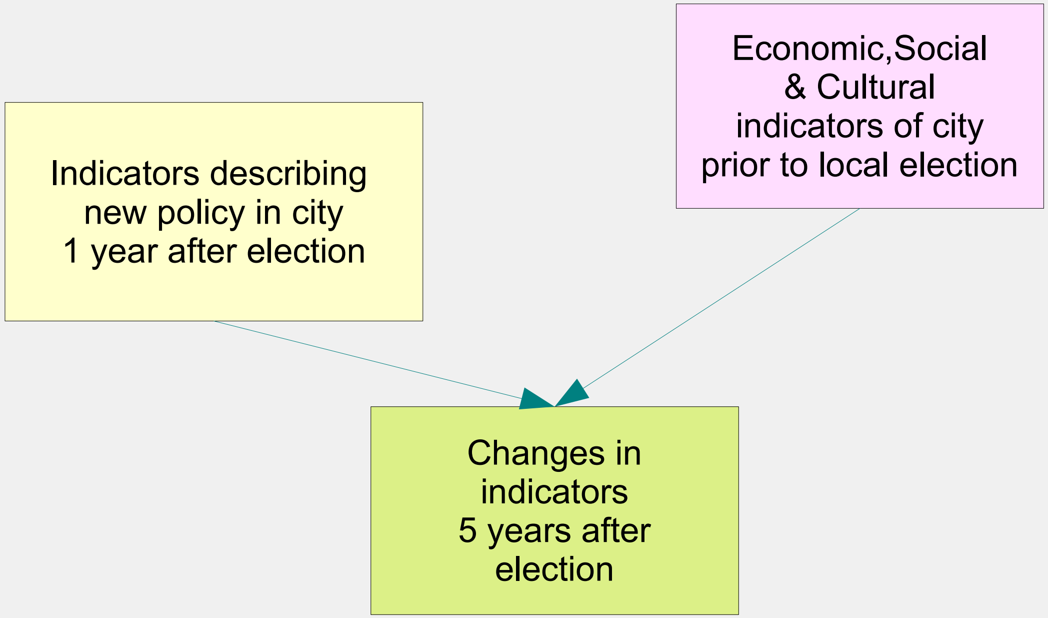
Example: *n* cities described through indicators:

Thematic equation 2



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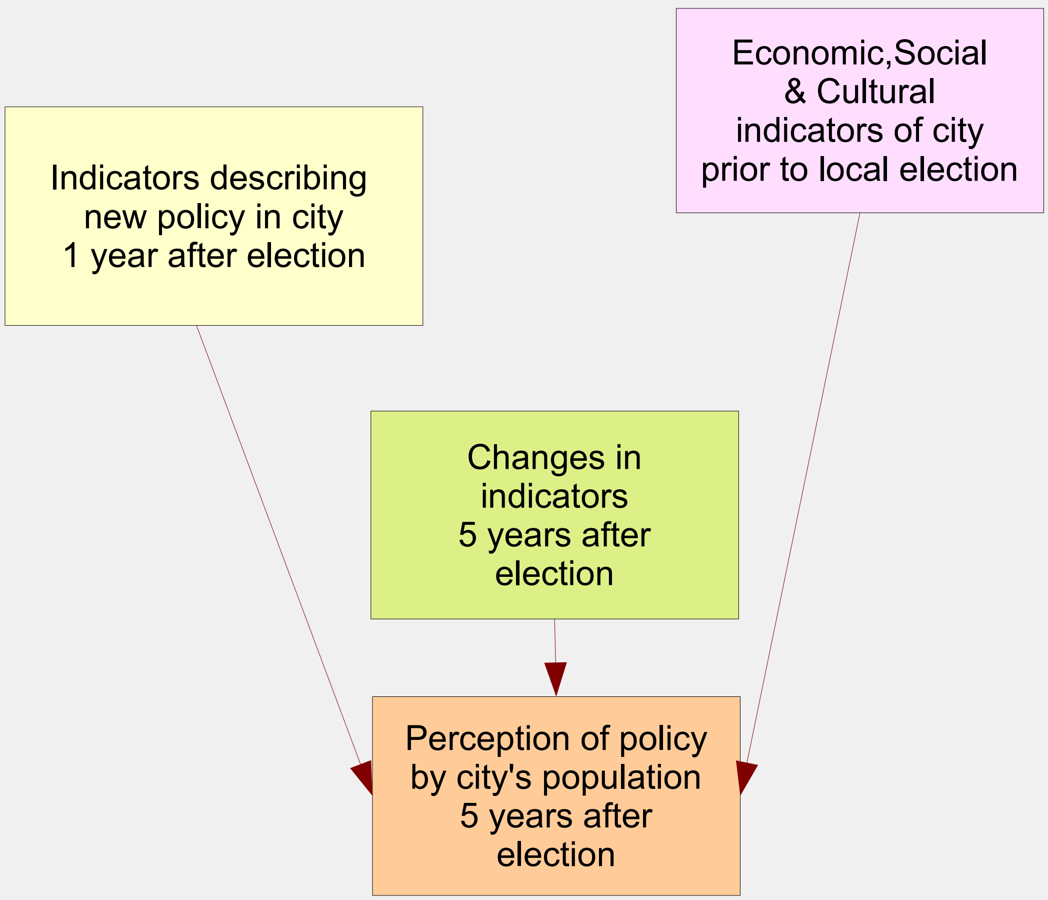
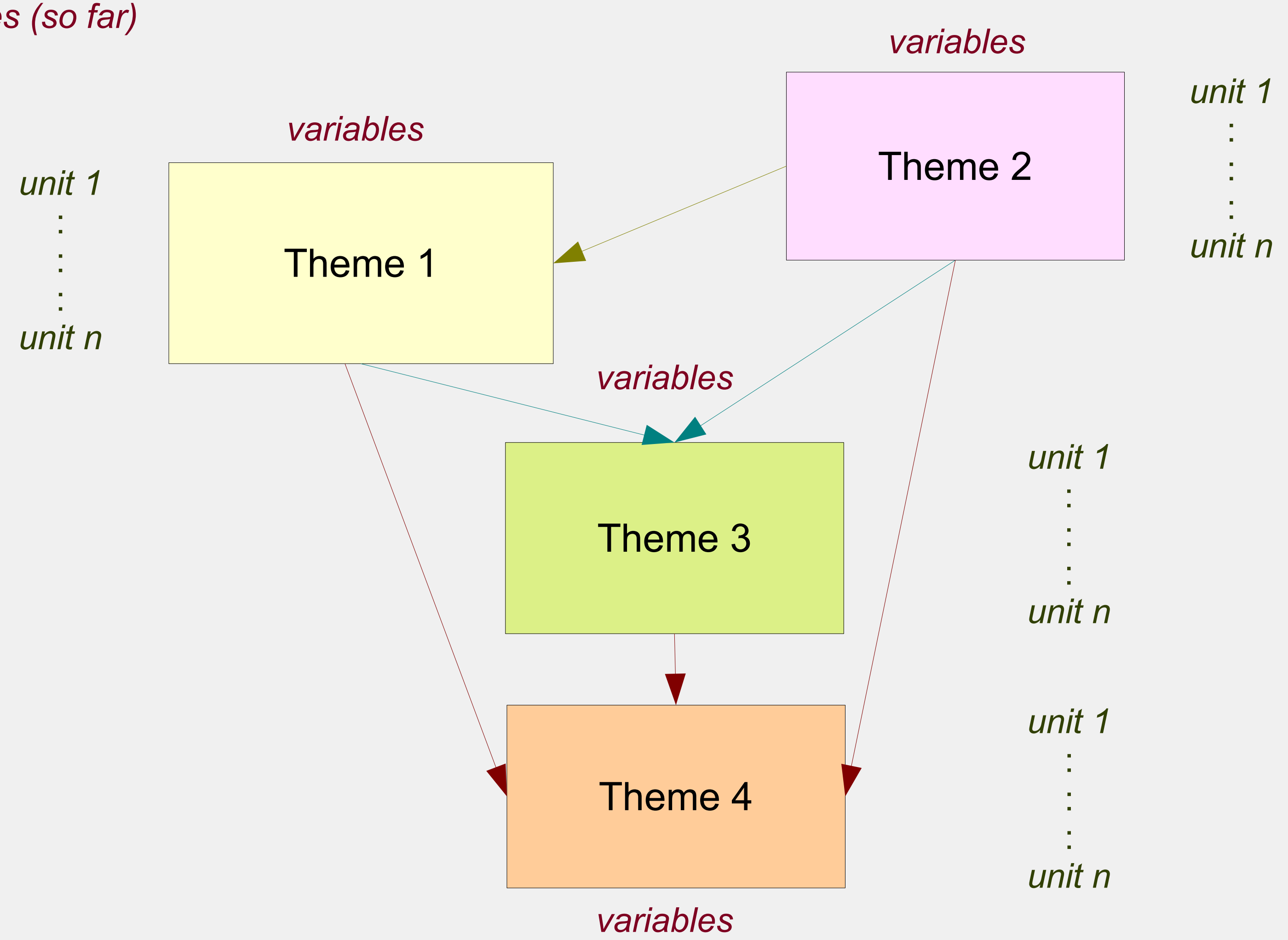


Thematic equation 3

Data and Problem:

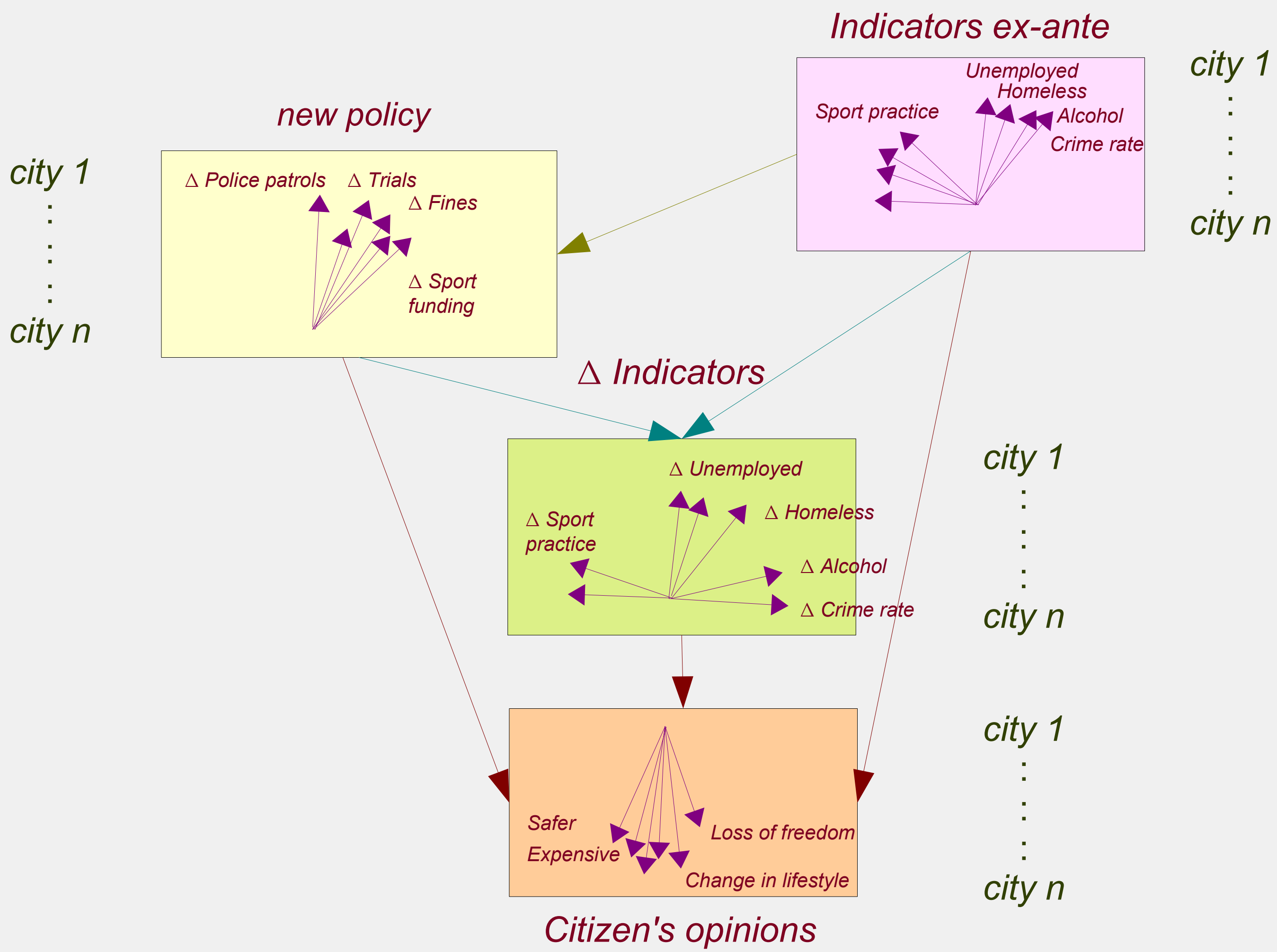
1. Conceptual model of a situation = Thematic Model

Numeric variables (so far)



Data and Problem:

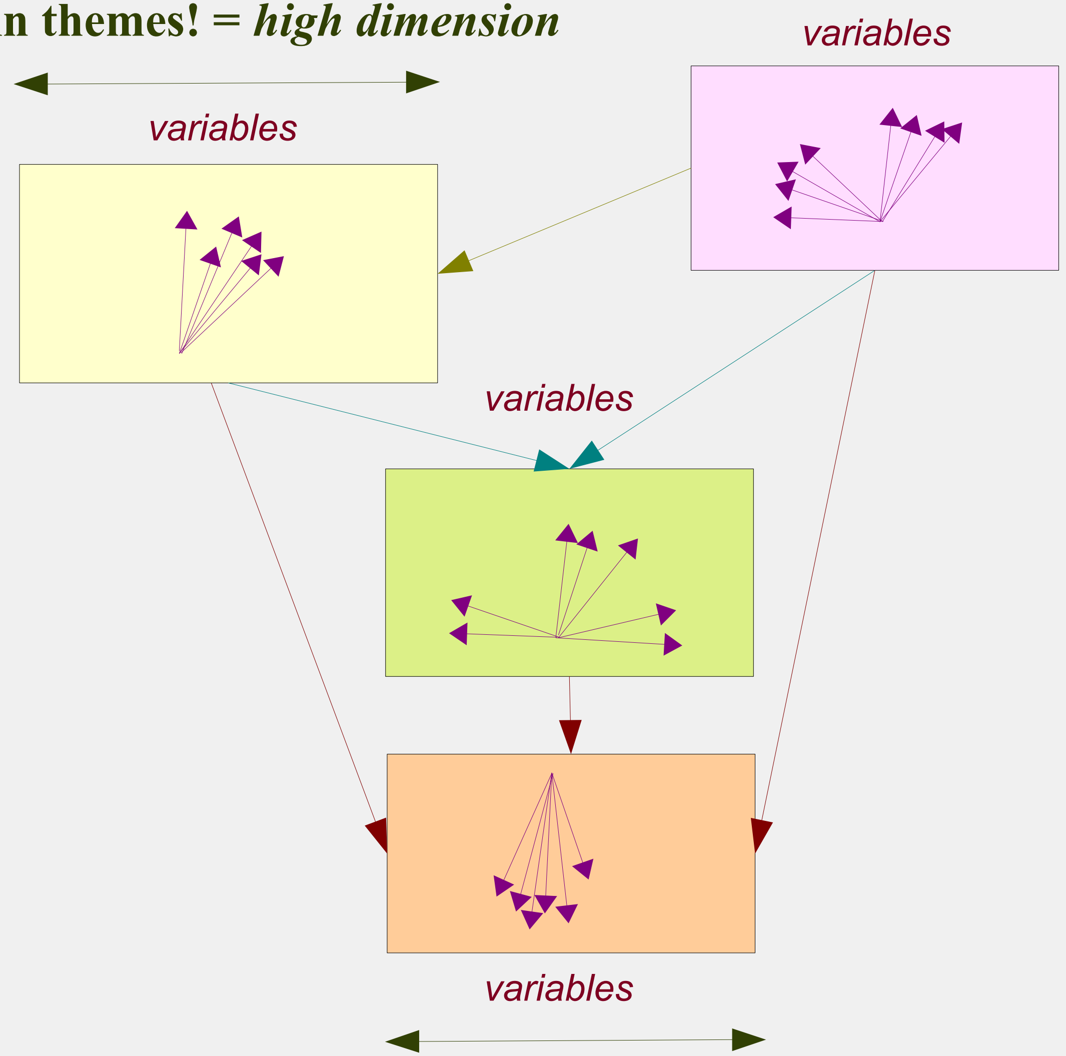
2. The Path-Modelling problem



Data and Problem:

2. The Path-Modelling problem

- **Too many variables in themes! =** ***high dimension***



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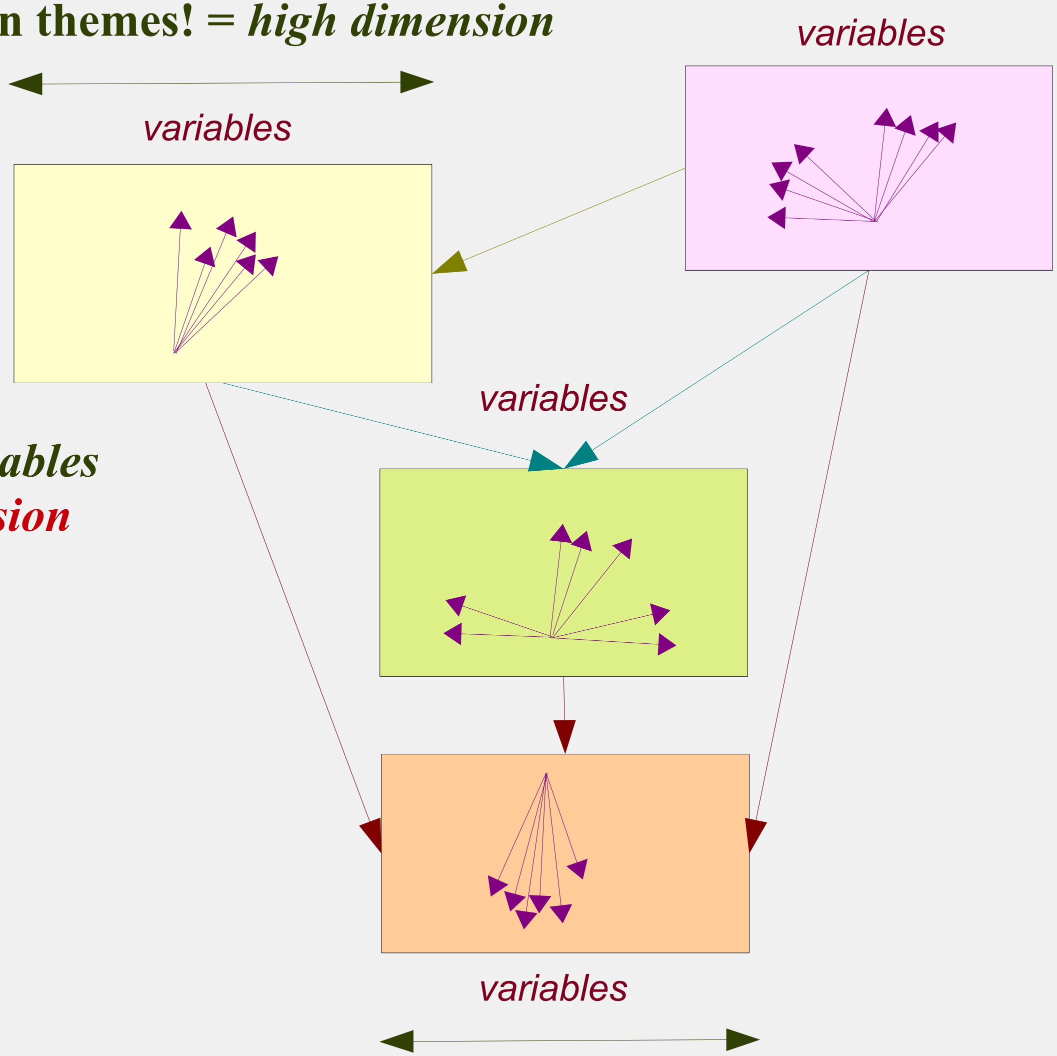

1) *Redundancy of variables*
→ instability of regression model coefficients.

Data and Problem:

2. The Path-Modelling problem

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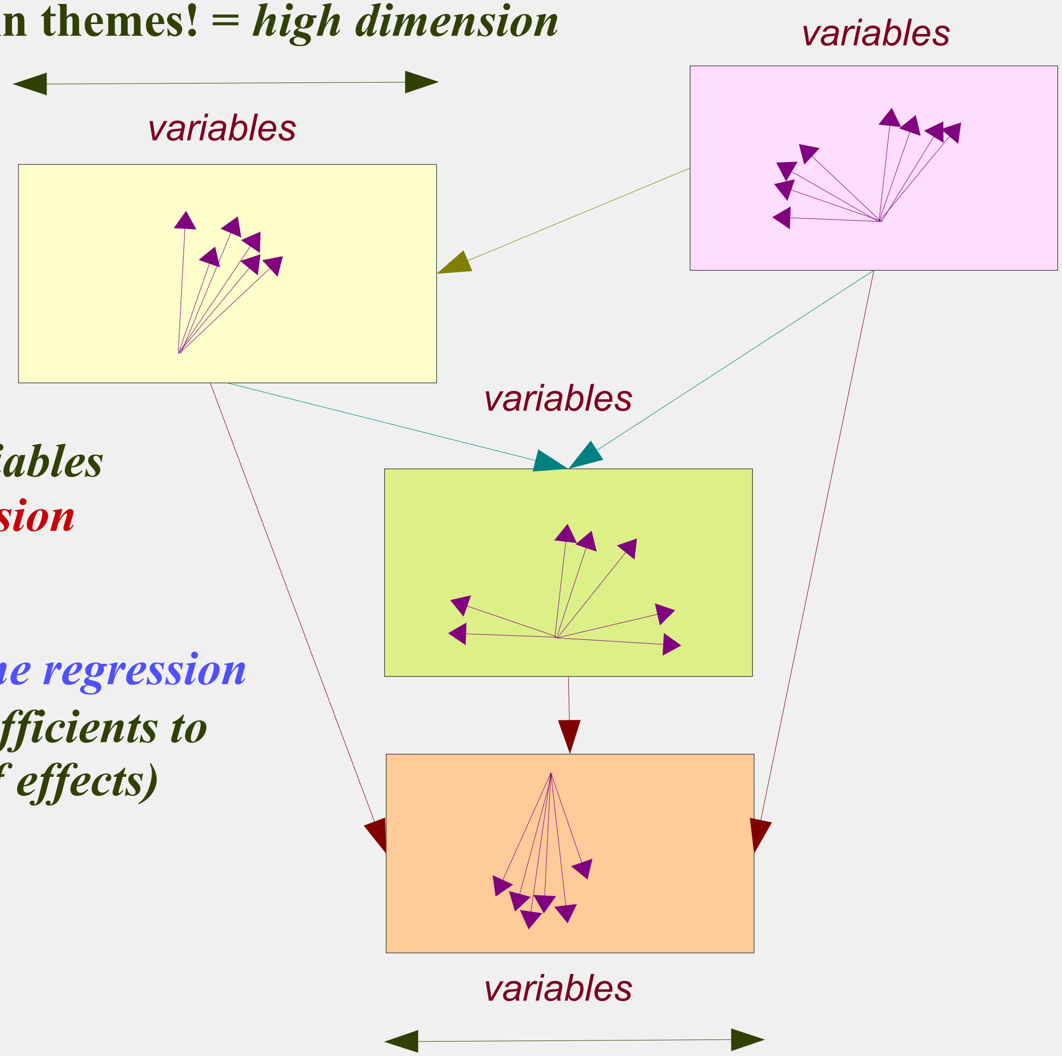
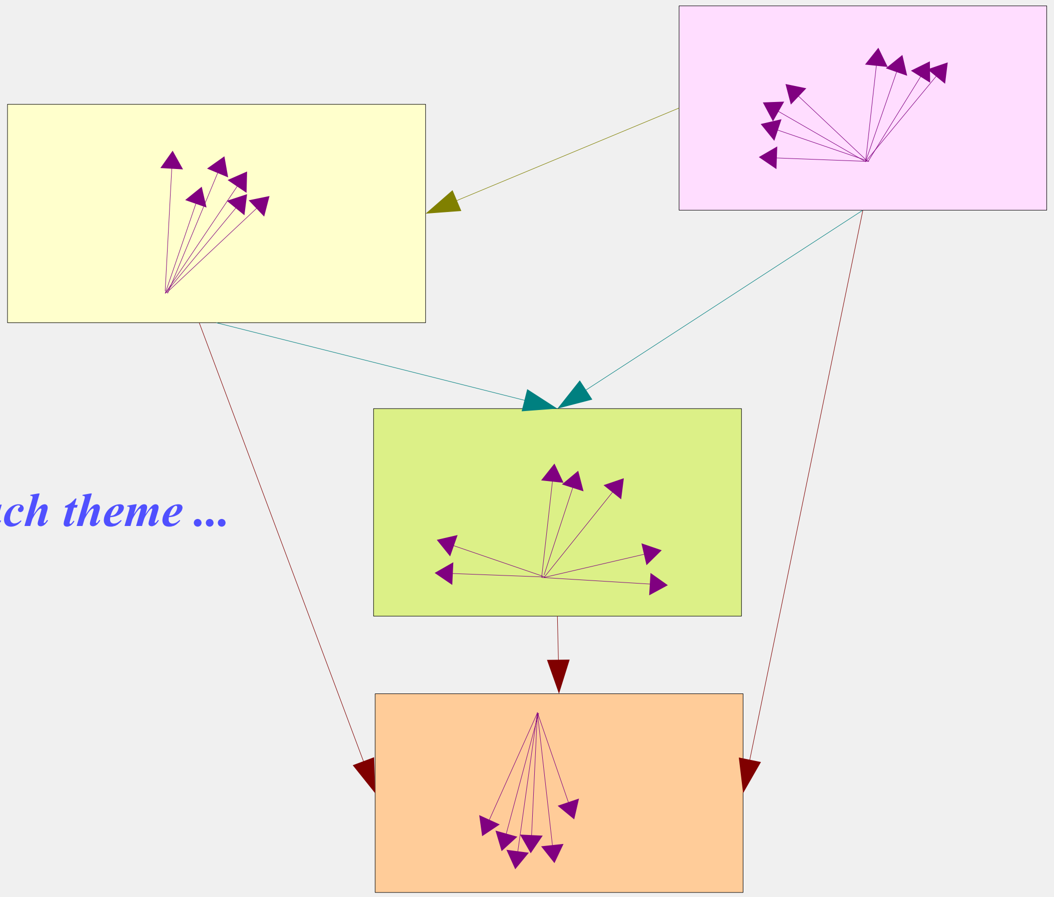


1) *Redundancy of variables*
→ *instability of regression model coefficients.*

⇒ *Regularisation of the regression models (shrinking coefficients to minimise confusion of effects)*

Data and Problem:

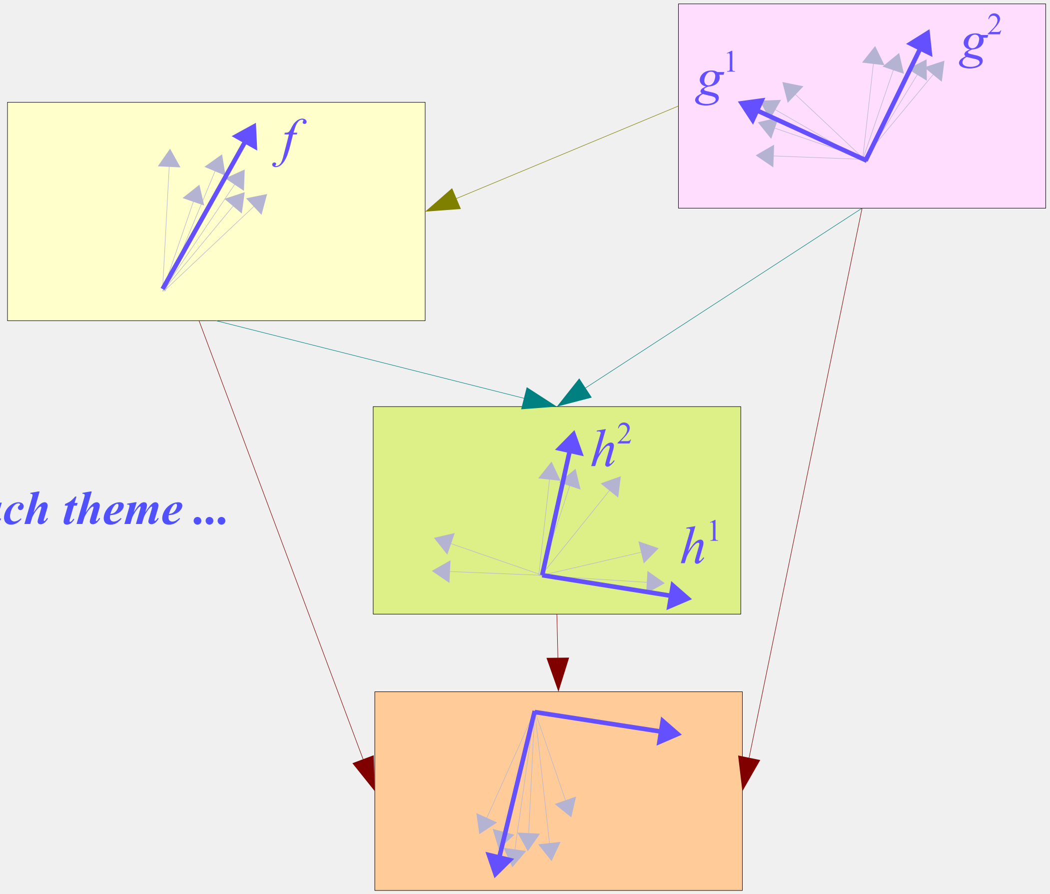
2. The Path-Modelling problem



2) *High dimension*
⇒ *Reduce dimension in each theme ...*

Data and Problem:

2. The Path-Modelling problem

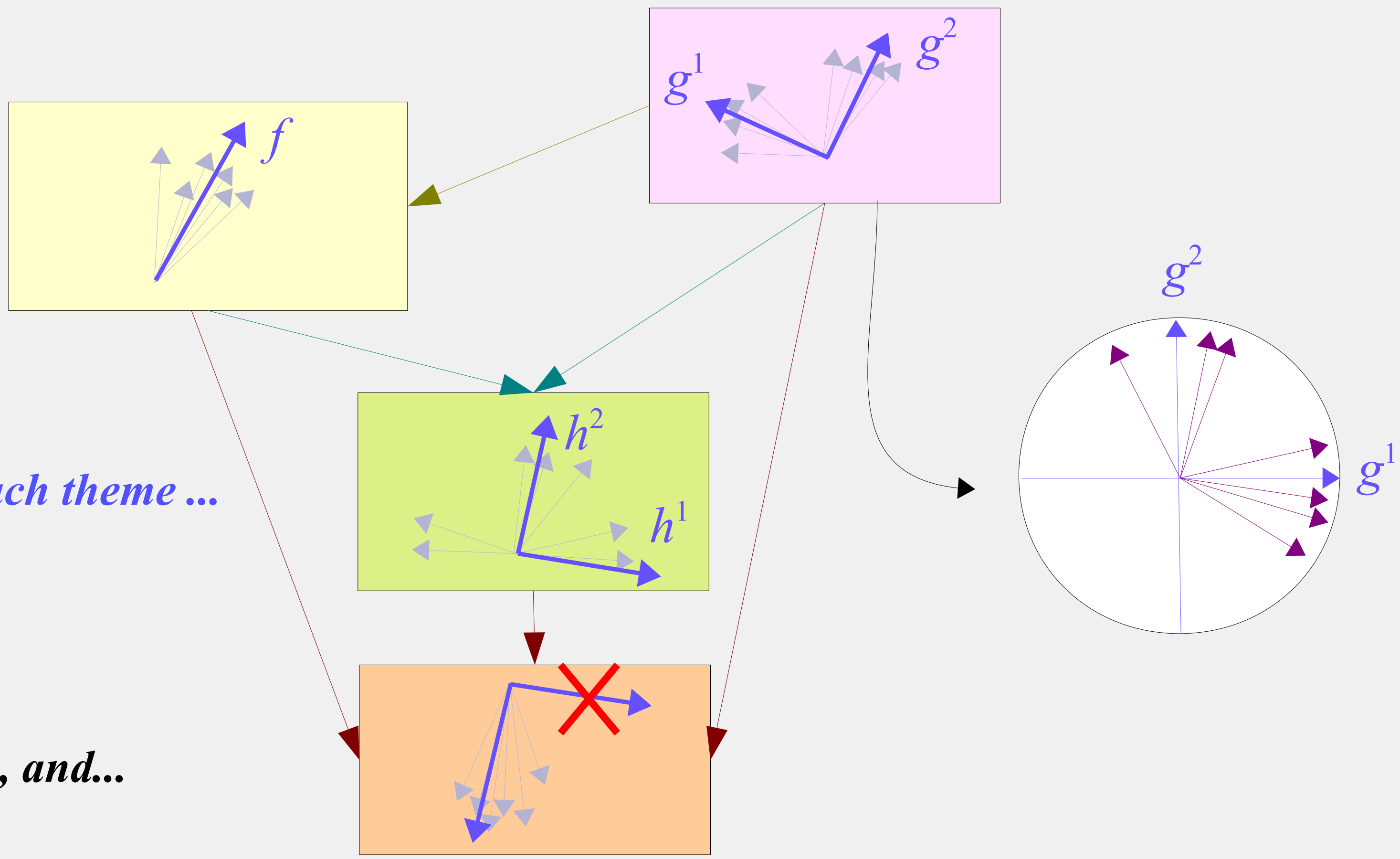


2) ***High dimension***
⇒ ***Reduce dimension in each theme ...***

through a few
Thematic Components

Data and Problem:

2. The Path-Modelling problem



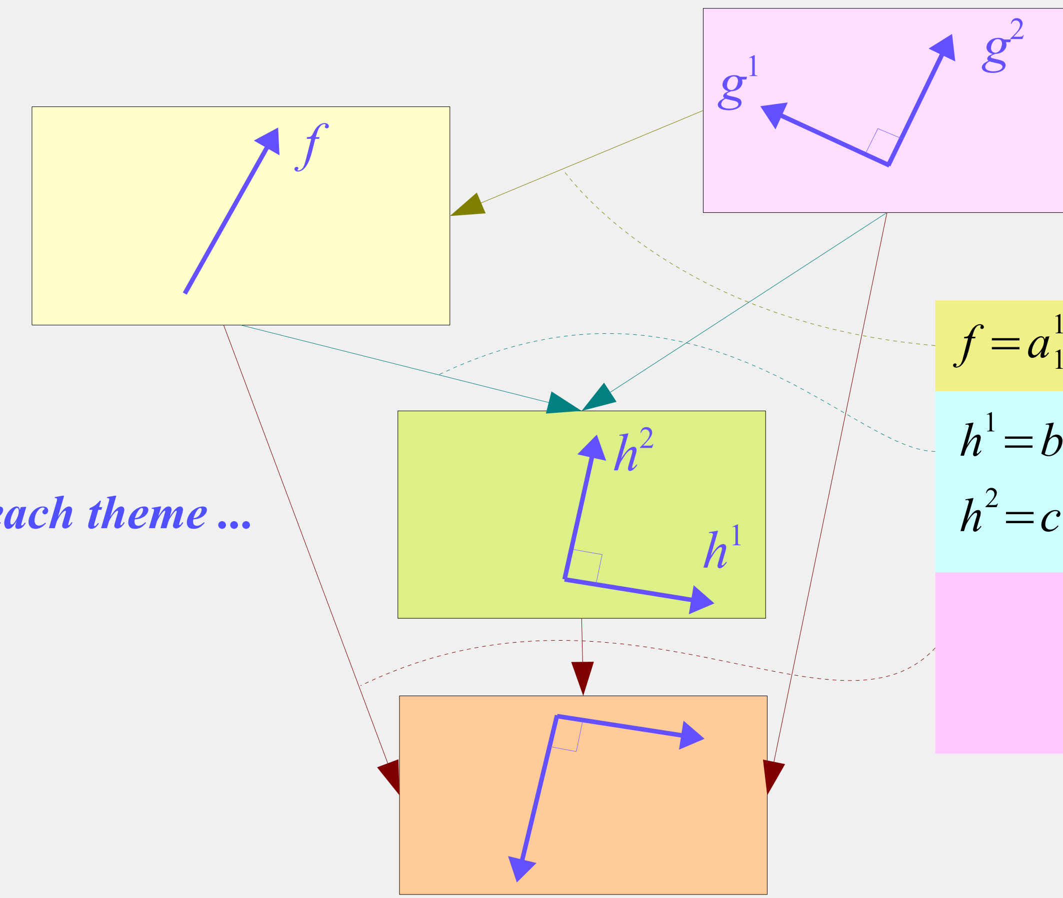
2) ***High dimension***
⇒ *Reduce dimension in each theme ...*

through a few
Thematic Components

... *non-redundant*, *strong*, *and...*

Data and Problem:

2. The Path-Modelling problem



$$f = a_1^1 g^1 + a_2^1 g^2 + \varepsilon_f$$

$$h^1 = b_0 f + b_1 g^1 + b_2 g^2 + \varepsilon_{h1}$$

$$h^2 = c_0 f + c_1 g^1 + c_2 g^2 + \varepsilon_{h2}$$

etc.

2) *High dimension*
⇒ *Reduce dimension in each theme ...*

through a few
Thematic Components

... *satisfying the model*.

Data and Problem:

2. The Path-Modelling problem

The advantage of *Thematic Components* :

- ***Thematic*** **: a clear conceptual interpretation**

Data and Problem:

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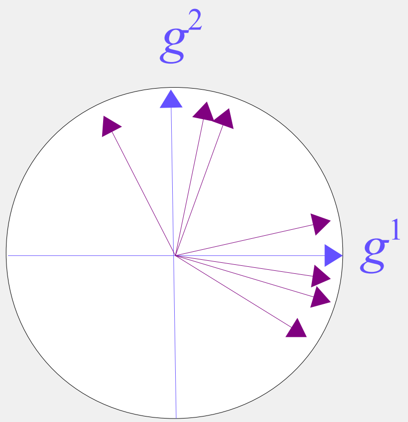
- ***Thematic*** **: a clear conceptual interpretation**
- ***Components*** *= linear combinations of variables estimating a latent variable* **:**

→ closer to the observed variables: easier to interpret substantially



Data and Problem:

2. The Path-Modelling problem

The advantage of ***Thematic Components*** **:**

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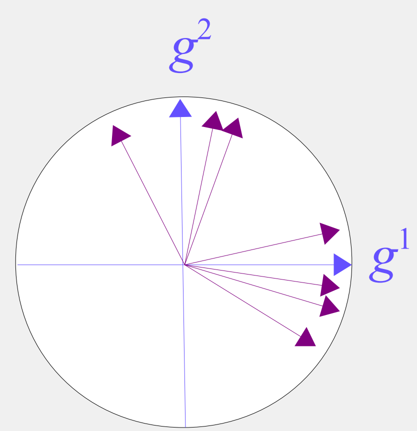
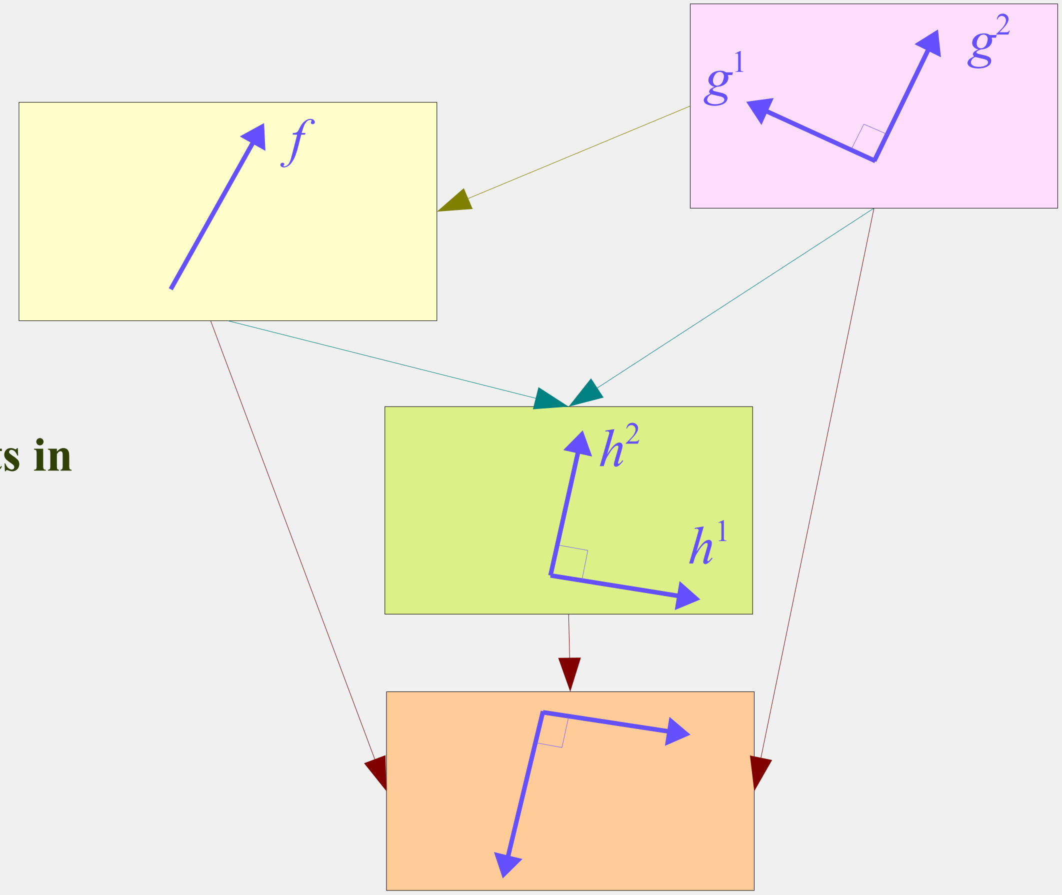


→ possibility to calculate the value of the components from those of the observed variables (contrary to standard SEM estimations)
→ possibility to predict the dependent variables...
... through ***regularised regression models*****!**

Data and Problem:

2. The Path-Modelling problem

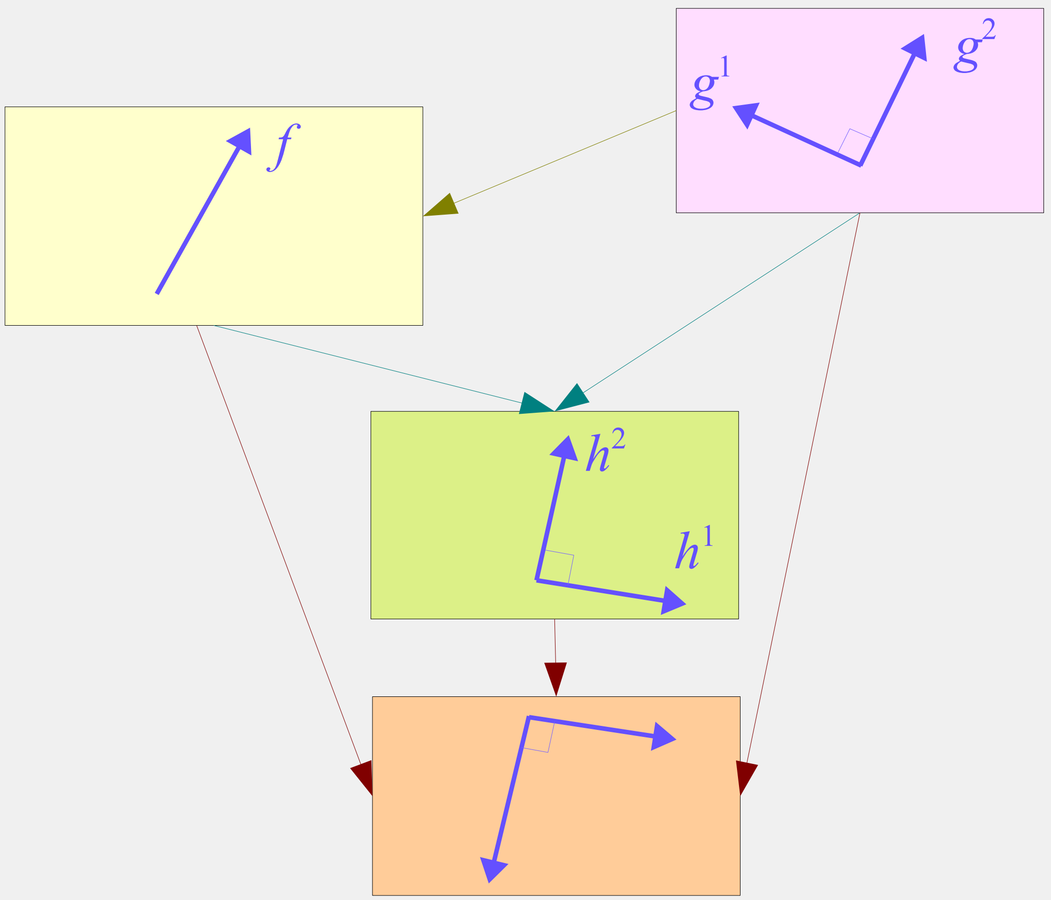


⇒ **How many components in each theme?**

... and which?

Data and Problem:

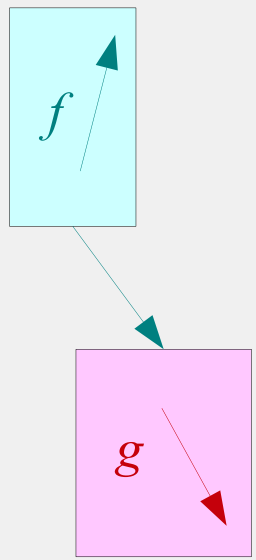
2. The Path-Modelling problem

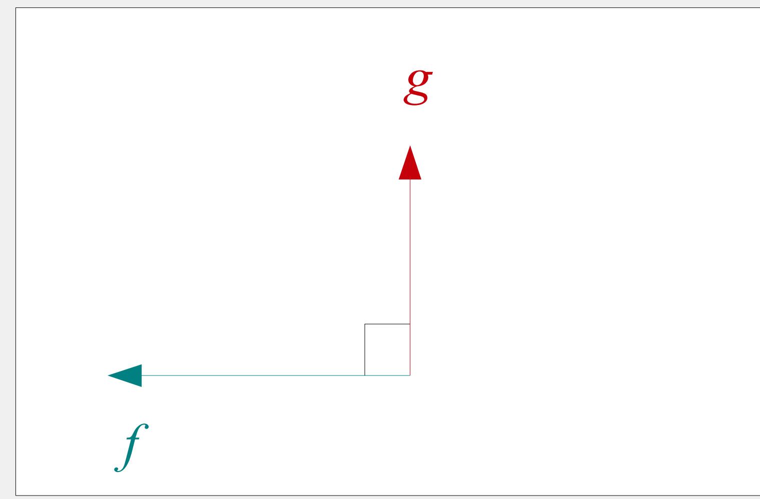


Pb: Every useful component partly depends on all others connected to it, directly or not...

How THEME works

2. The Path-Modelling problem





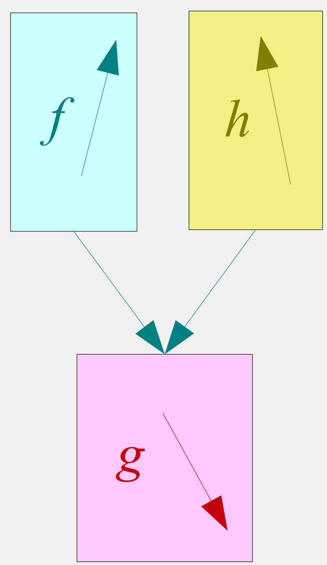
$$\rho^2(g, f) = 0$$

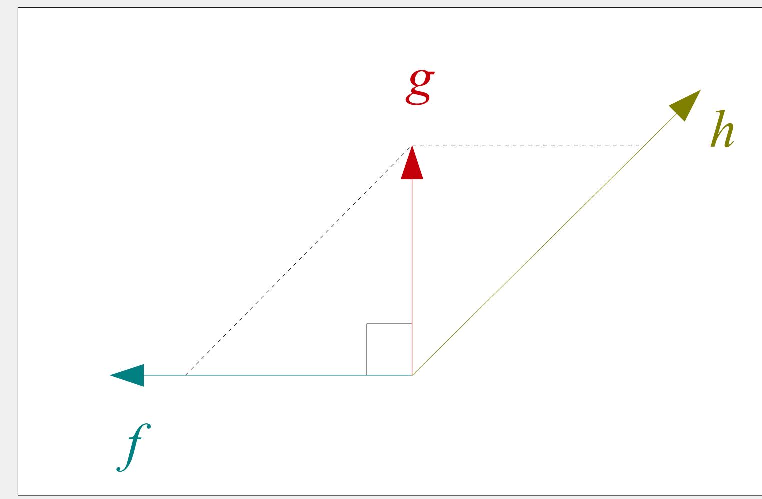
Pb: Every useful component partly depends on *all* others connected to it, directly or not...

No bivariate correlation $\rho(f,g)$

How THEME works

1. Goodness of Fit of the Component Model





$R^2(g\,|f,h) = 1$

Pb: Every useful component partly depends on *all* others connected to it, directly or not...

No bivariate correlation $\rho(f,g)$

*Important partial effect of f on g, **conditional on h***

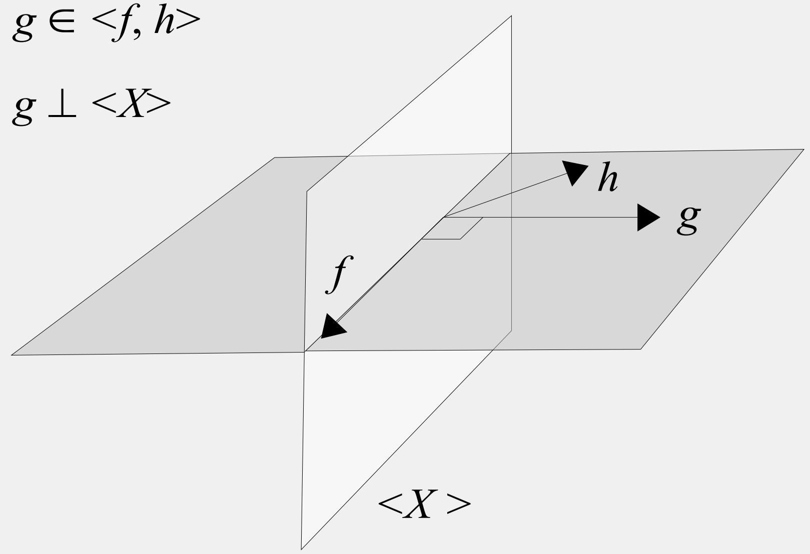
How THEME works

1. Goodness of Fit of the Component Model

A very simple case : $g = af + bh$

$g \in \langle f, h\rangle$

$g \perp \langle X\rangle$



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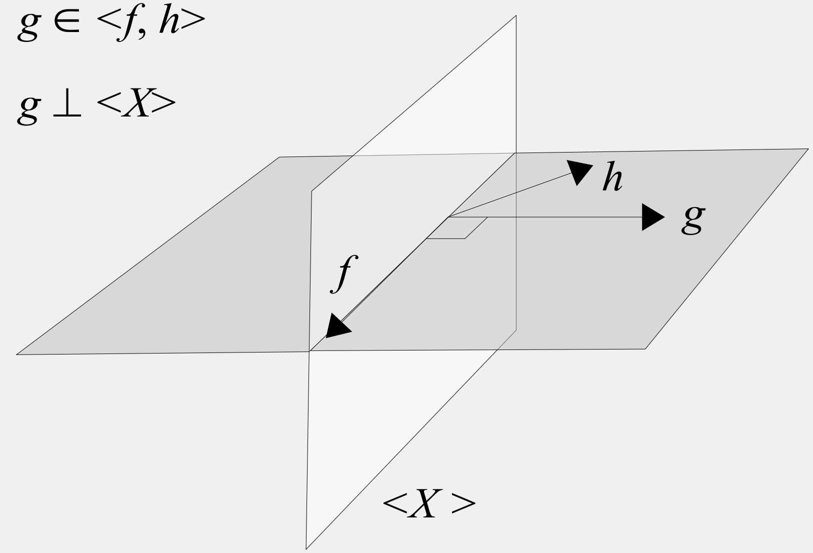

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A thematic model that should lead to f : $g = \langle X , h \rangle$

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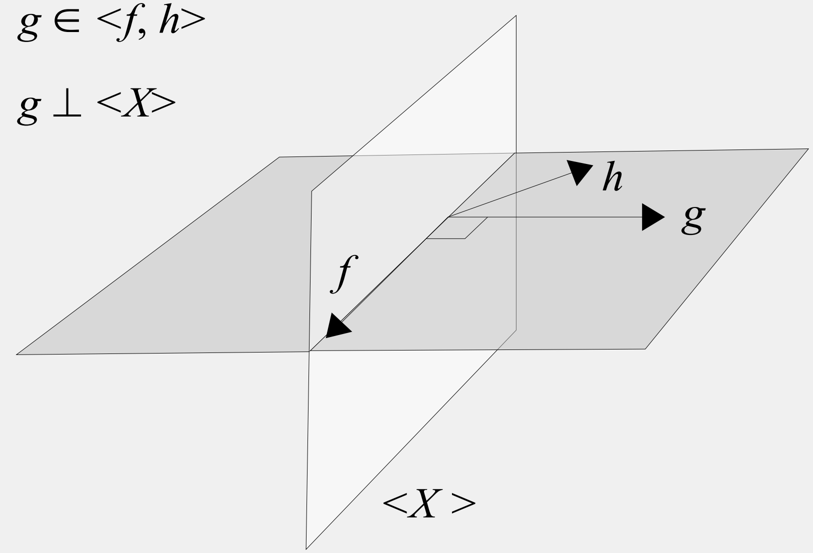

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Here, f can never be found within $\langle X \rangle$ by means of single bivariate correlation with g.

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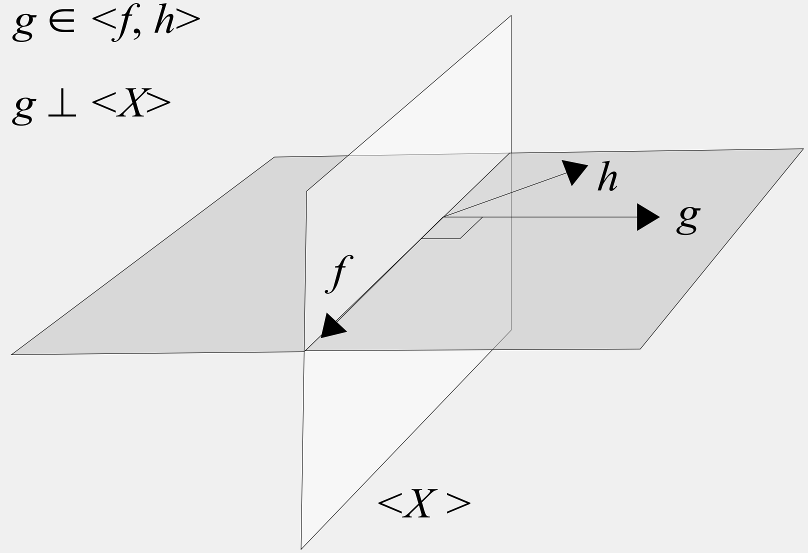

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*Proper (partial) effects cannot be correctly captured through **bivariate** correlations with the dependent components.*

$\Rightarrow$ *Exeunt: PLS Path-Modeling, Multiblock PLS, RGCCA...*

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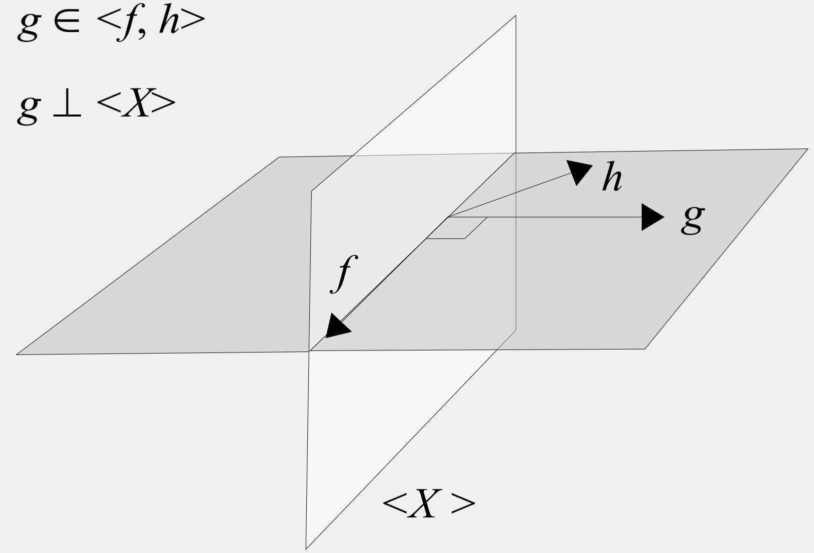

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*Proper (partial) effects cannot be correctly captured through **bivariate** correlations with the dependent components.*

⇒ *Exeunt: PLS Path-Modeling, Multiblock PLS, RGCCA...*

⇒ THEME uses a Goodness-of-Fit criterion ψ capturing *partial* component-relationships

How THEME works

1. Goodness of Fit of the Component Model

... for a single dependent component per equation

- Goodness of fit of one equation:

Equation q : $\mathbf{M}^q : X_{d^q} = \langle \{ X_r ; r \in \mathbf{P}^q \} \rangle$

→ GOF: $\psi_q = g\left(R_q^2\right)$, where g is any positive strictly increasing function

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- Goodness of fit of the component-model:

$$\psi = g^{-1}\left(\sum_{q=1}^{Q} \varpi_q \psi_q \right)$$

weight of equation q

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weight of equation q

Particular cases:

- Arithmetic averaging: $\forall q : \varpi_q = \frac{1}{Q} \; ; \; g = id \quad \Rightarrow \quad \psi = \frac{1}{Q} \sum_q R_q^2$
- Geometric averaging: $\forall q : \varpi_q = \frac{1}{Q} \; ; \; g = \ln \quad \Rightarrow \quad \psi = \left(\prod_q R_q^2 \right)^{\frac{1}{Q}}$

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... for any number of dependent components per equation

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$F_{\mathbf{P}^q}$ = all explanatory components of eq. q

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→ GOF: $$\psi_q = g\left(h^{-1}\left(\sum_{k=1,\ldots K_{d^q}} h\left(R^2\left(f^k_{d^q} \middle| F_{\mathbf{P}^q} \right) \right) \right) \right)$$

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Particular case: when $h = id$: $\psi_q = g\left(tr\left(\Pi_{F_{d^q}} \Pi_{\langle F_{\mathbf{P}^q} \rangle} \right) \right)$

Classic link between sub-spaces

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Classic link between sub-spaces

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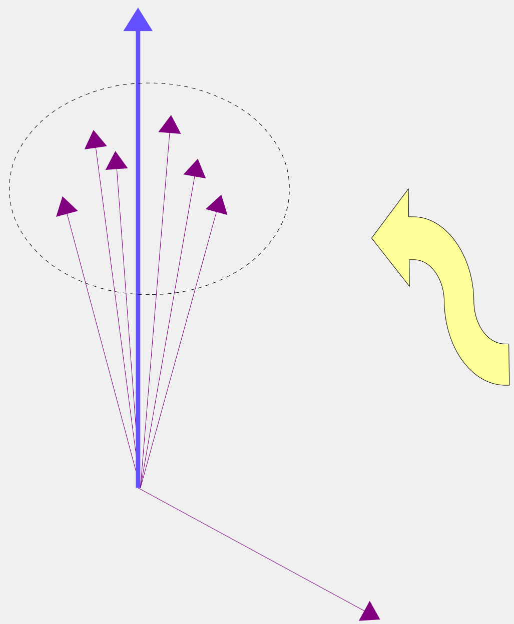
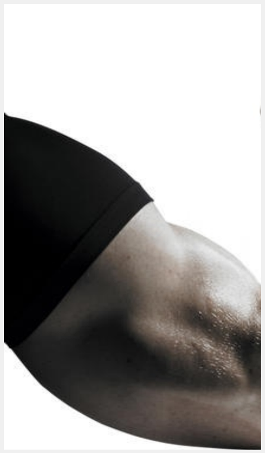
How THEME works

2. Structural relevance of components

To be interpretable, components must be *structurally strong*, e.g. close to *observed variables bundles*





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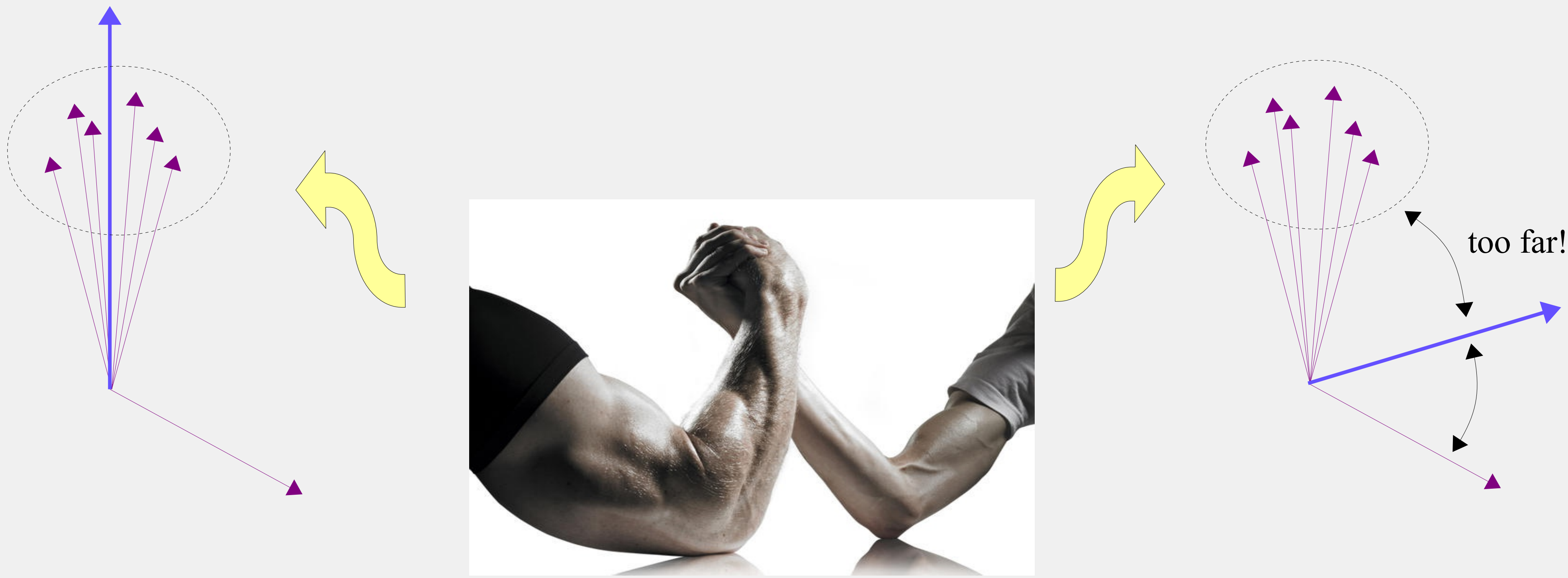

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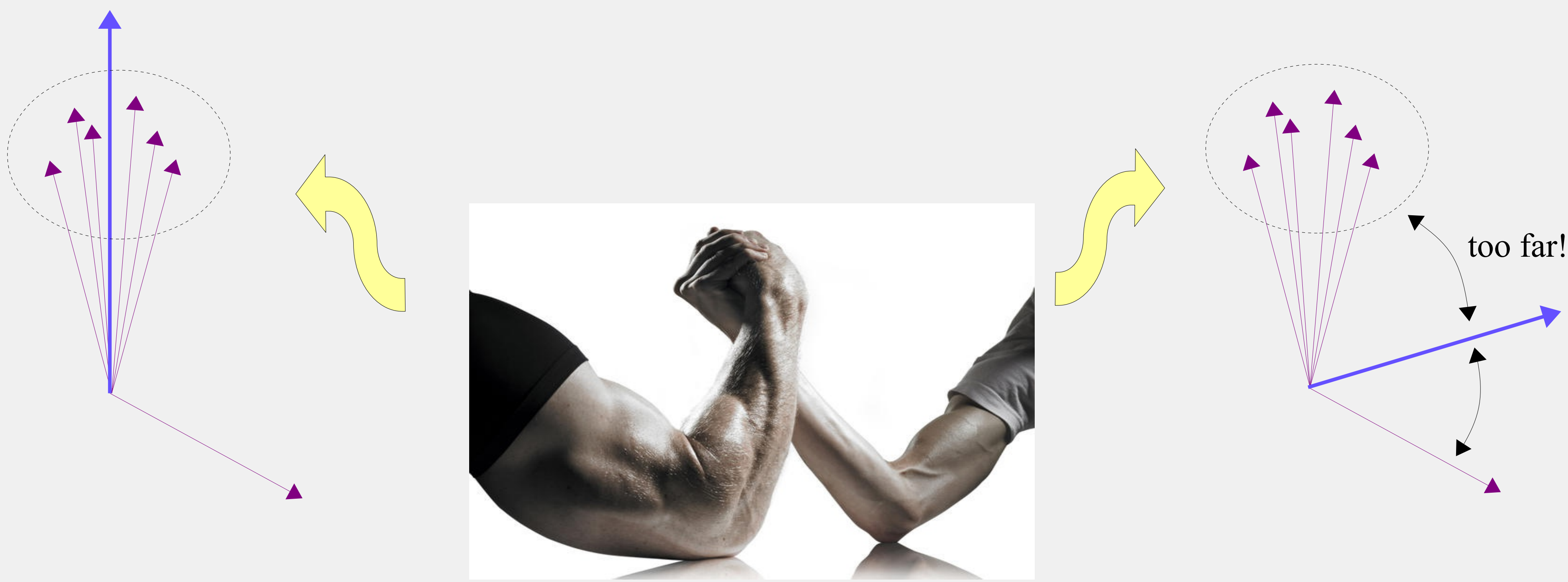

THEME uses an indicator of structural strength, $\boldsymbol{\phi} \simeq$ closeness to bundles.

How THEME works

2. Structural relevance of components

To be interpretable, components must be *structurally strong*, e.g. close to *observed variables bundles*

- *Component in a theme* X : $f = Xv$
- *Identification / regularisation constraint* : $v' M^{-1} v = 1$

with $M^{-1} = \tau A^{-1} + (1-\tau) X' W X$

where A is such that PCA of (X,A,W) is relevant to X's data

→ • ***The Structural Relevance Indicator:***

$$\phi(v) := \left(\sum_{j=1}^{J} \omega_j (v' N_j v)^l \right)^{\frac{1}{l}} \quad \text{s.t. constraint} \quad v' M^{-1} v = 1$$

weights

N_j's code the directions components should focus on

Structural Relevance of components

2. Structural relevance of components

- **Purpose of N_j's = ?**

$$\phi(v) := \left(\sum_{j=1}^{J} \omega_j (v' N_j v)^l \right)^{\frac{1}{l}}$$

The N_j's are coding directions of concern

Examples:

- Component's variance: $\phi(v) = V(f) = \| X v \|_W^2 = v' (X' W X) v$

$\| v \|^2 = 1 \ \Rightarrow \ M = I$

$\rightarrow$ directions of discrepancy of observations

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→ directions of discrepancy of observations

- Variable Powered Inertia: $\phi(v) = \left(\sum_{j=1}^{p} \omega_j \rho^{2l}(f, x^j) \right)^{\frac{1}{l}}$

locality parameter

$$= \left(\sum_{j=1}^{p} \omega_j (v' \underbrace{X' W x^j x^{j\,\prime} W X}_{N_j} v)^l \right)^{\frac{1}{l}}$$

$$\|f\|_W^2 = 1 \;\Rightarrow\; M = (X'WX)^{-1}$$

→ directions of observed variables.

Structural Relevance of components

2. Structural relevance of components

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The N_j's are coding directions of concern

Examples:

Variable Powered Inertia can be extended to:

- Variable Powered Covariance: $\phi(v) = \left(\sum_{j=1}^{p} \omega_j \langle f | x^j \rangle_W^{2l} \right)^{\frac{1}{l}}$

locality parameter

$$= \left(\sum_{j=1}^{p} \omega_j (v' \underbrace{X' W x^j x^{j\prime} W X}_{N_j} v)^l \right)^{\frac{1}{l}}$$

$$M^{-1} = \tau A^{-1} + (1-\tau)(X'WX)$$

Regularisation parameter

Matrix suitable for the PCA of X

Structural Relevance of components

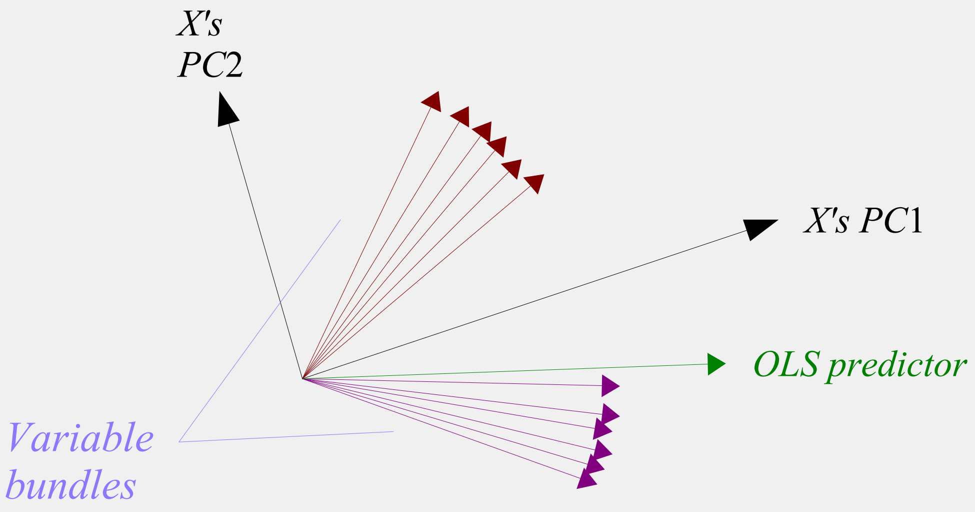
2. Structural relevance of components

- **Purpose of *l* = ?**

$$\phi(v) := \left(\sum_{j=1}^{J} \omega_j (v' N_j v)^l \right)^{\frac{1}{l}}$$

A disturbing phenomenon when regularising regression in the PLS way...

What happens:



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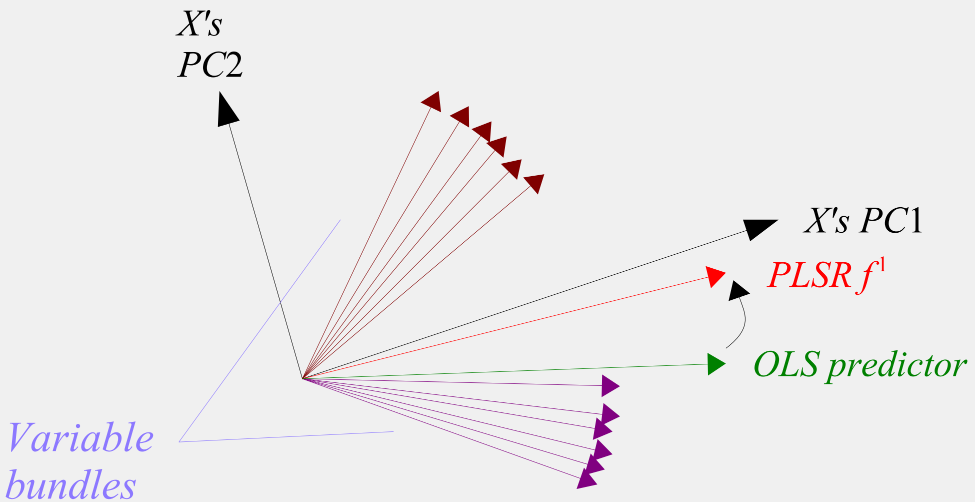

A PC is too ***global*** a direction to fit bundle structures.

 We must go beyond component variance.

Structural Relevance of components

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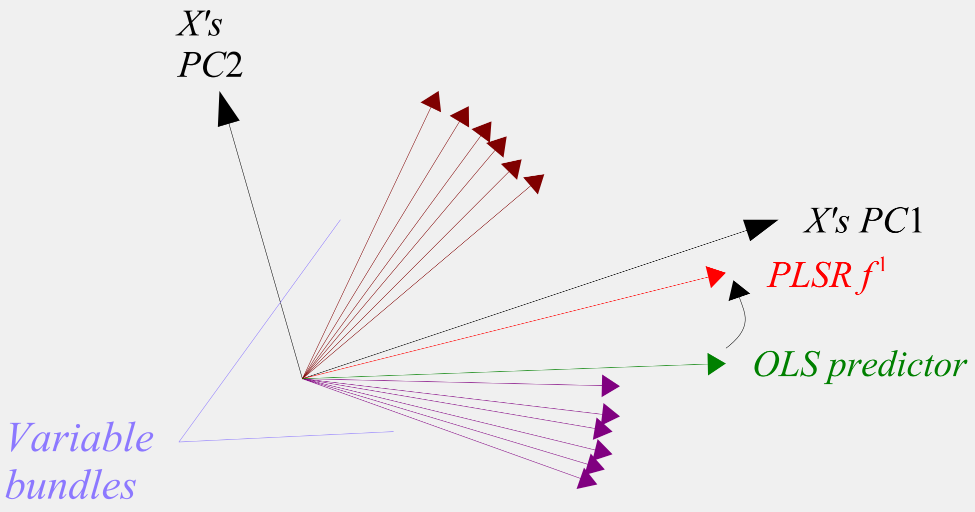
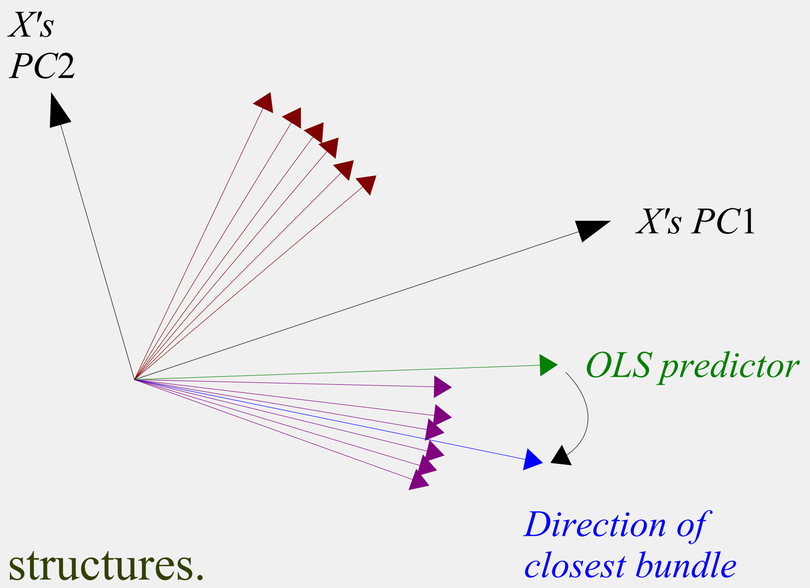


What we would like to happen :



A PC is too ***global*** a direction to fit bundle structures.

□ We must go beyond component variance.

Structural Relevance of components

2. Structural relevance of components

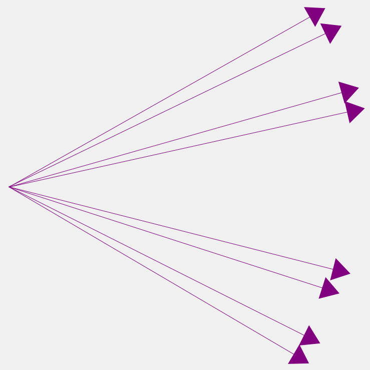
- **Purpose of *l* = ?**

$$\phi(v) := \left(\sum_{j=1}^{J} \omega_j (v' N_j v)^l \right)^{\frac{1}{l}}$$

l : tunes the "locality" of the bundles of directions to focus on

locality = ± the "width" of the bundles of directions considered structurally interesting.

Had this set of directions rather be considered...



How THEME works

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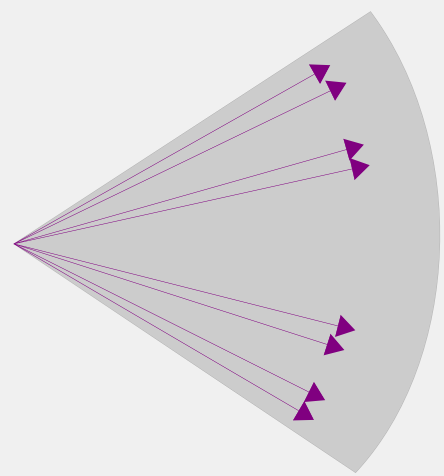

... one bundle? (*l* <<)

How THEME works

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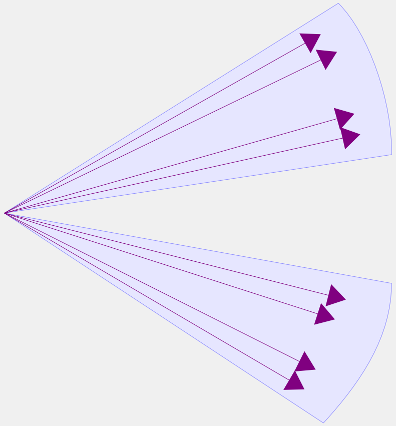

... two bundles? ($l \uparrow$)

How THEME works

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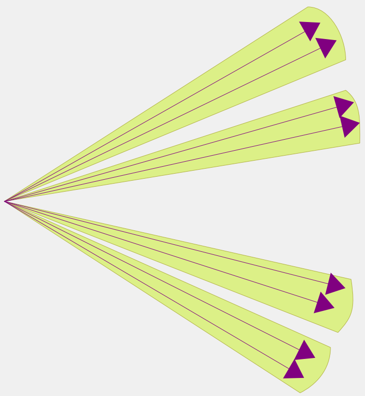

... four bundles? (l ↑↑)

How THEME works

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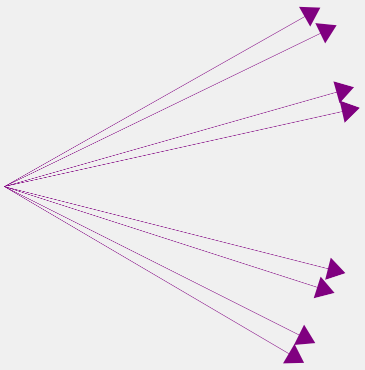

... eight bundles, each one being a single direction? ($l \to \infty$)

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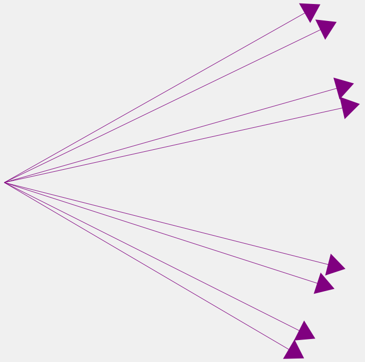


... eight bundles, each one being a single direction? ($l \to \infty$)

This ultimately depends on the data
⇒ Best l to be found through cross-validation.

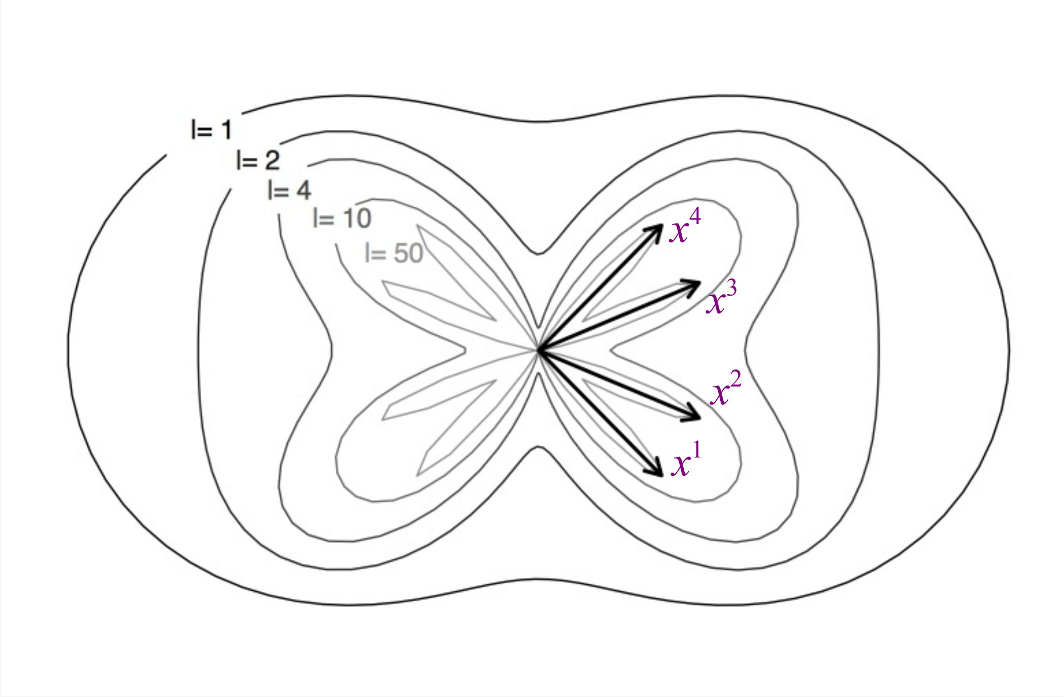
How THEME works

2. Structural relevance of components

l : tunes the "locality" of the bundles of directions to focus on

Example: 4 variables in a plane...

- VPI: $\phi_X^l(v)$ plotted in polar coordinates:



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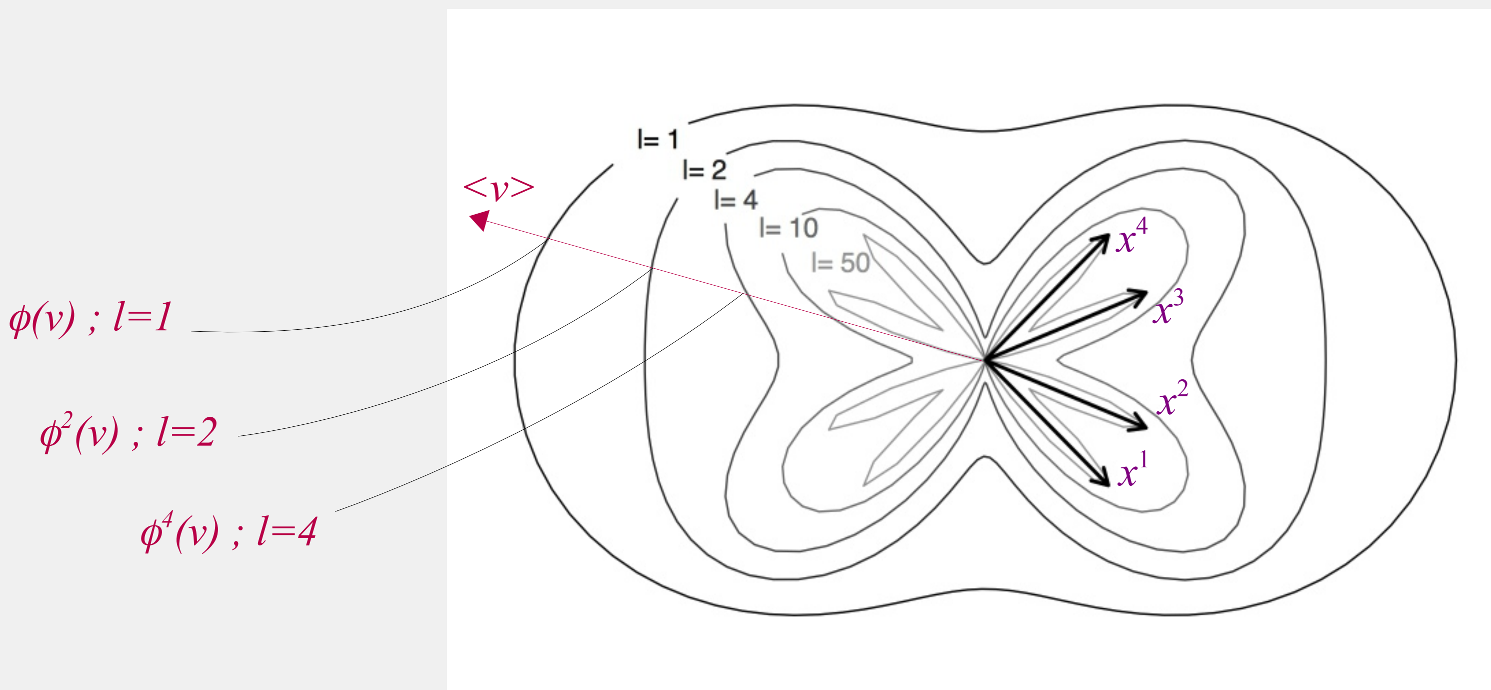

How THEME works

3. Combining goodness of fit ψ and structural relevance ϕ

The criterion to be maximised by a component $f = Xv$, *given ALL others*, must have the form:

$$\boxed{\psi(v)^{1-s}}\,\boxed{\phi(v)^{s}}$$

GoF SR importance given to the SR relative to the GoF .

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GoF SR importance given to the SR relative to the GoF .

$$\nabla \ln\left(\psi(f)\phi(f)^{s}\right)=0 \quad \Leftrightarrow \quad \frac{\nabla\psi(f)}{\psi(f)} = -\frac{s}{1-s}\frac{\nabla\phi(f)}{\phi(f)}$$

+1% on ϕ is compensated by -s/(1-s)% on ψ

Relative variations compensate at optimum

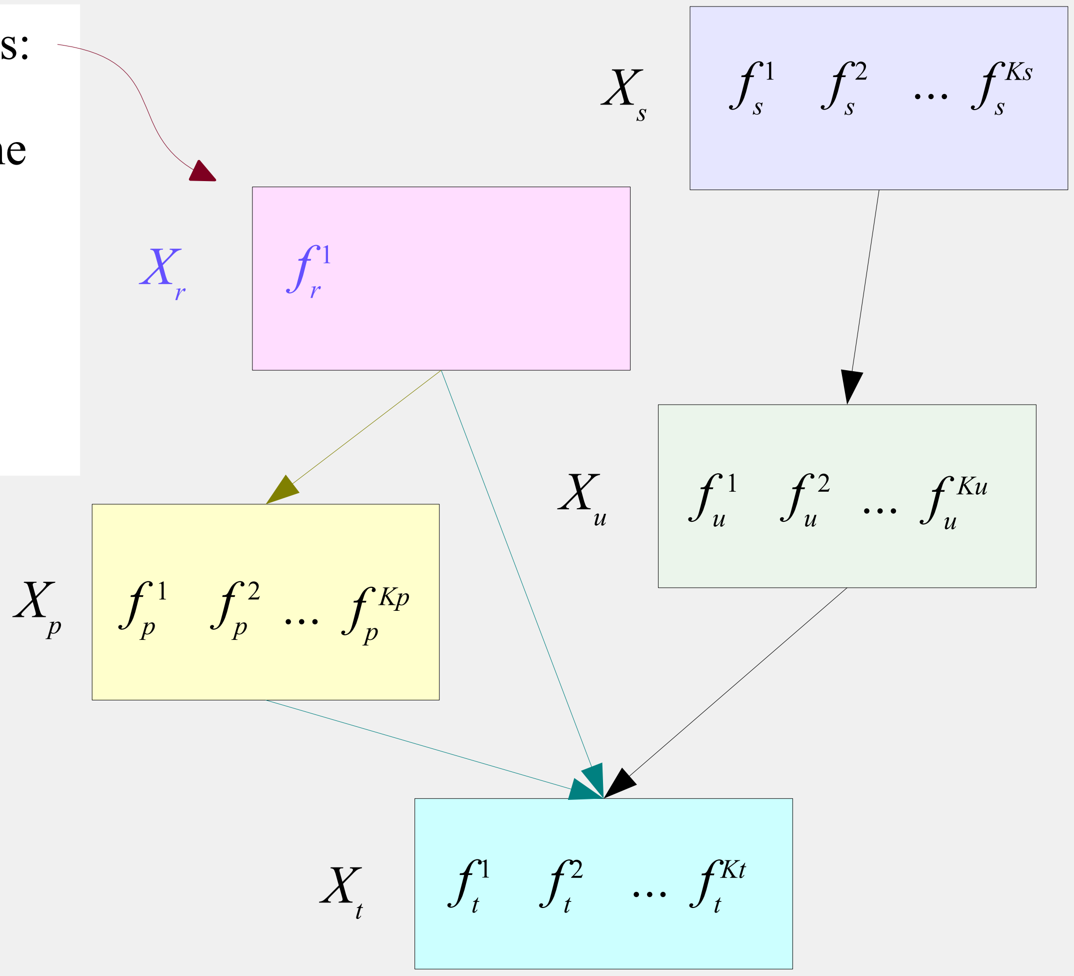
How THEME works

4. Algorithm → component hierarchy

- **The local-nesting (LocNes) principle:**

In X_r , given all components in other groups:

f_r^1 is the best component with respect to the criterion;



How THEME works

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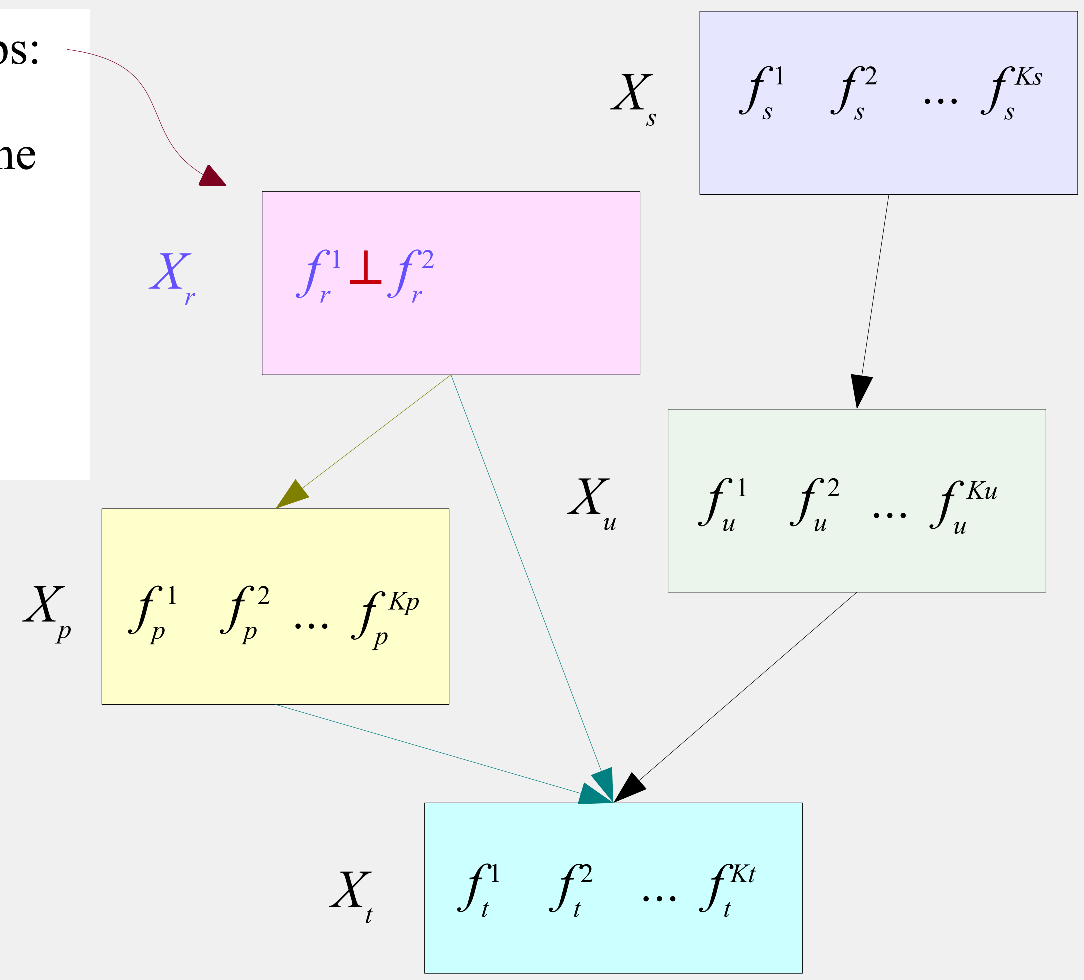

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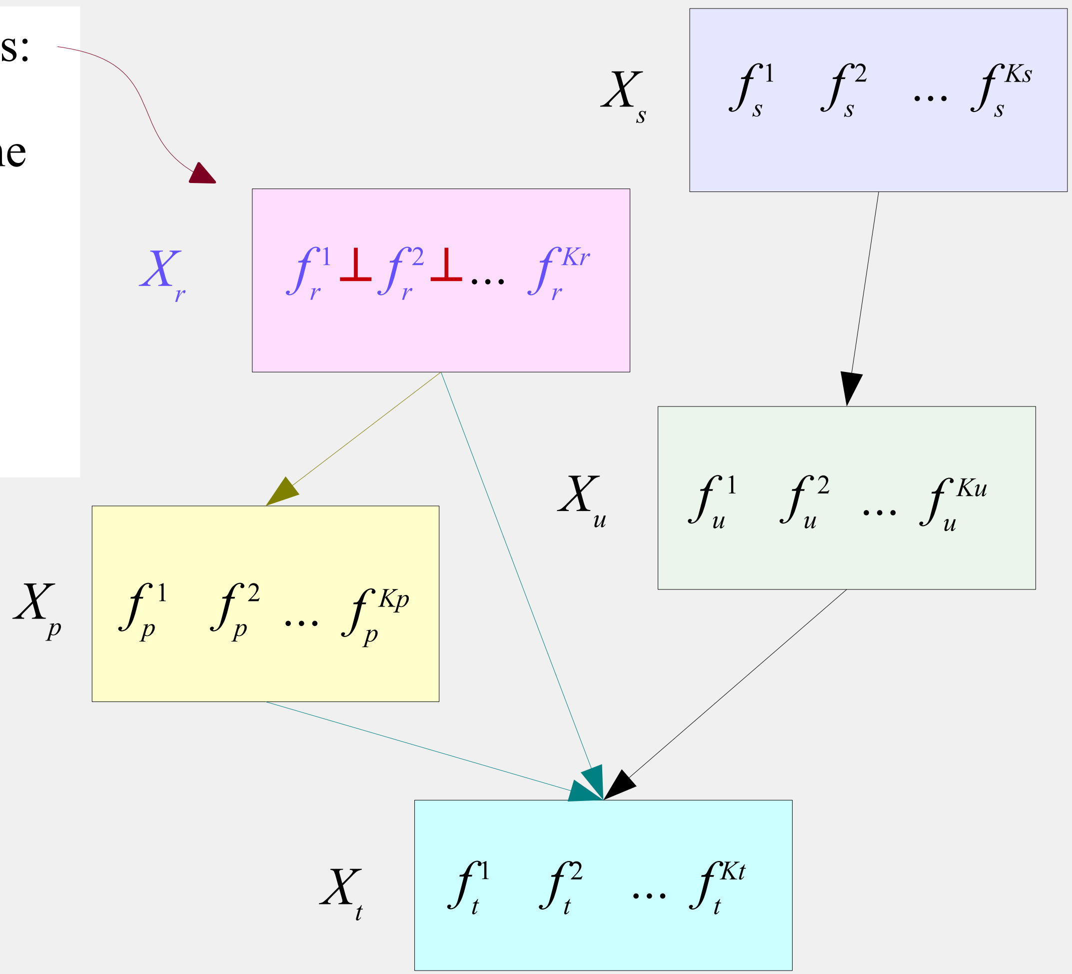

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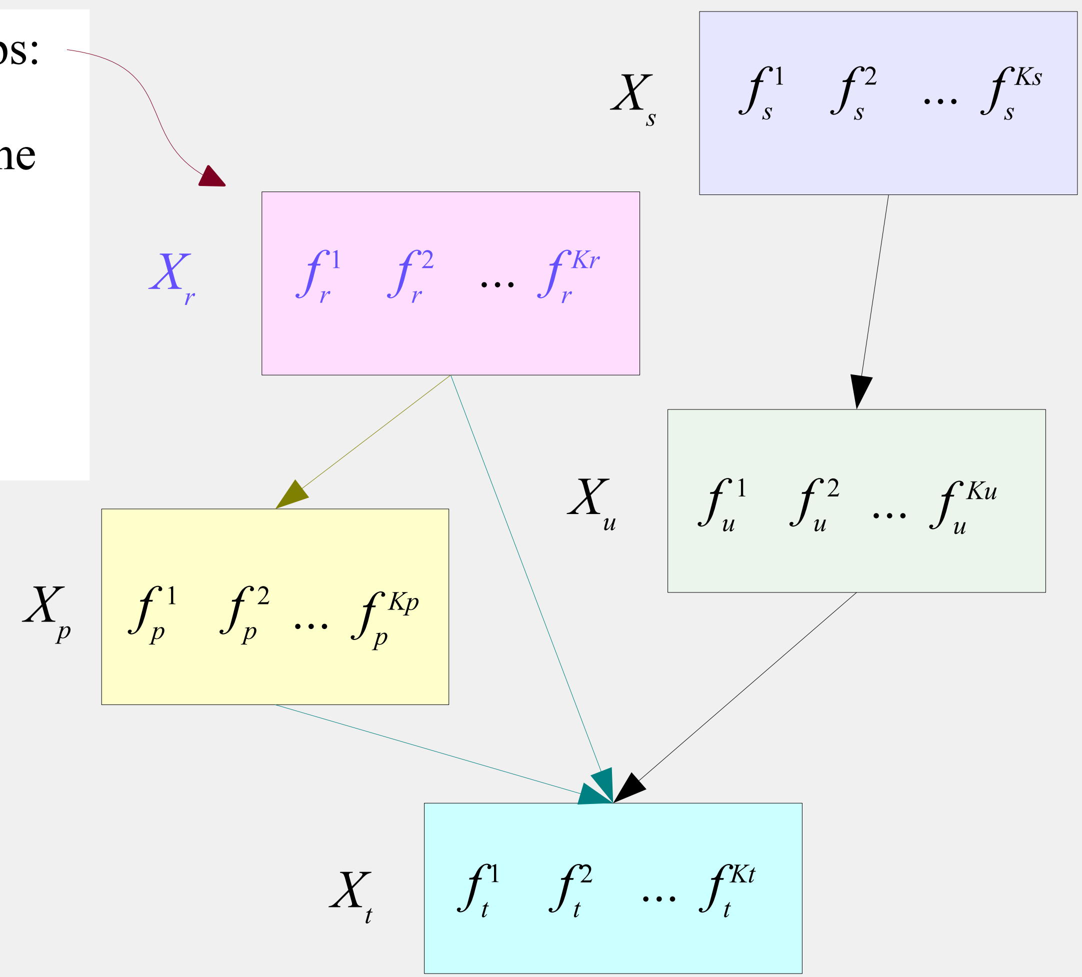


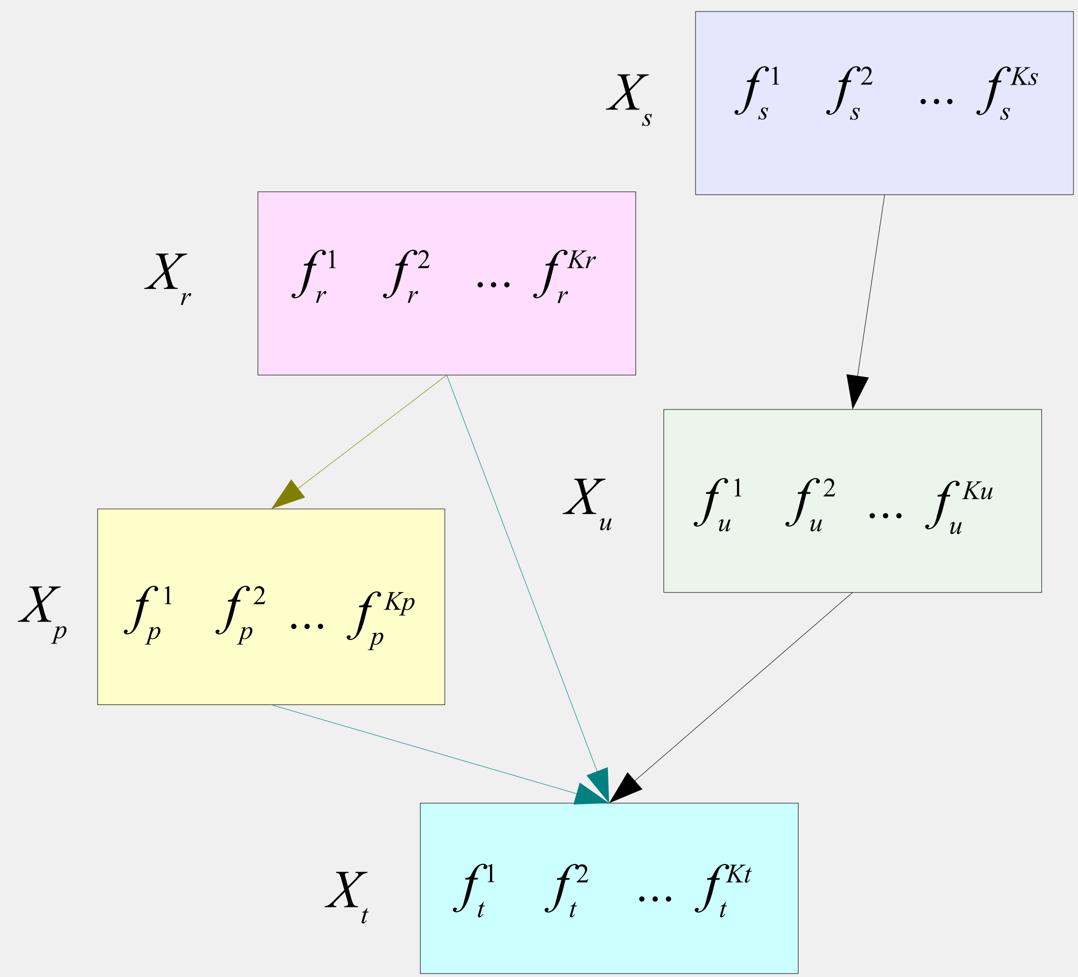
And the algorithm loops over groups X_r until convergence.

How THEME works

5. Backward component selection

- **How to select the suitable number of components in each group?**

Local nesting makes ***backward selection*** natural and easy:



How THEME works

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1) Calculate the model using (too large) K_r components in group X_r.

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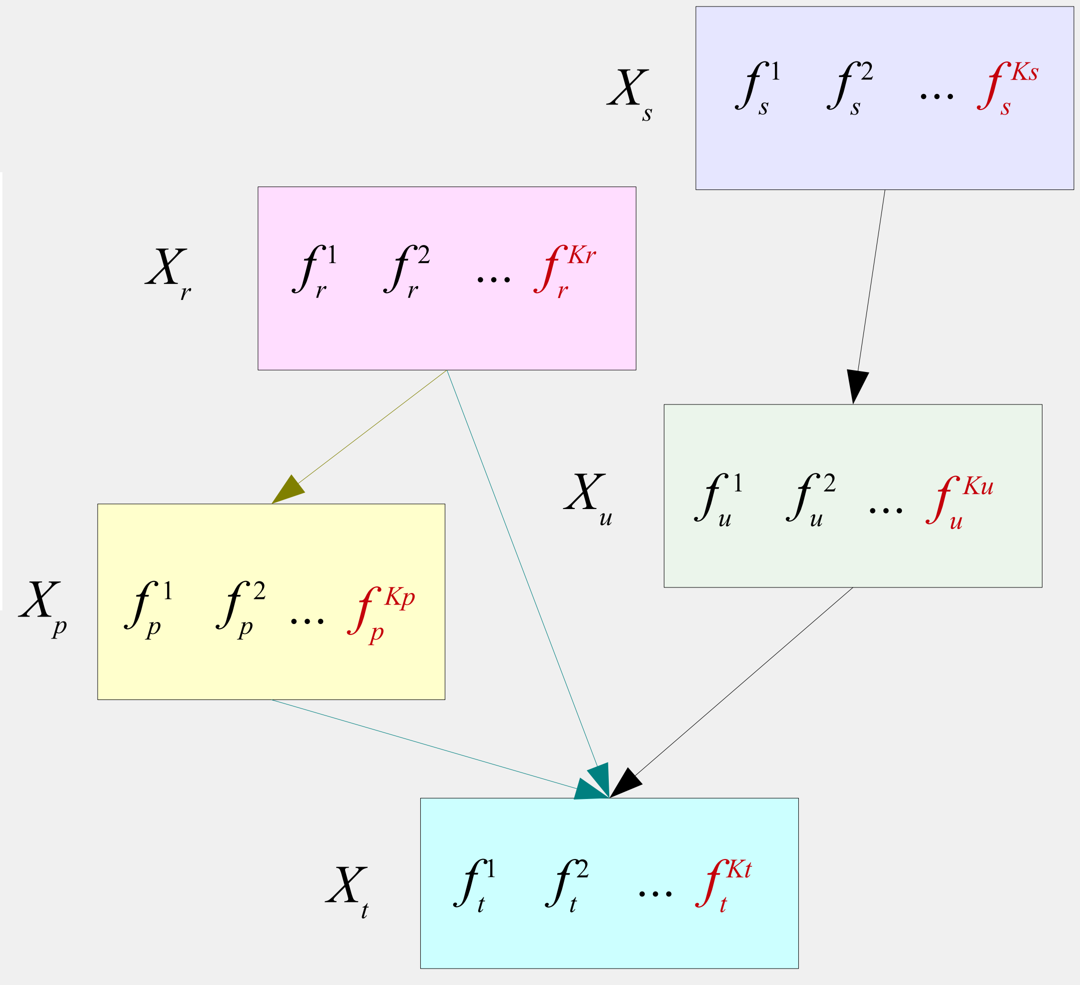

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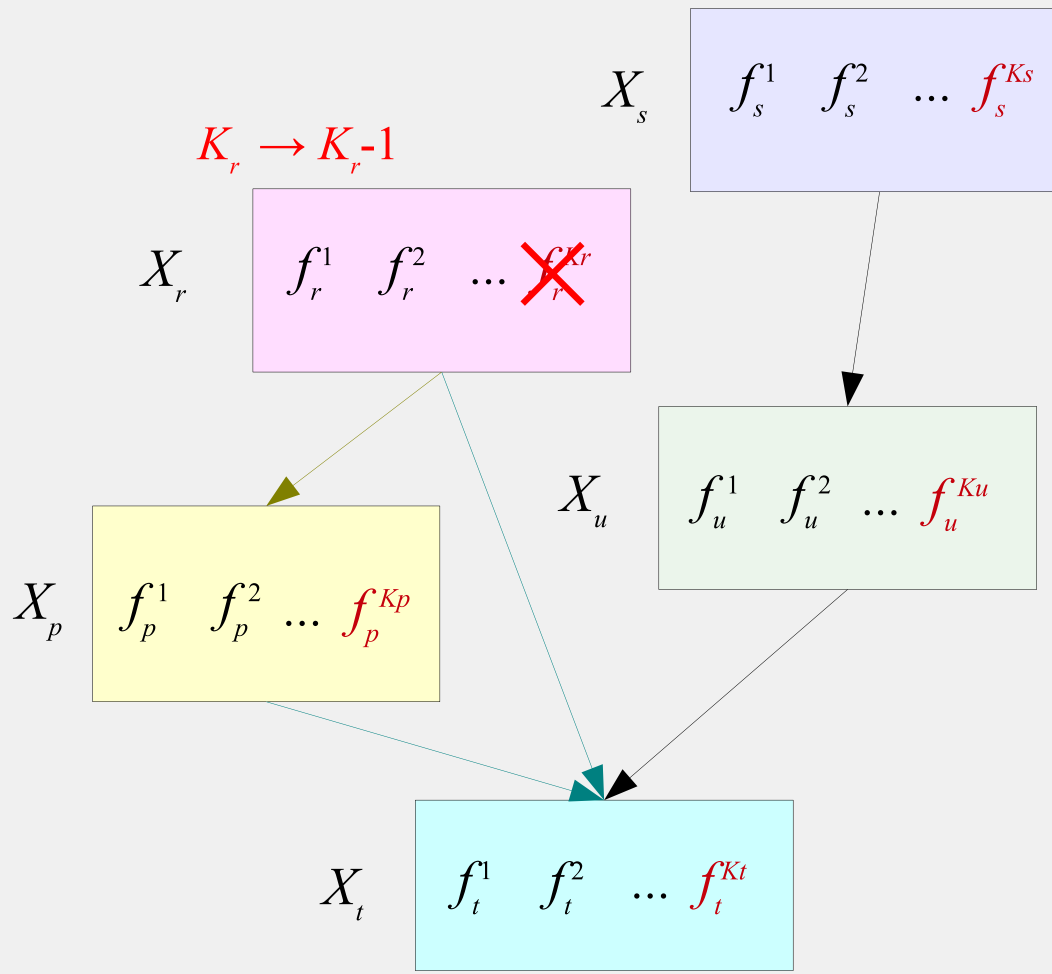
3) Compare these last components between groups with respect to some loss criterion.

4) Discard the least useful last component *if affordable*, and resume (1) with one less component in the corresponding group. Else, stop.



How THEME works

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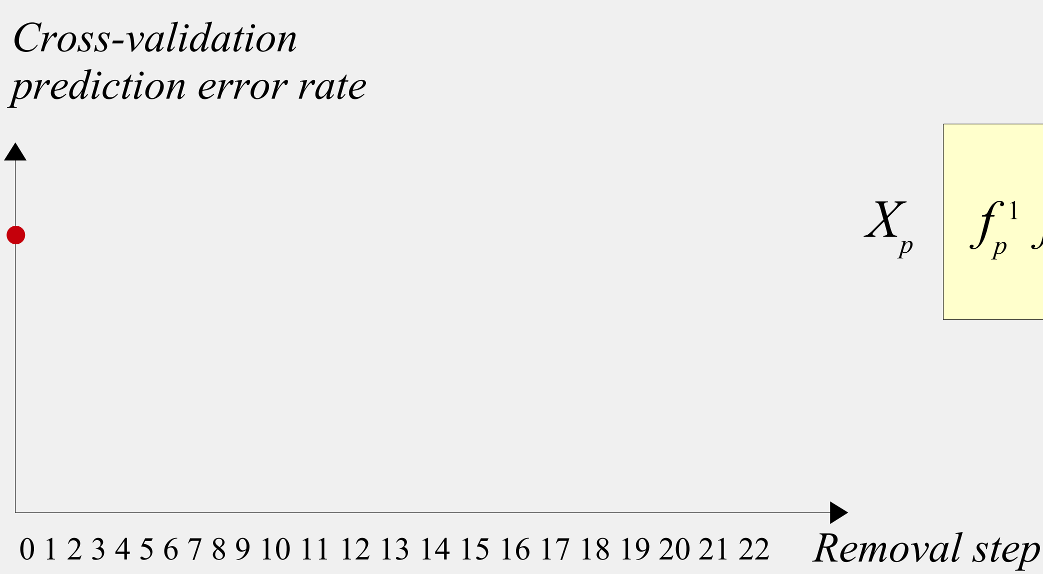
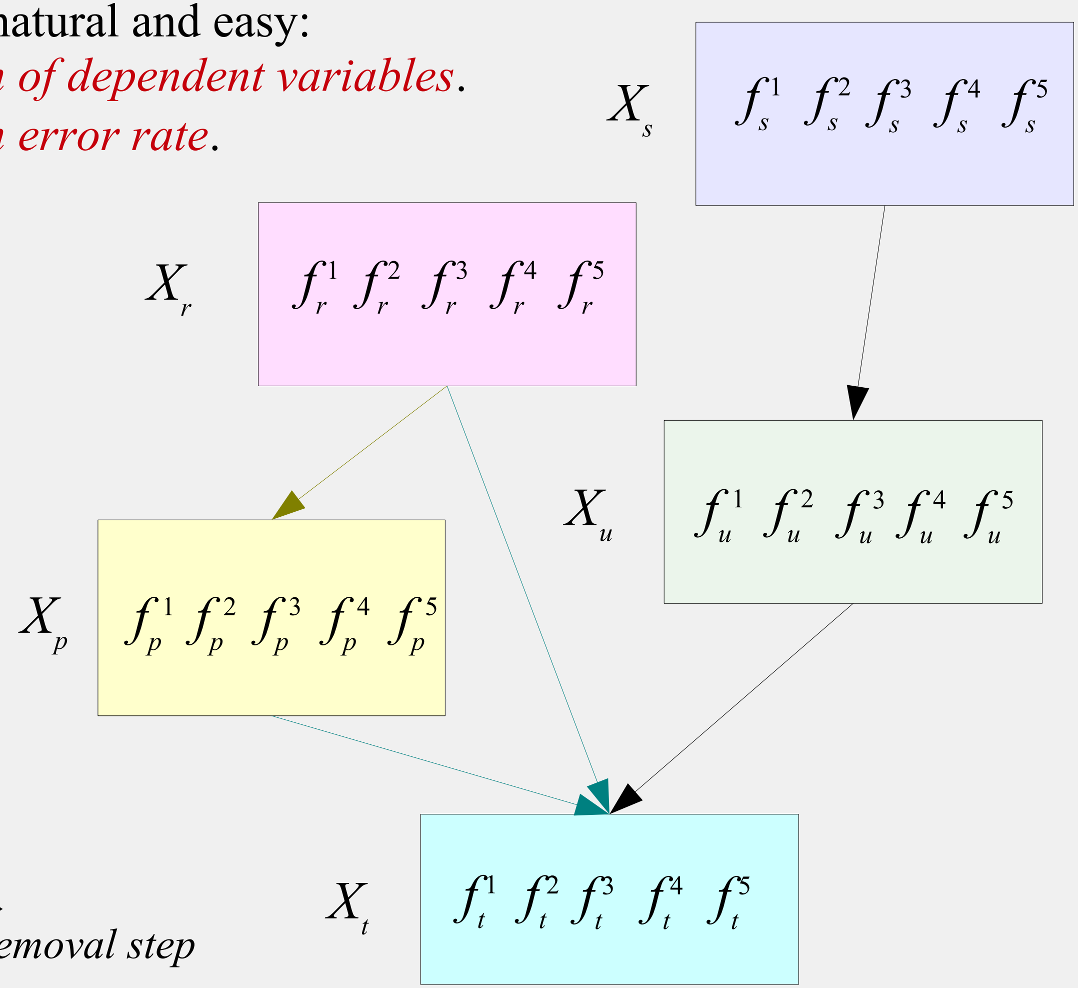
Local nesting makes ***backward selection*** natural and easy:

Explanatory components → *prediction of dependent variables*.

→ *prediction error rate*.

Example:





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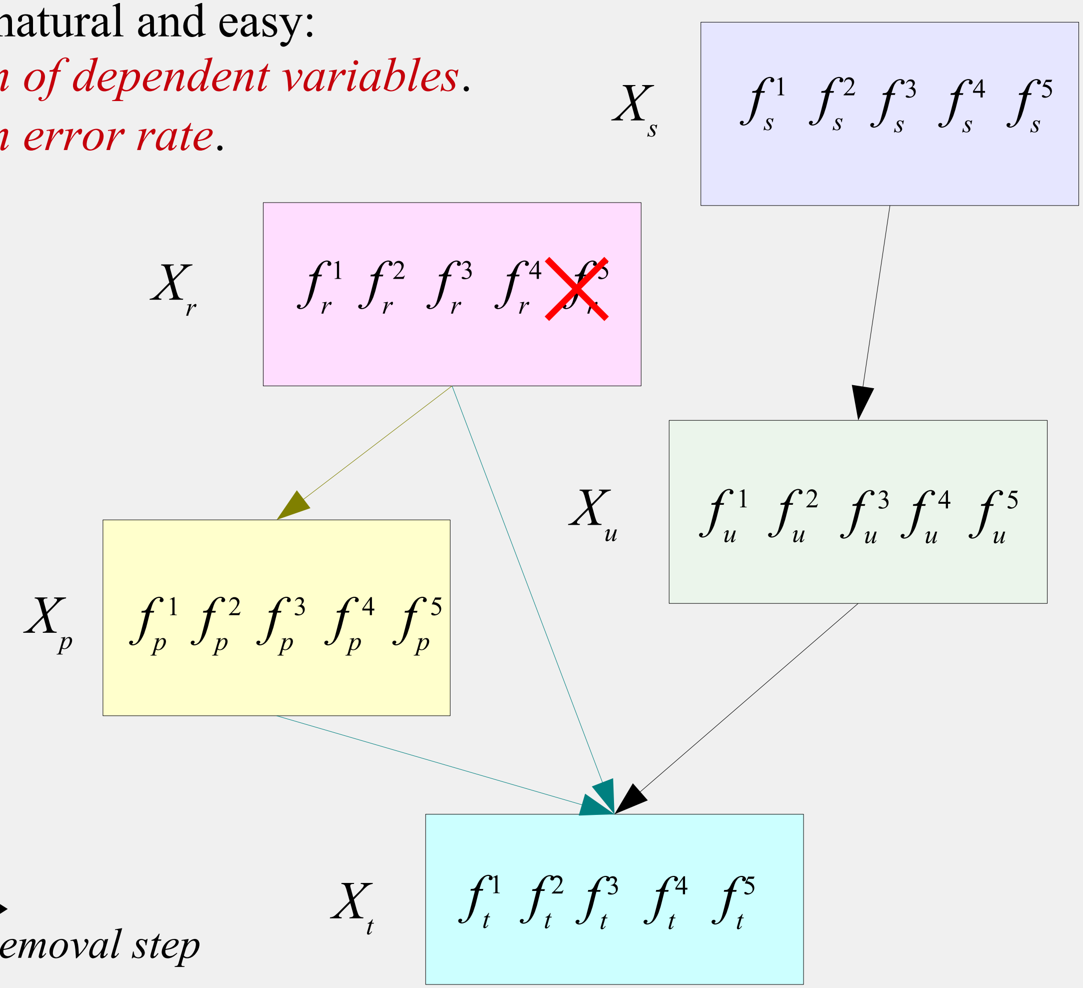

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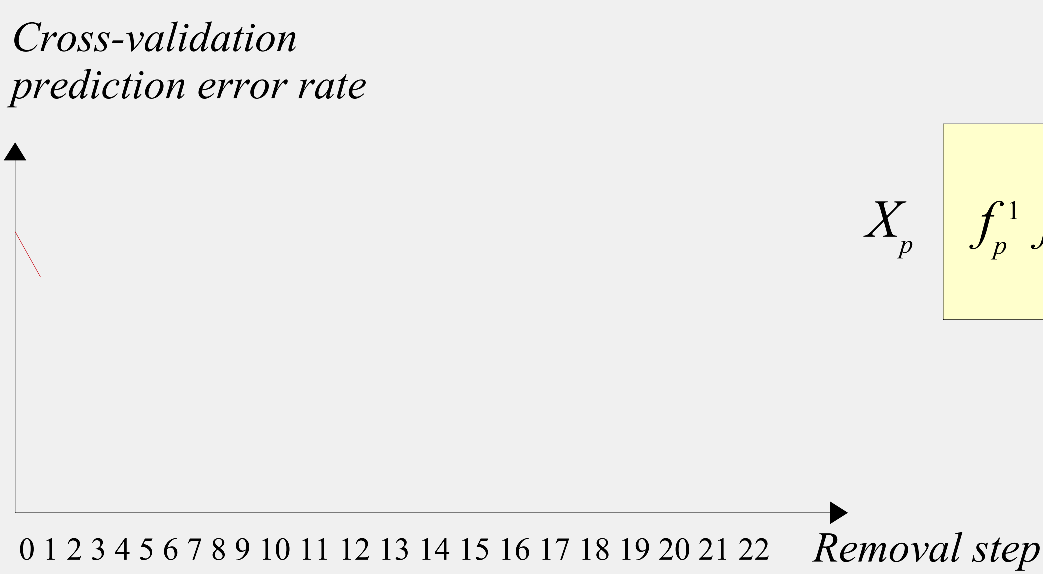

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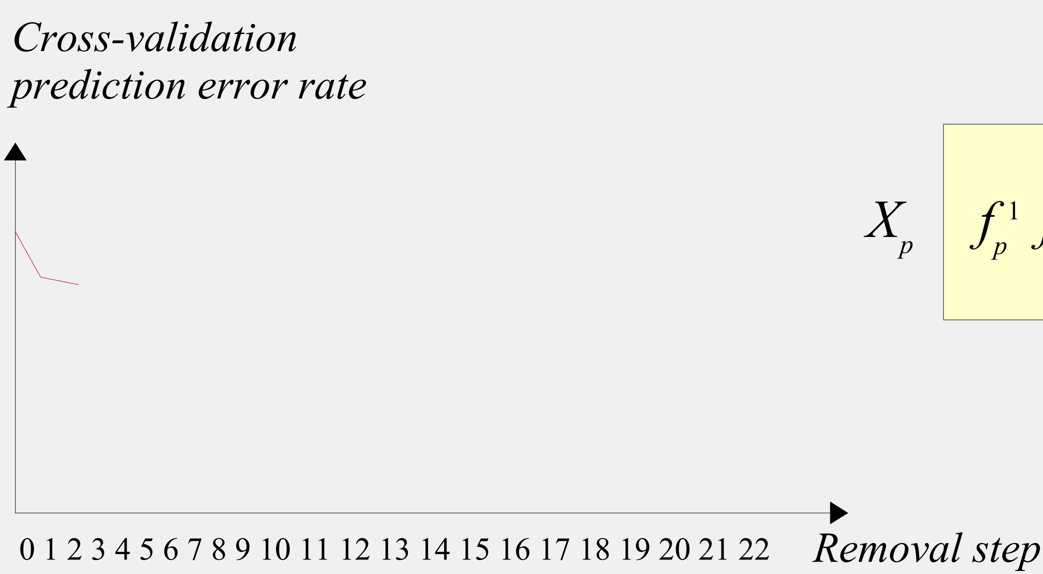

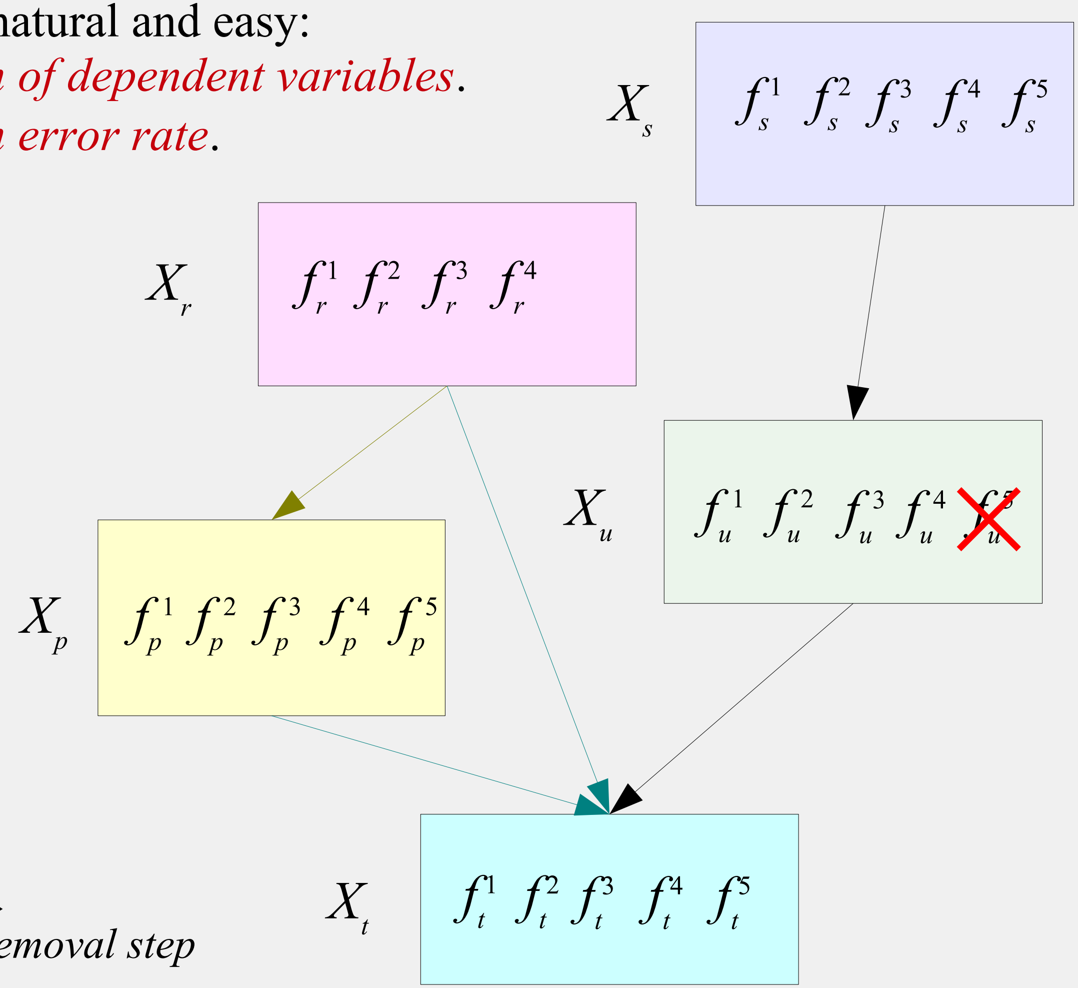

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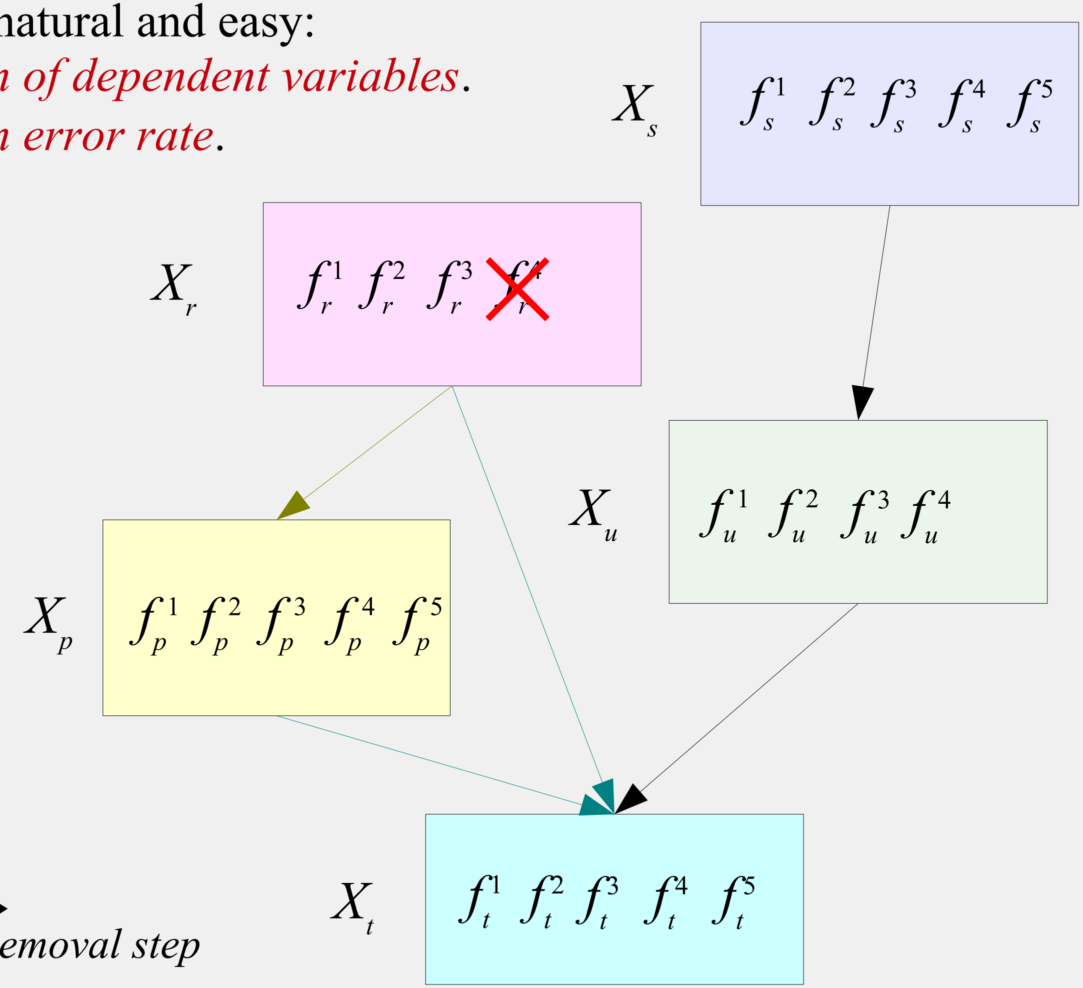
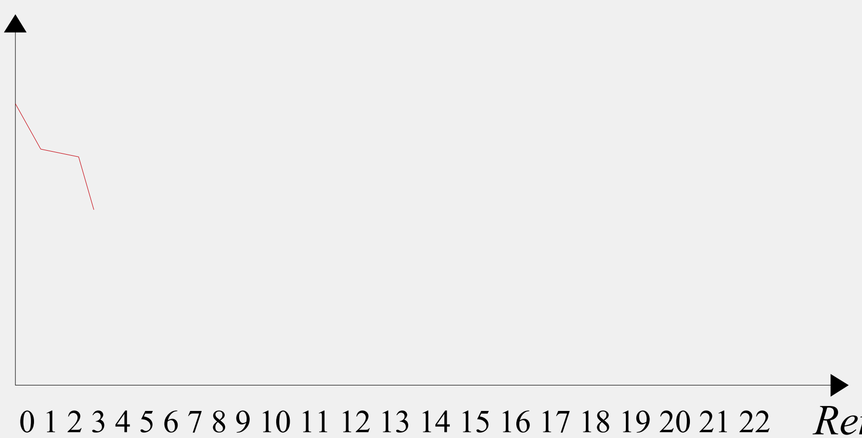


Example:

Cross-validation prediction error rate



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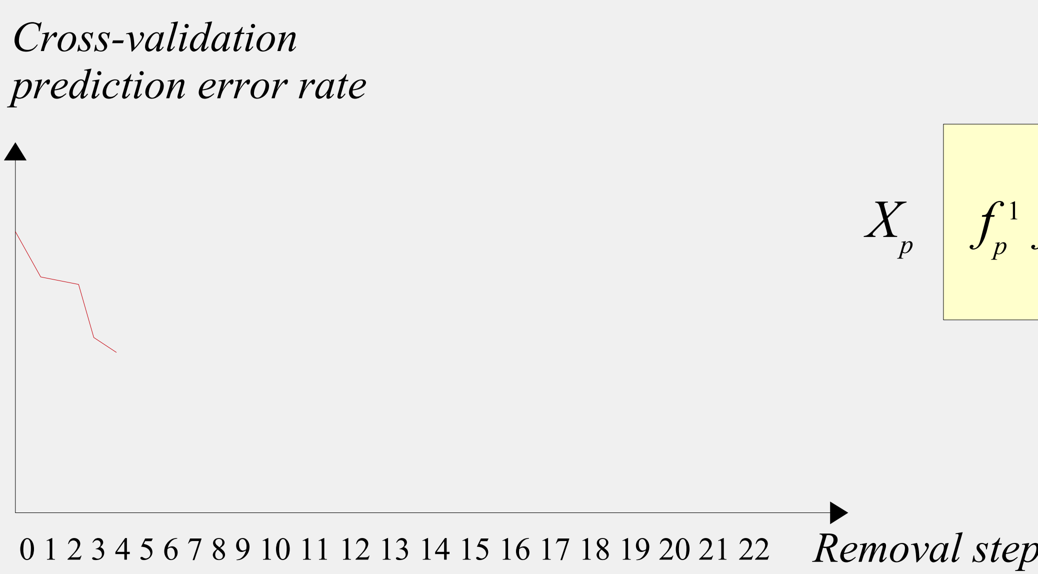

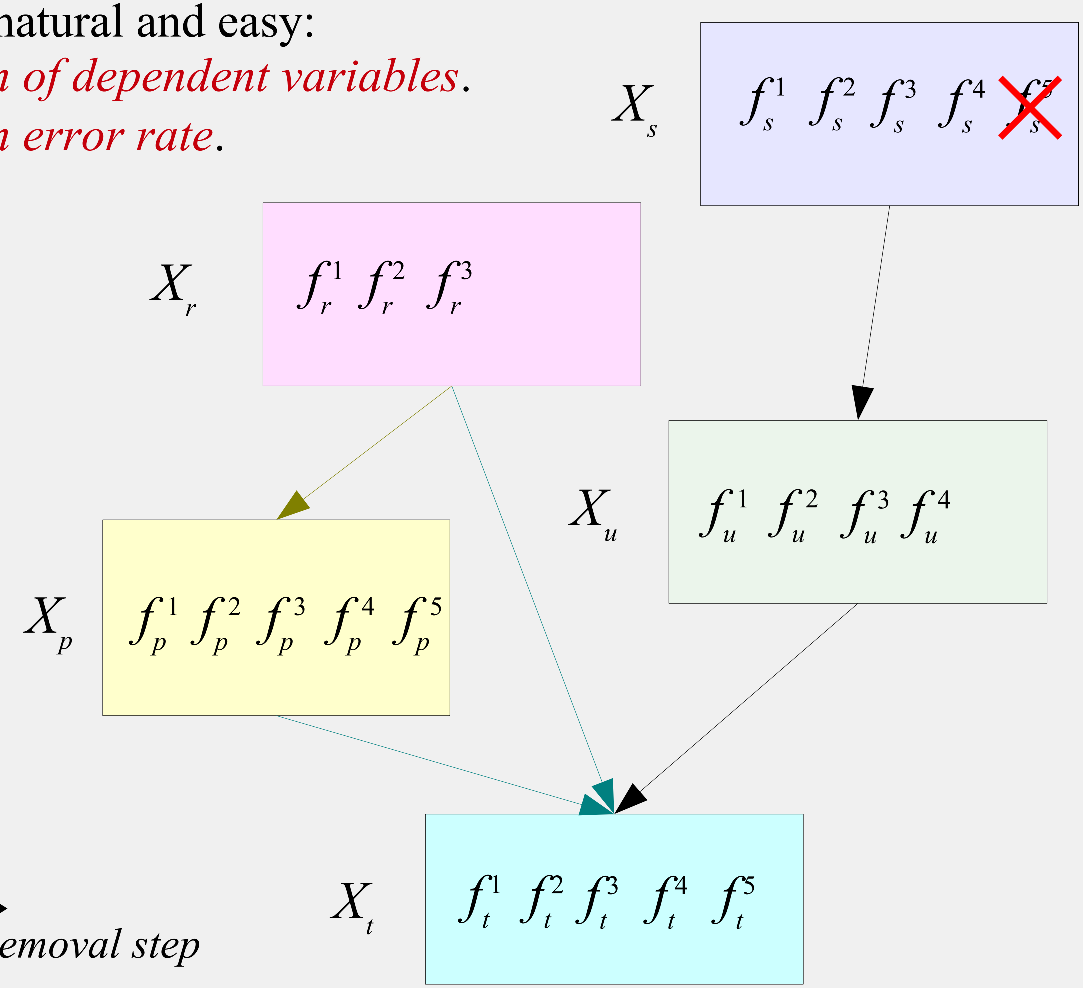

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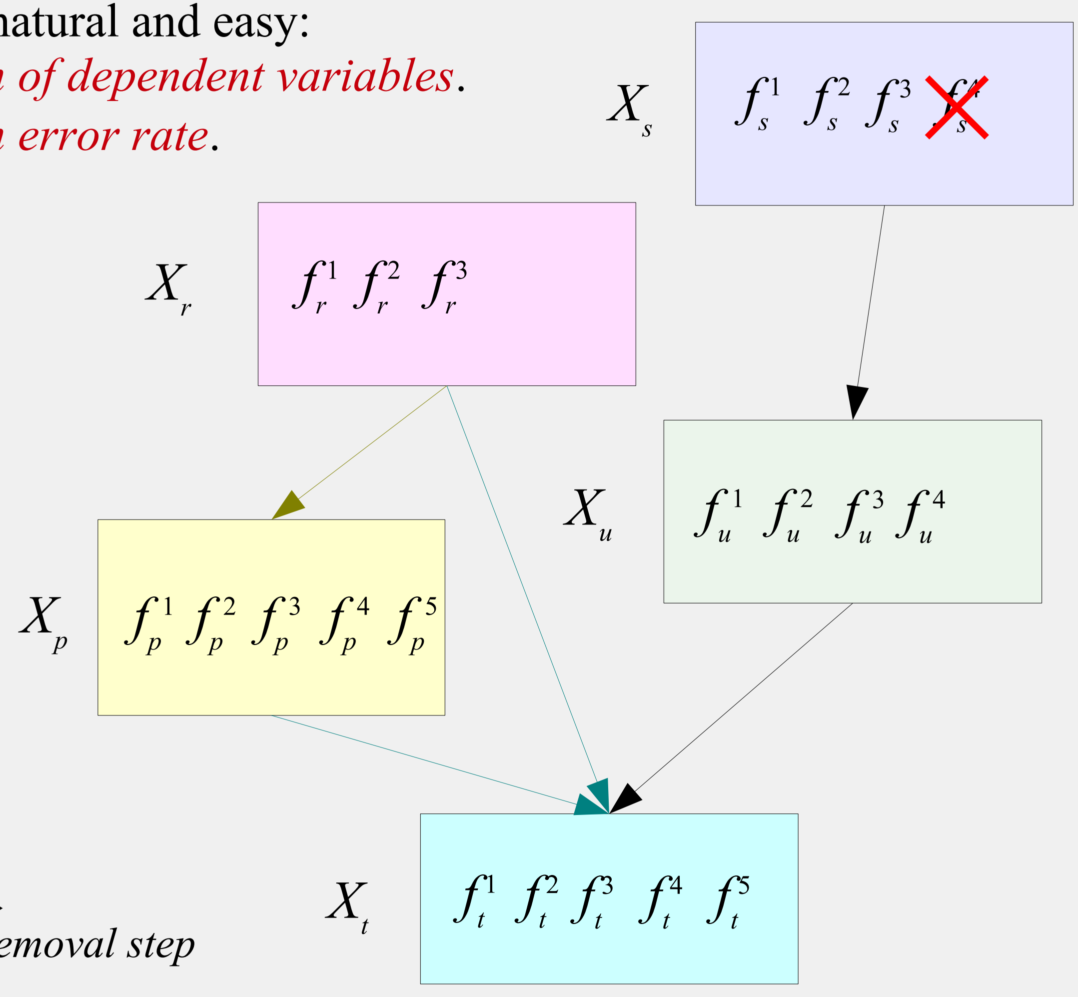

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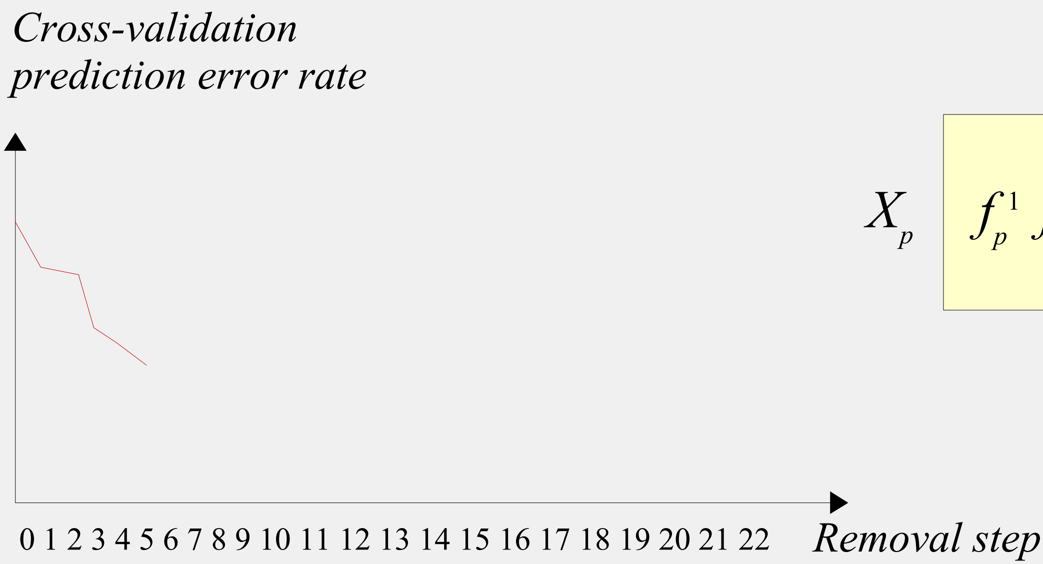

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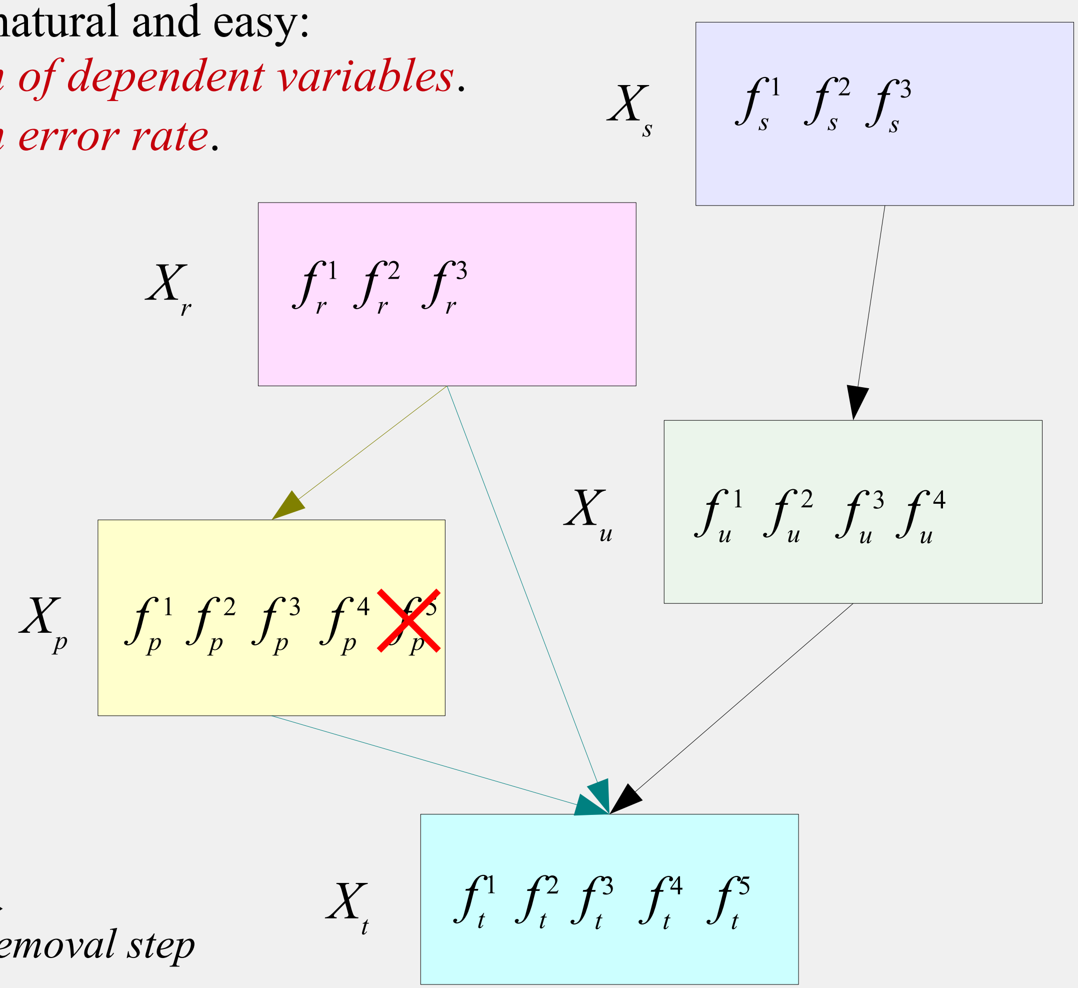

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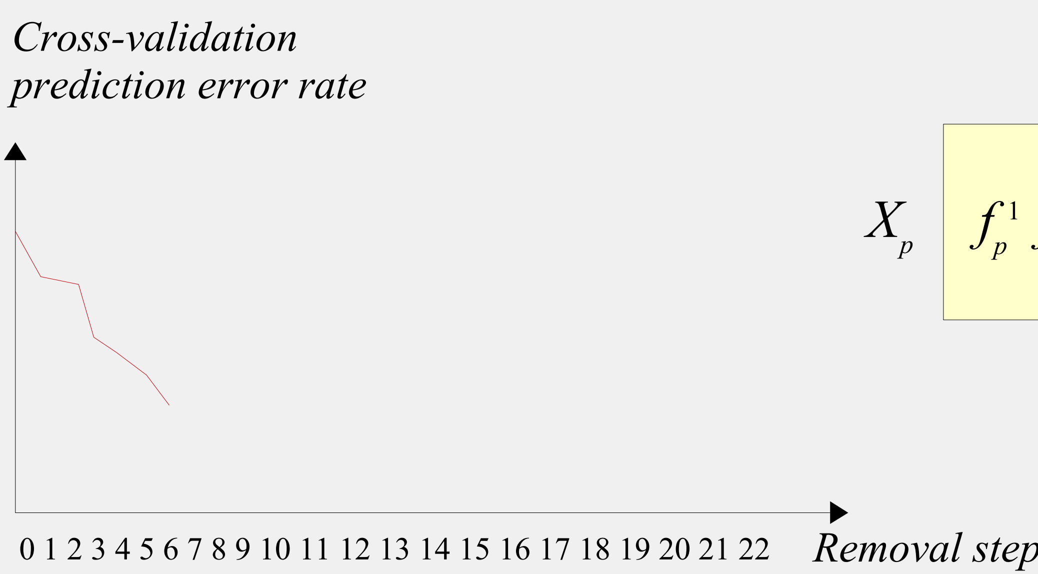

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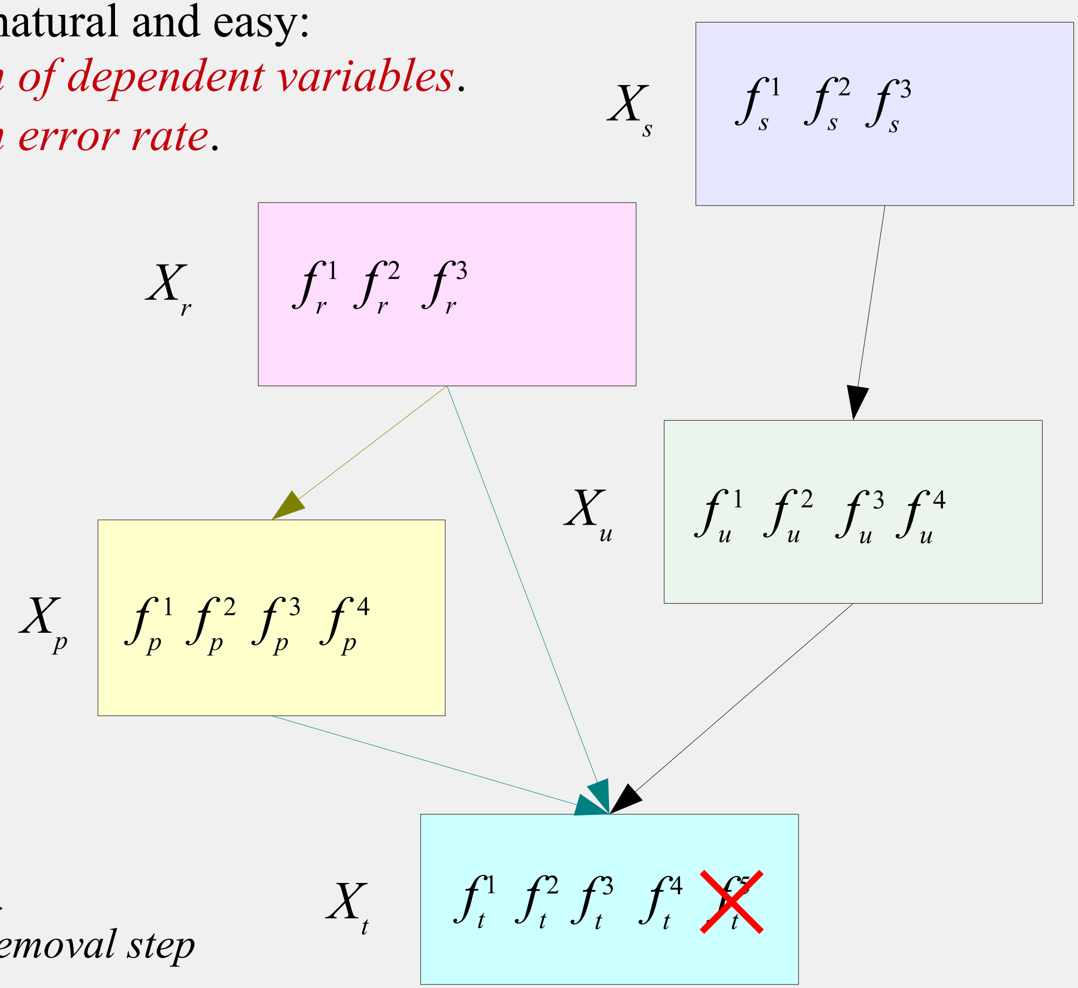

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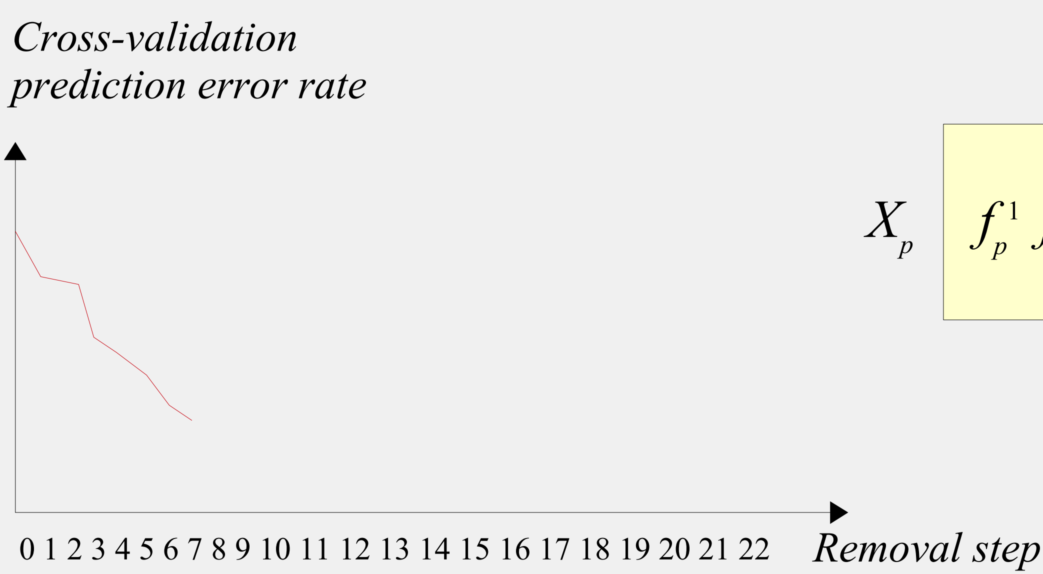

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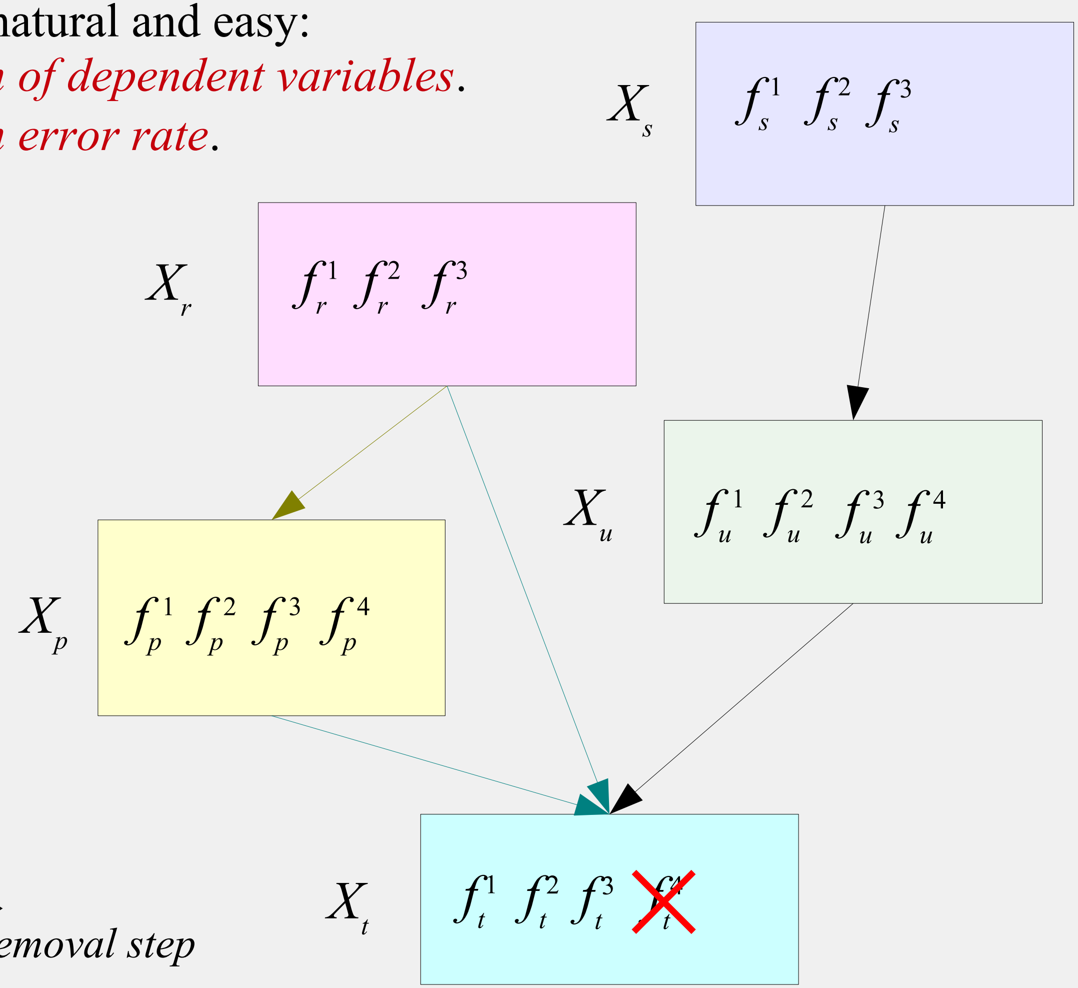

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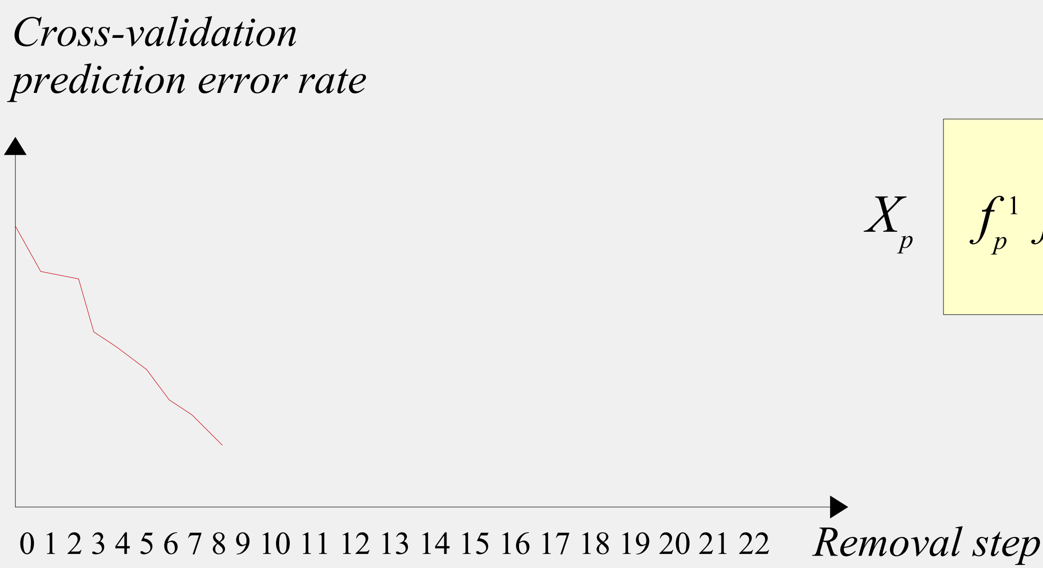

How THEME works

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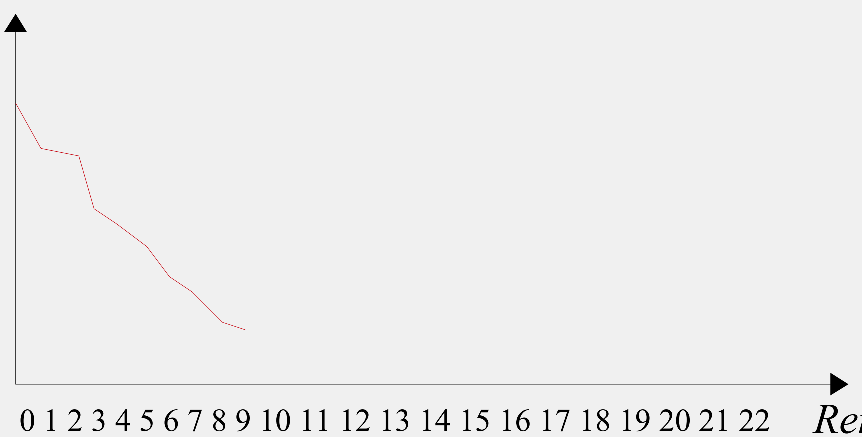
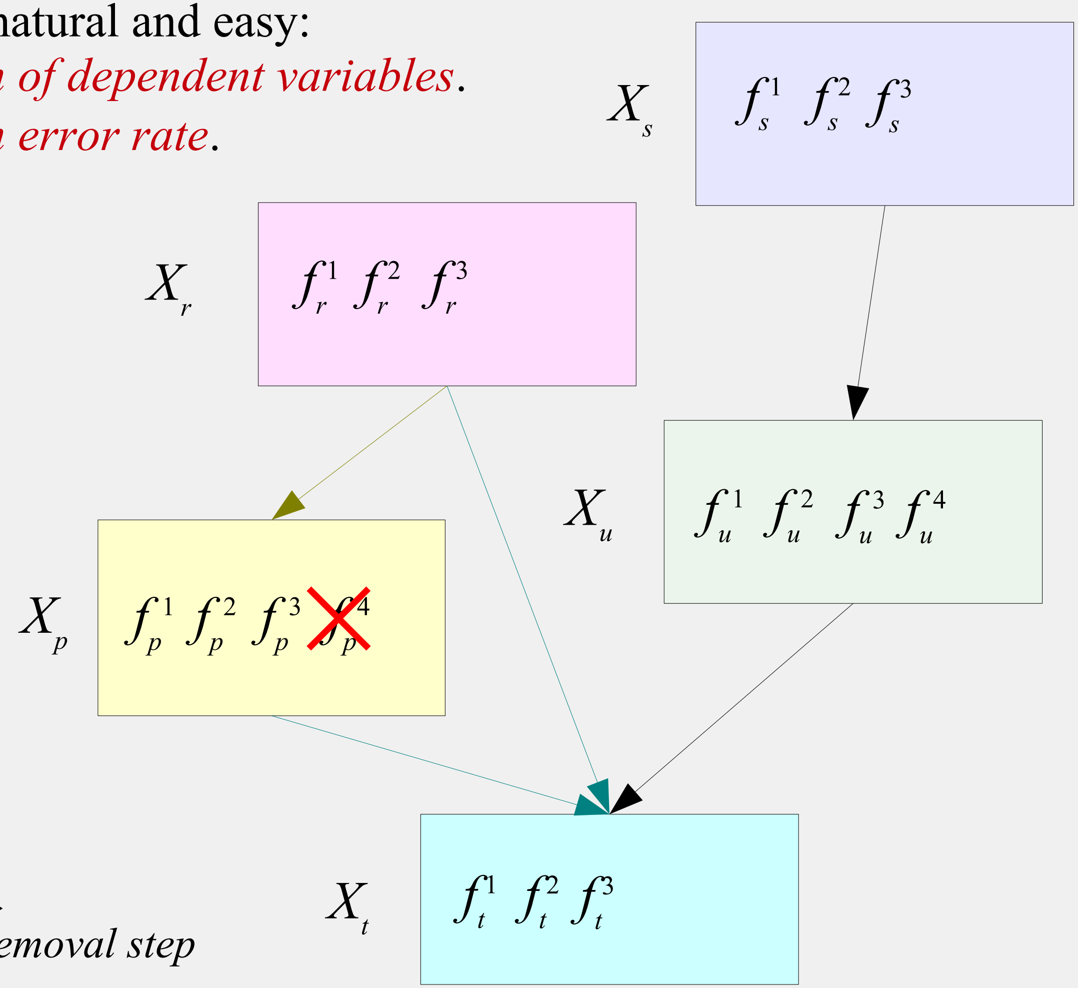
Example:

Cross-validation prediction error rate



Removal step



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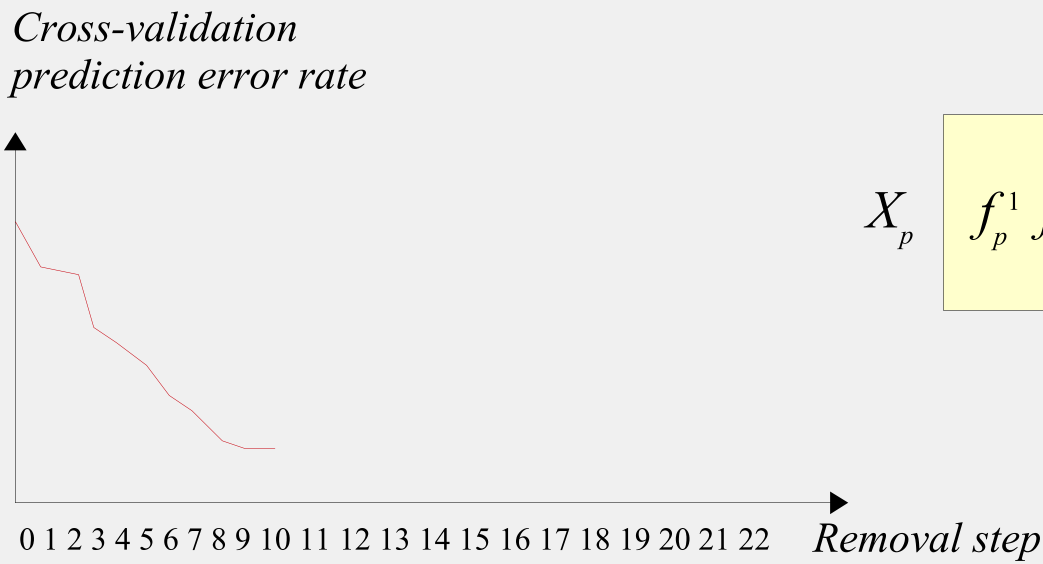

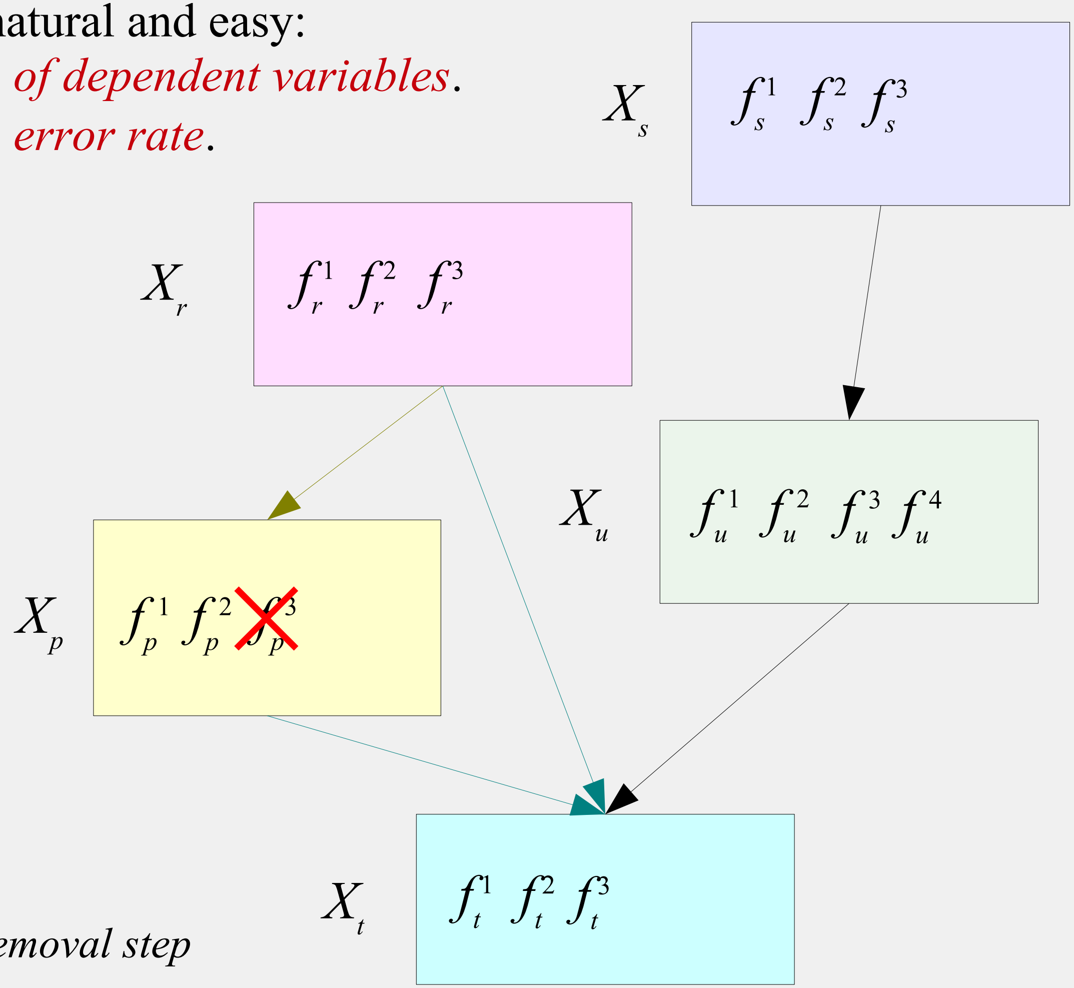

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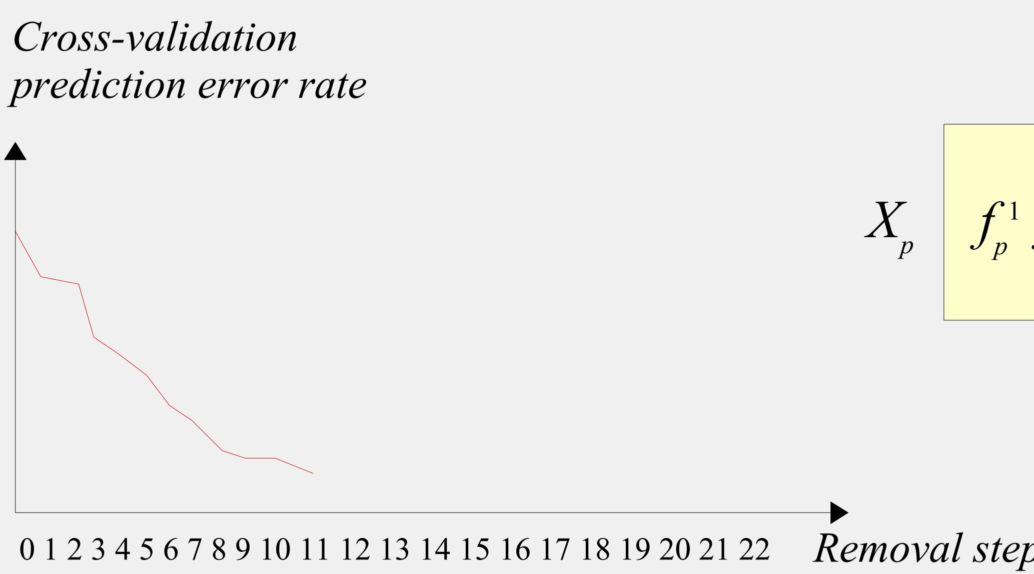

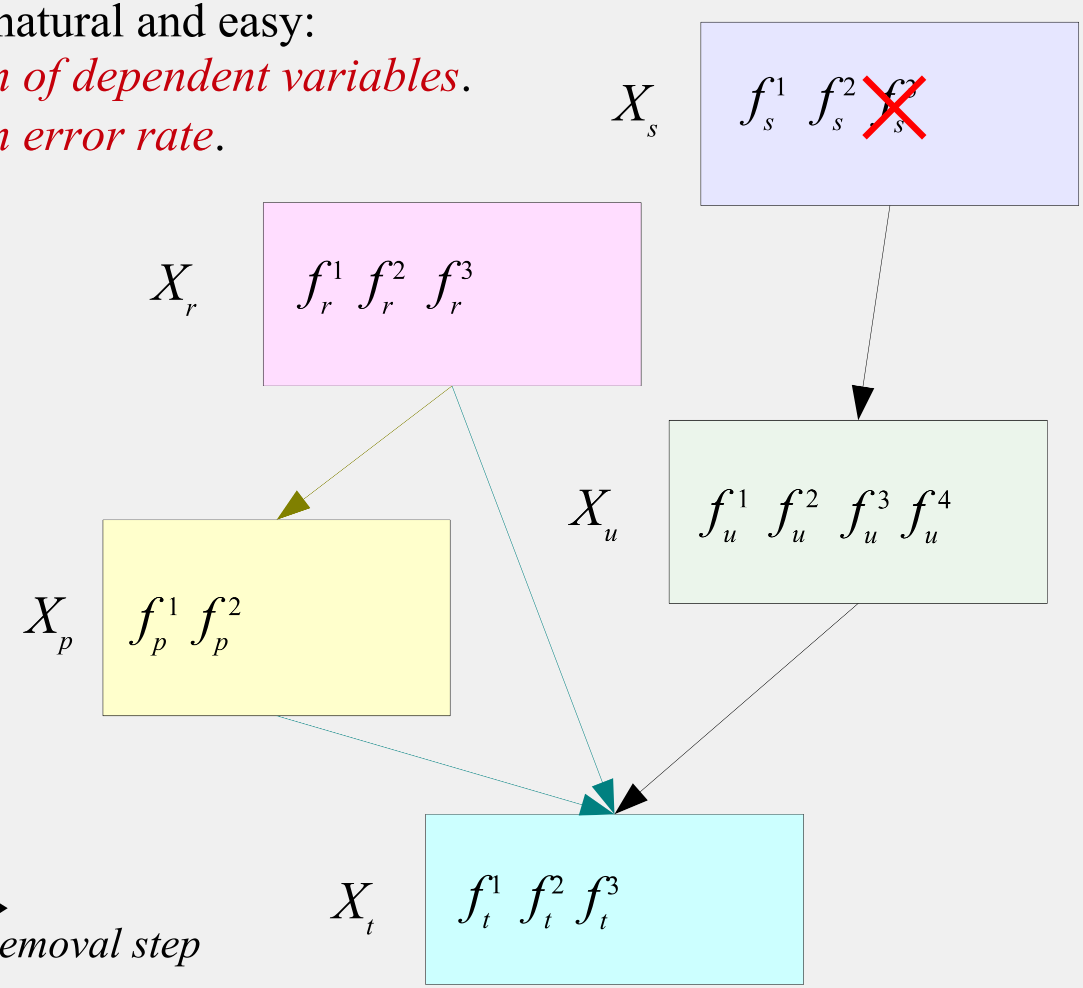

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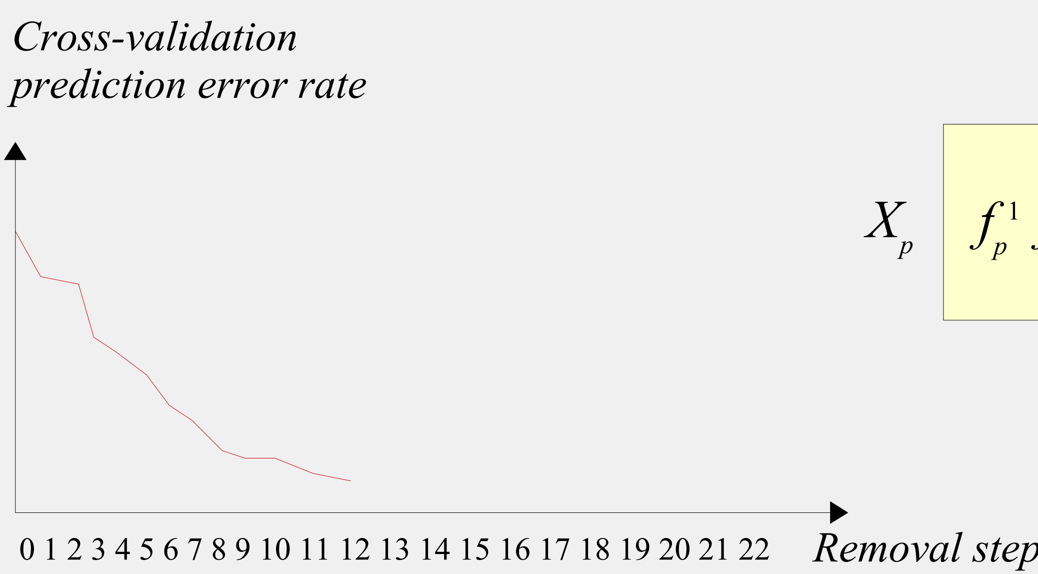

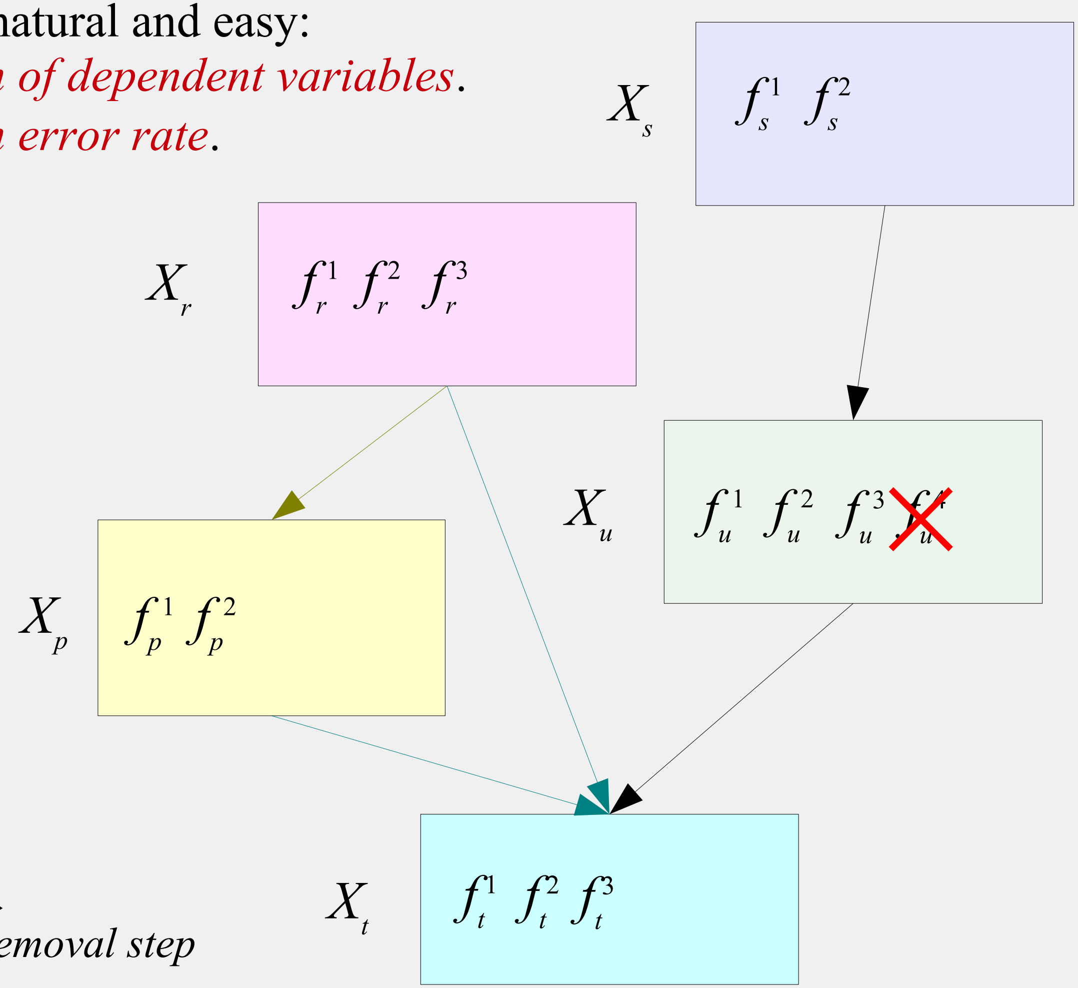

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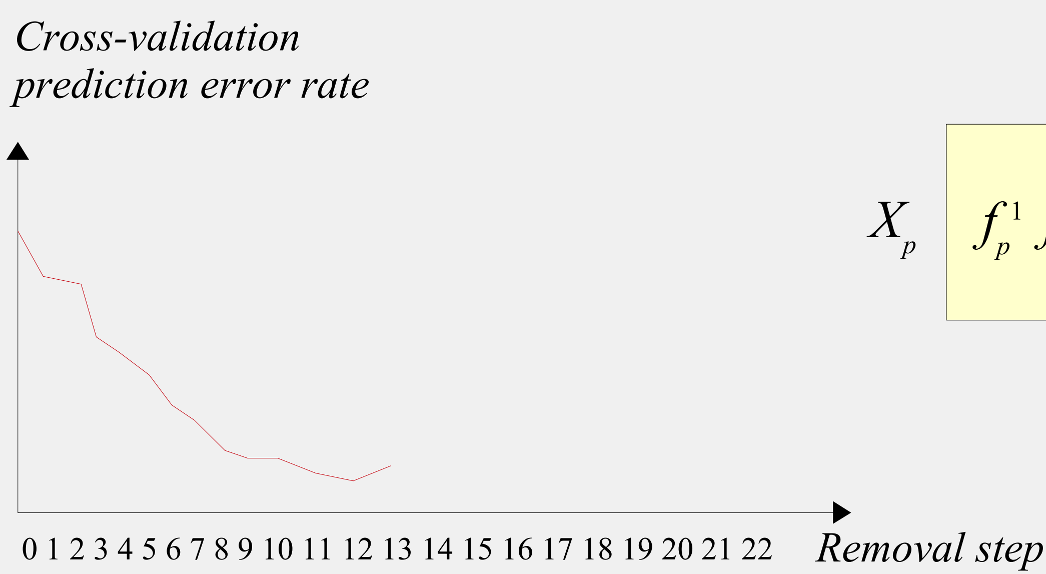

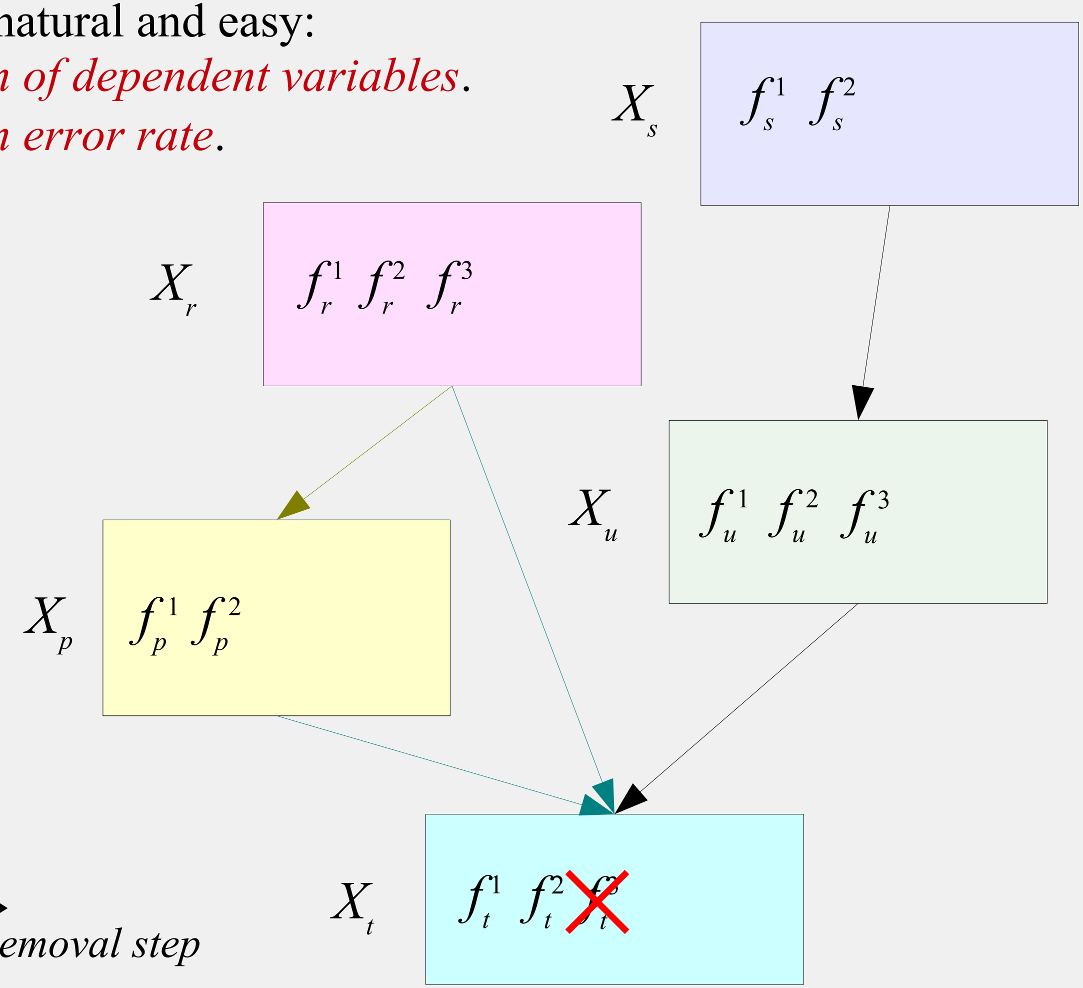

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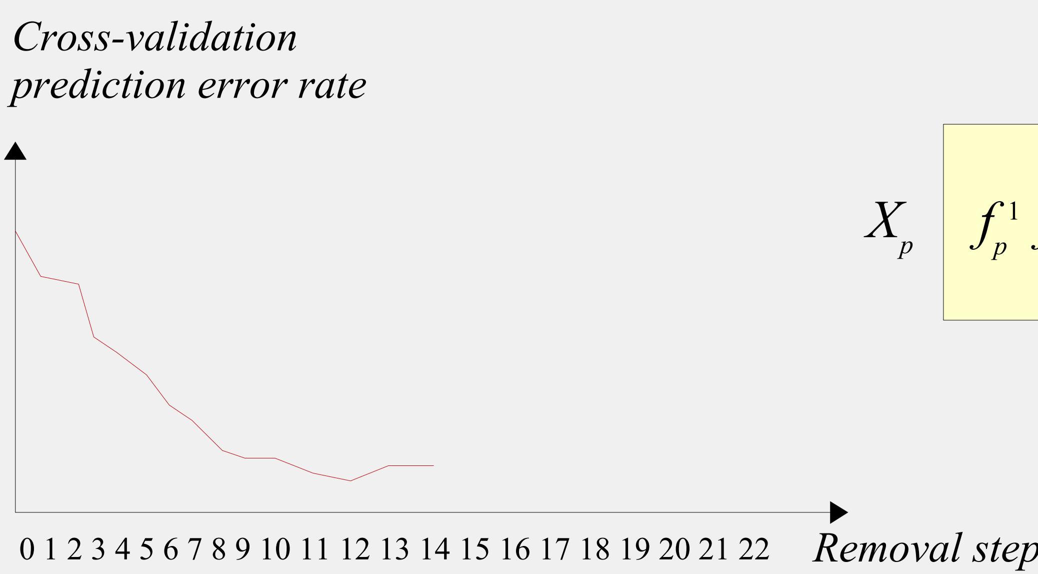

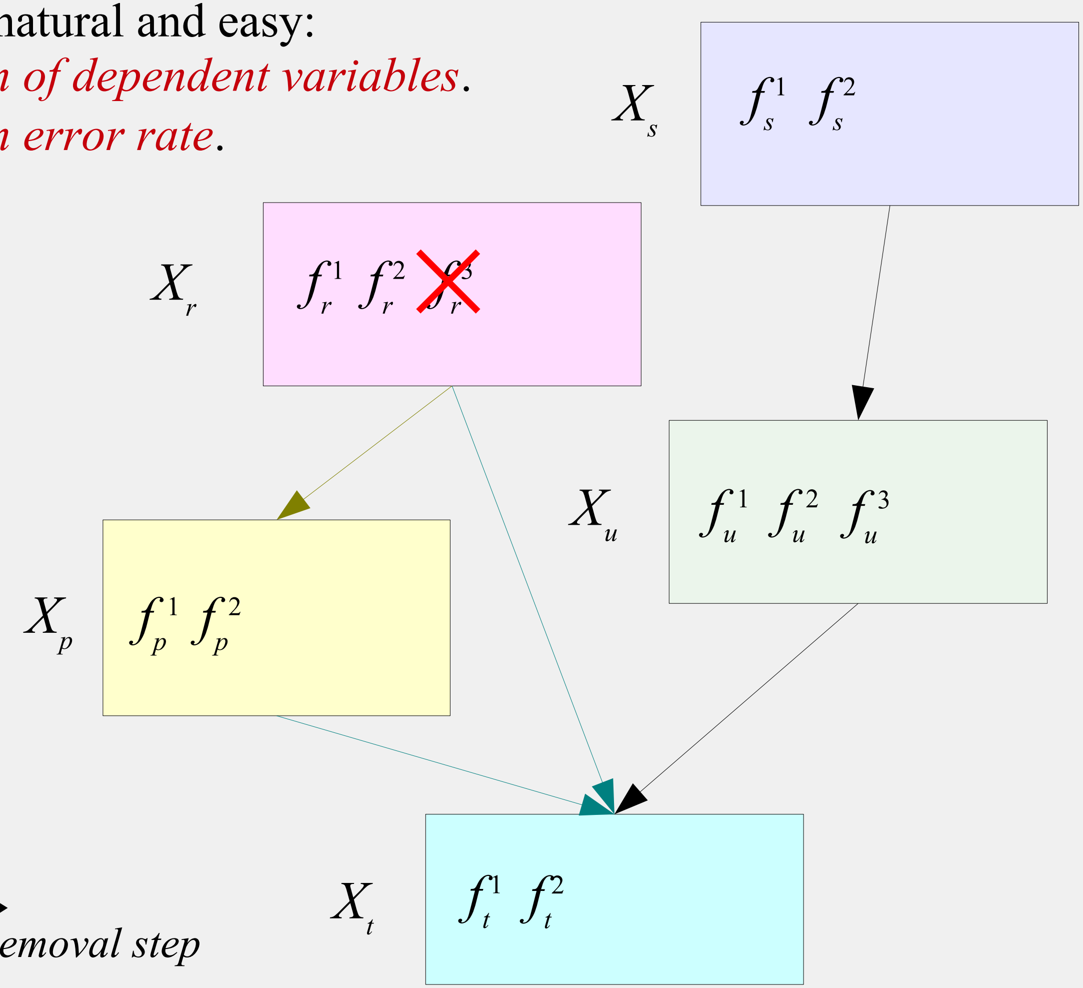

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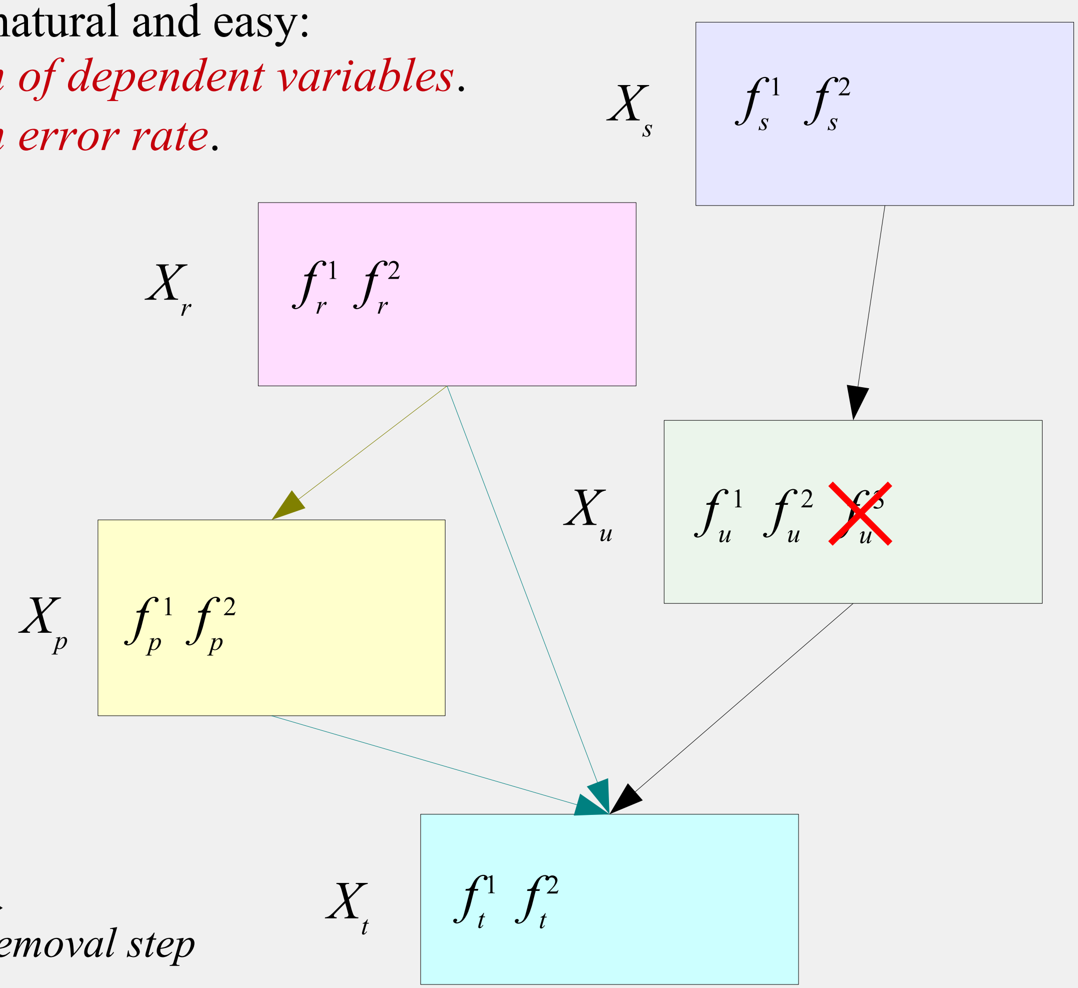

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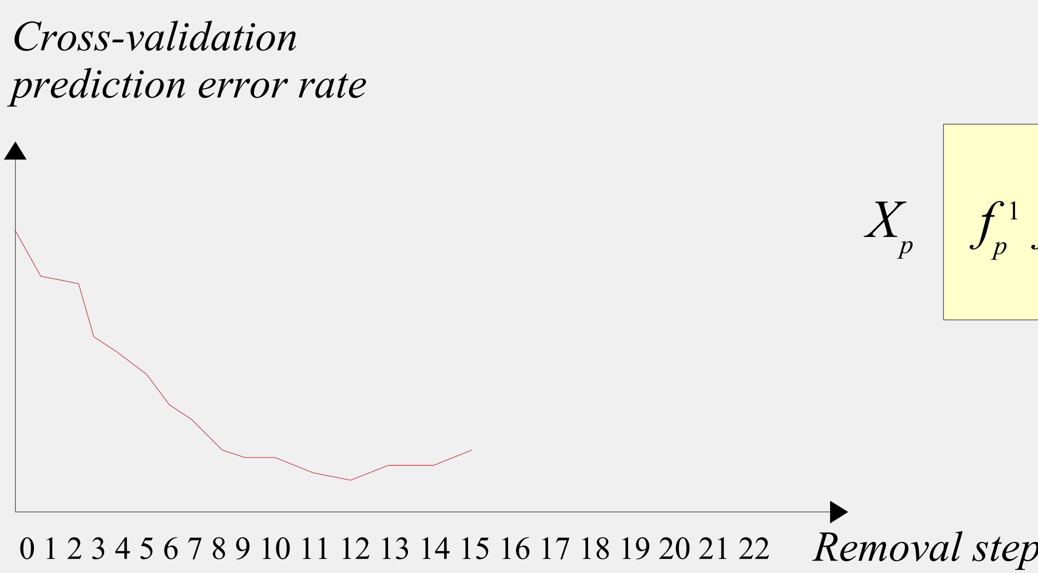

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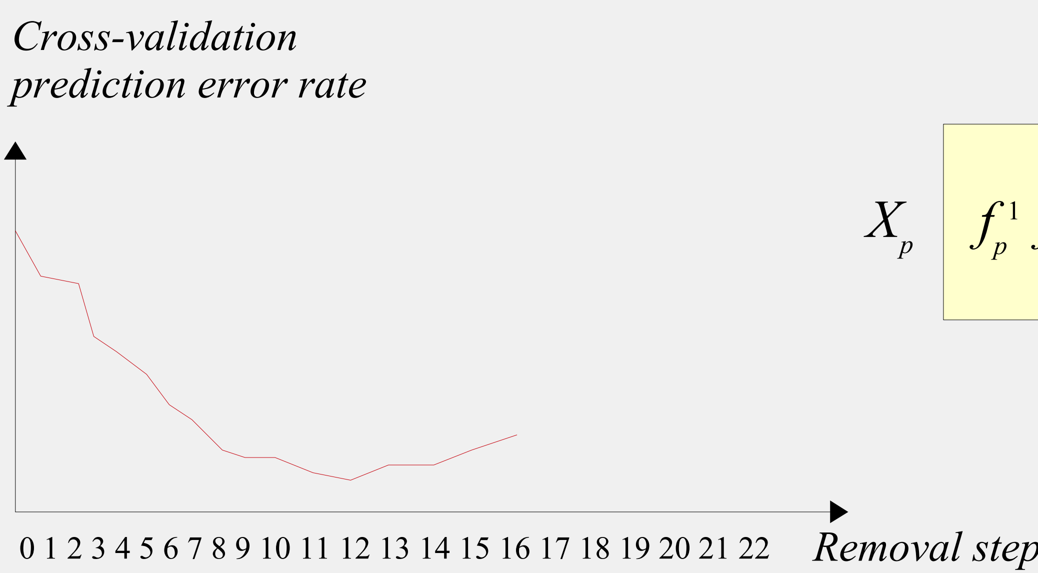
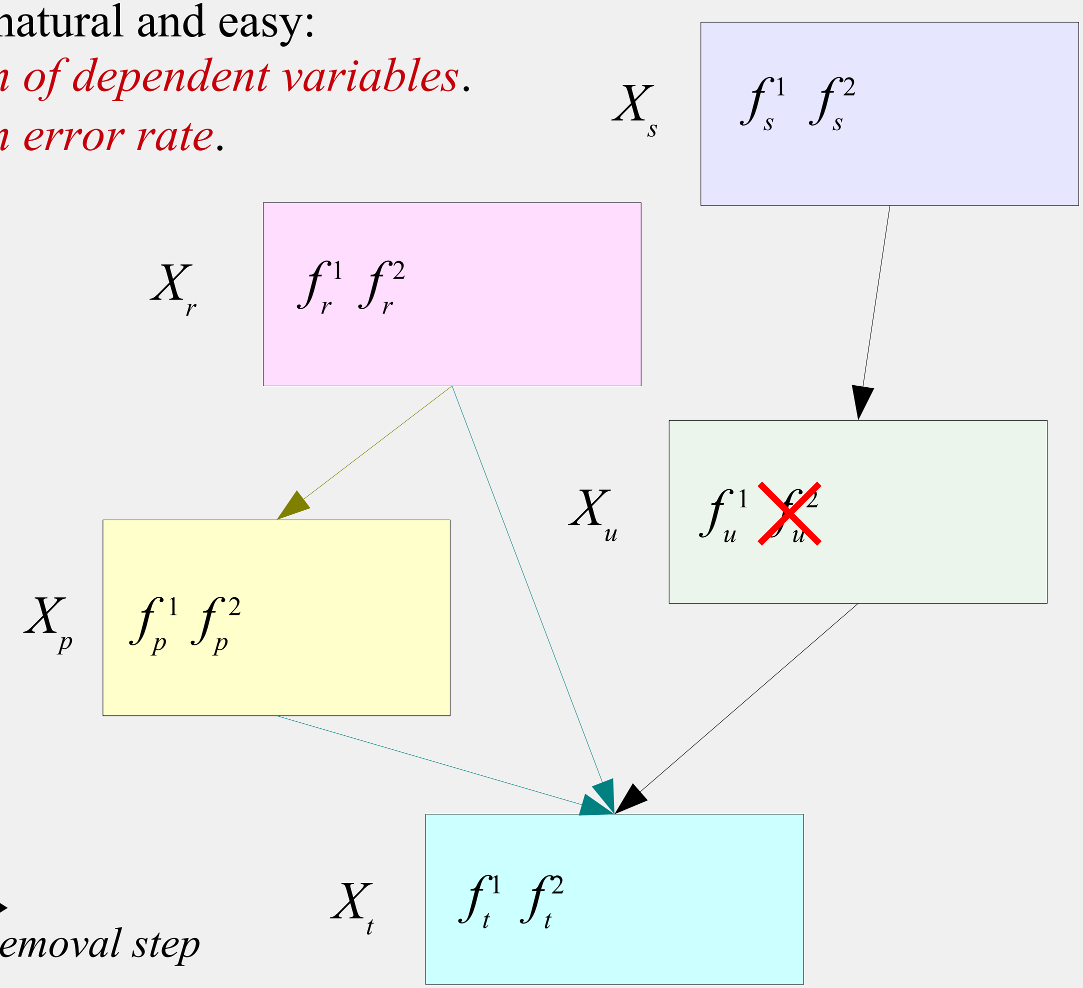


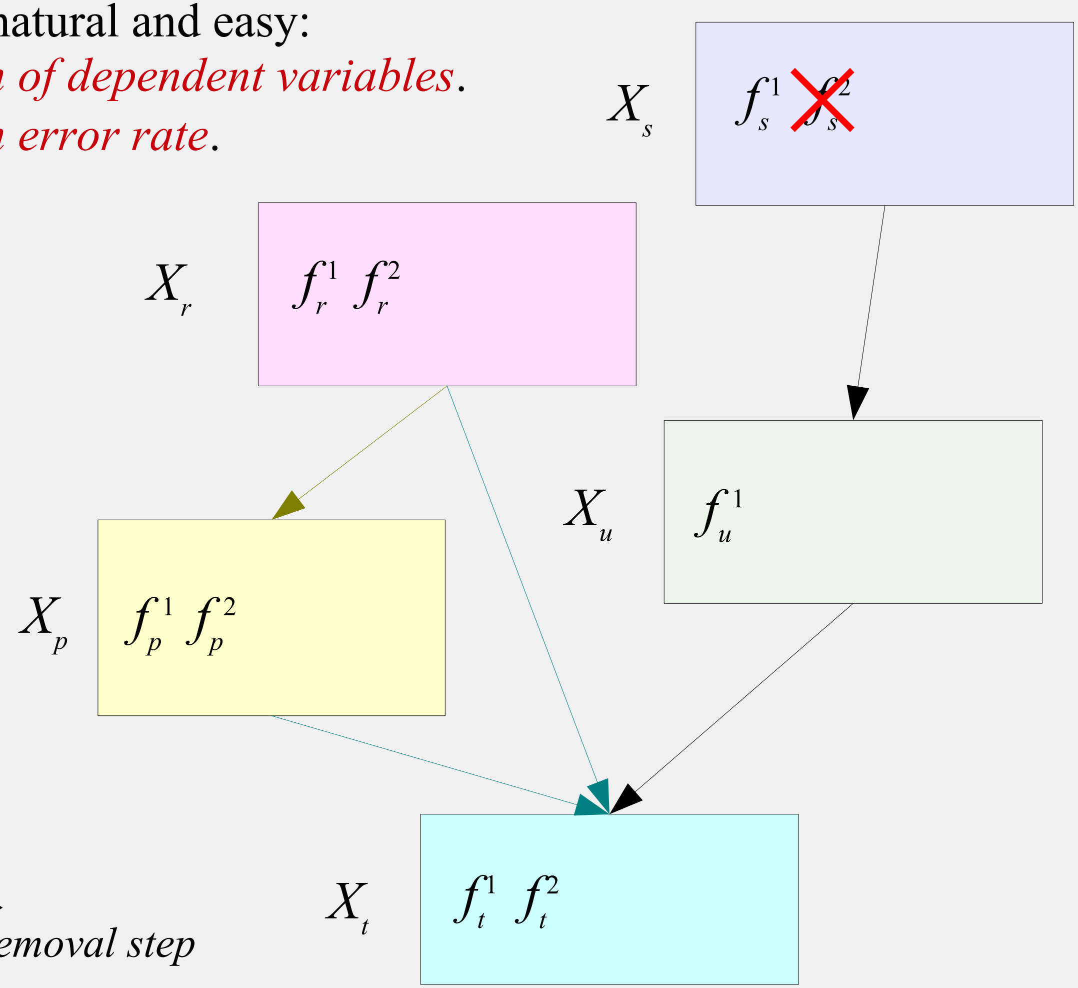


How THEME works

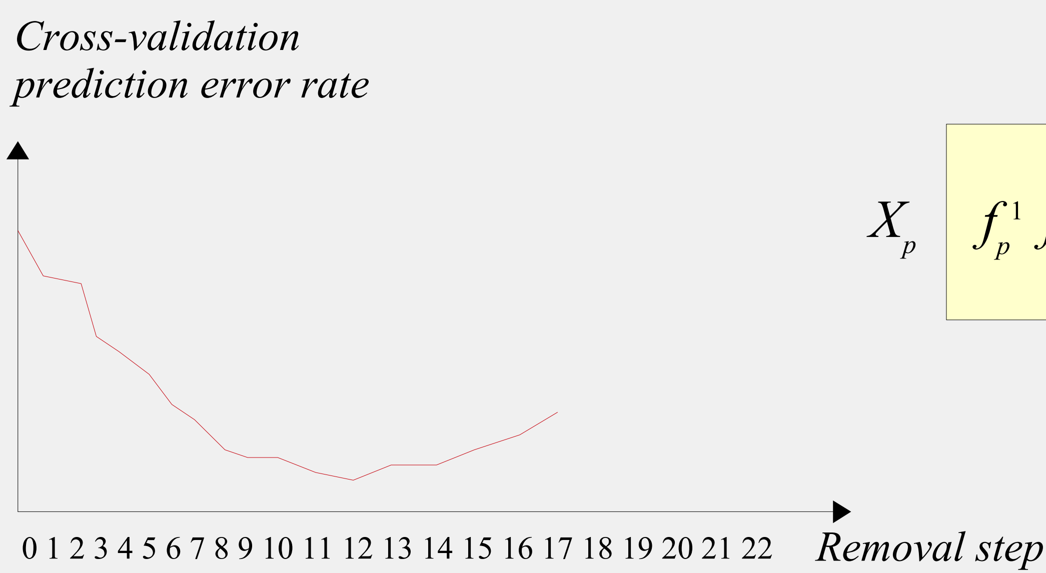
5. Backward component selection

- **How to select the suitable number of components in each group?**

Local nesting makes ***backward selection*** natural and easy:
Explanatory components → *prediction of dependent variables*.
→ *prediction error rate*.



Example:



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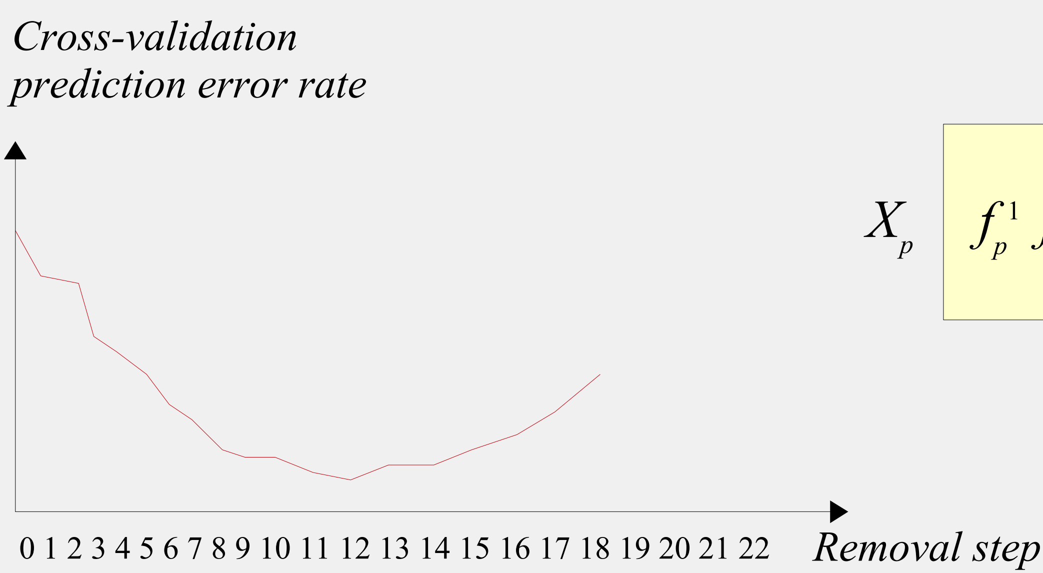

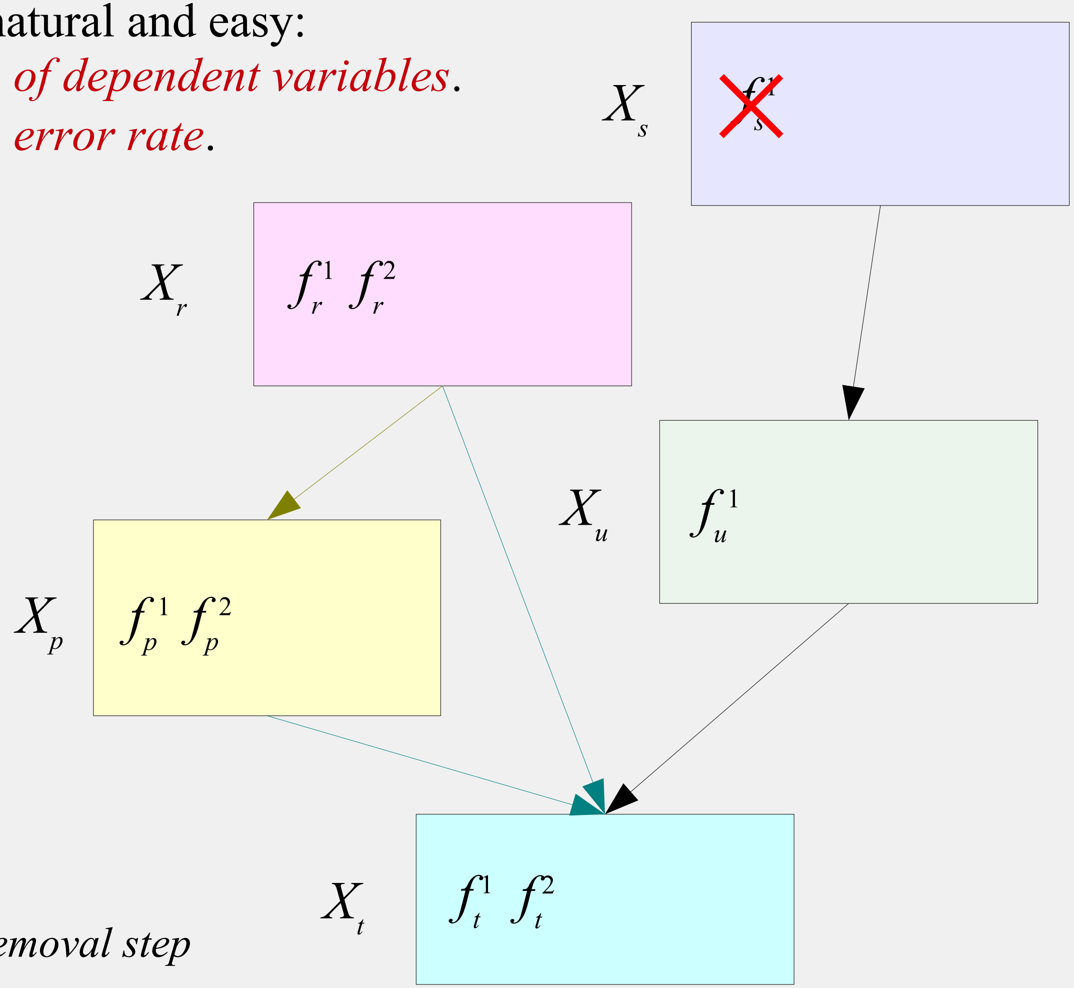

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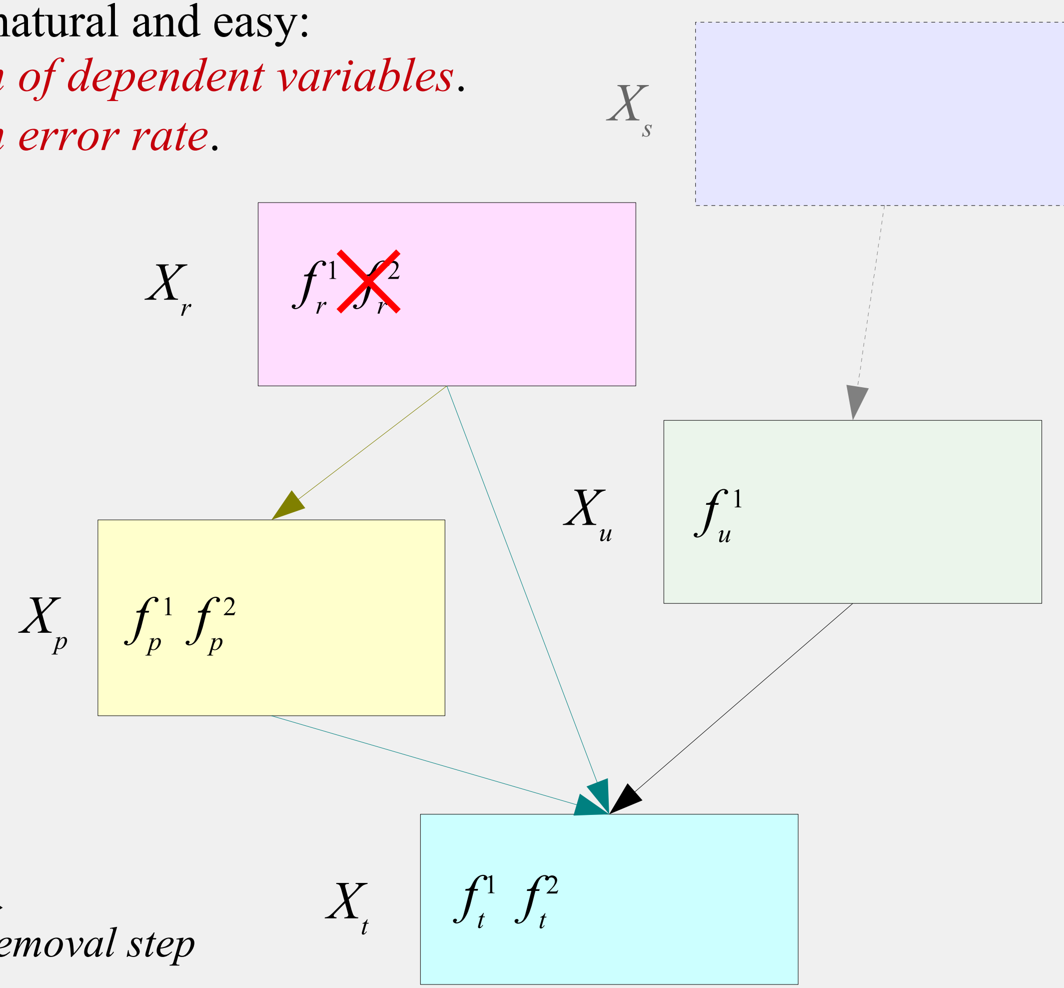

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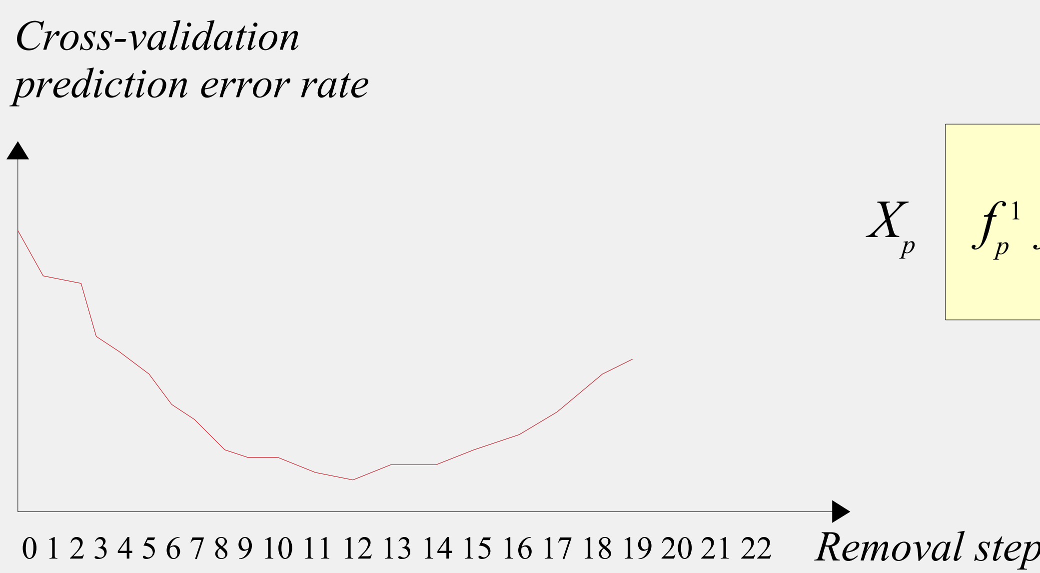

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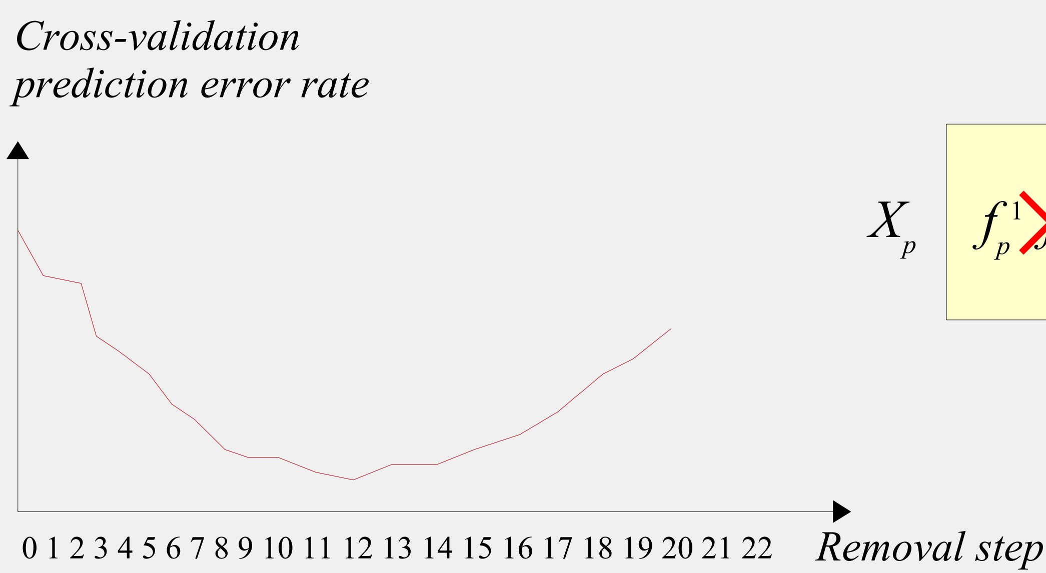

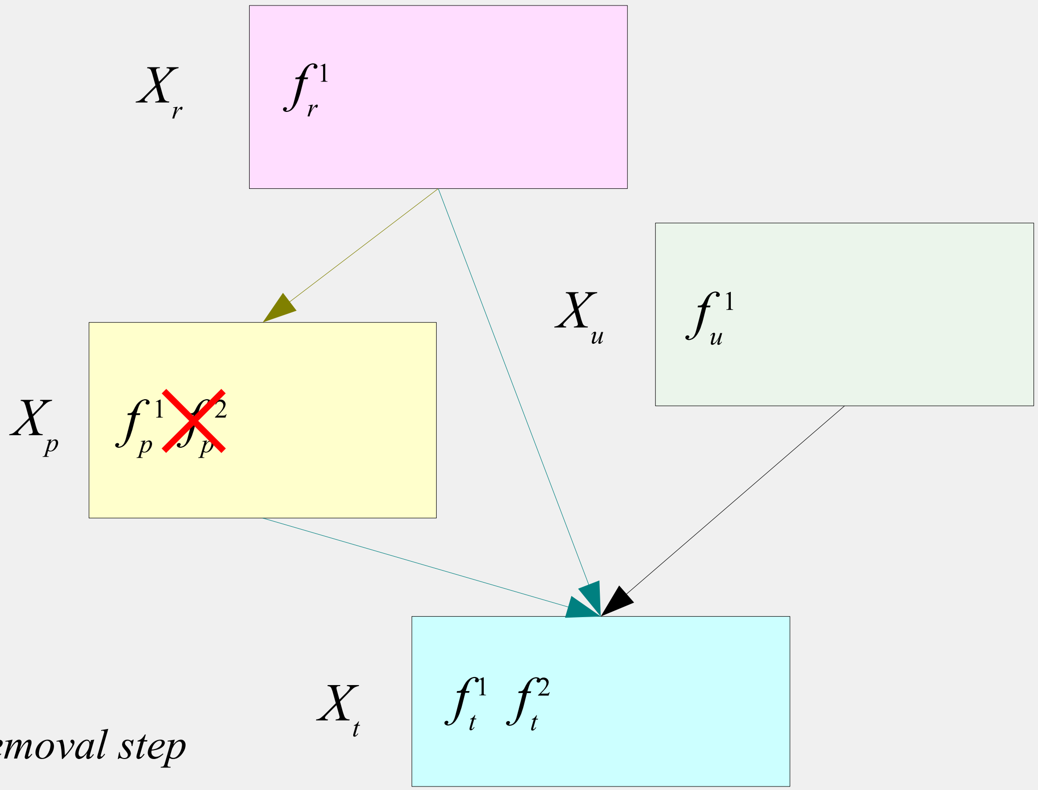

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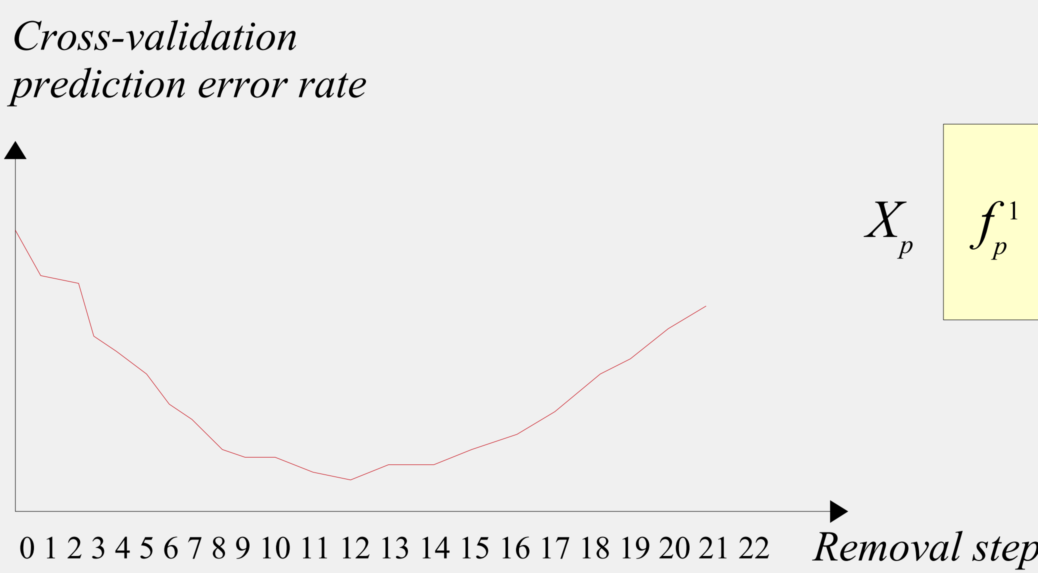

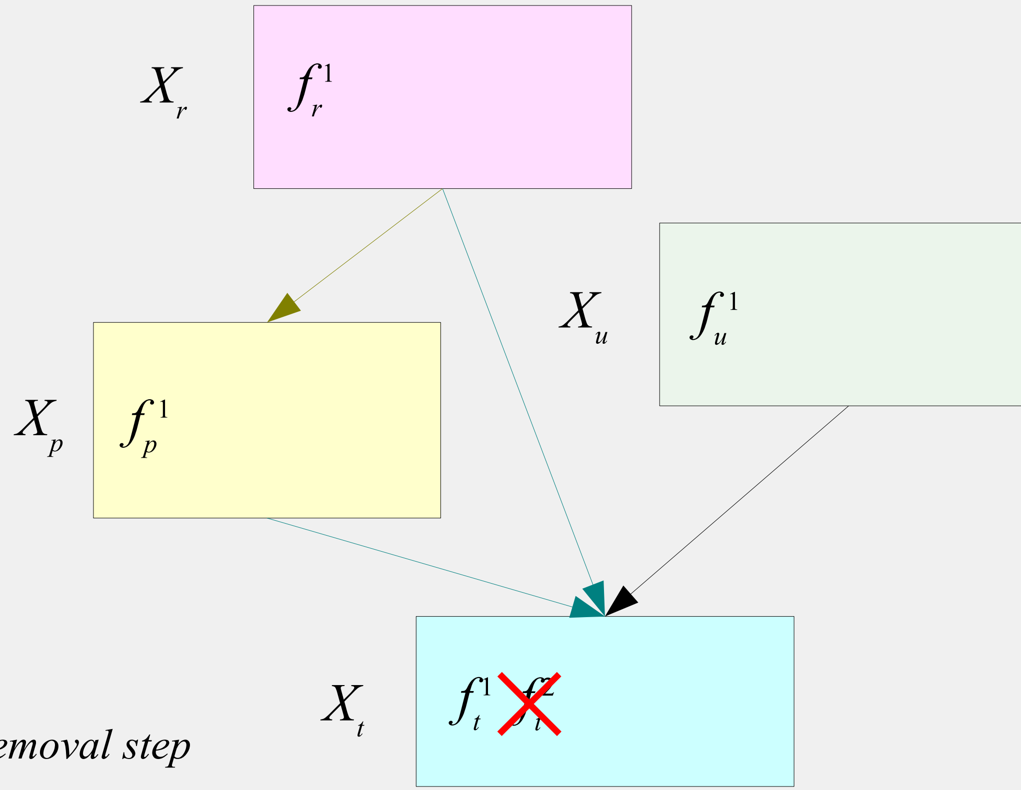

How THEME works

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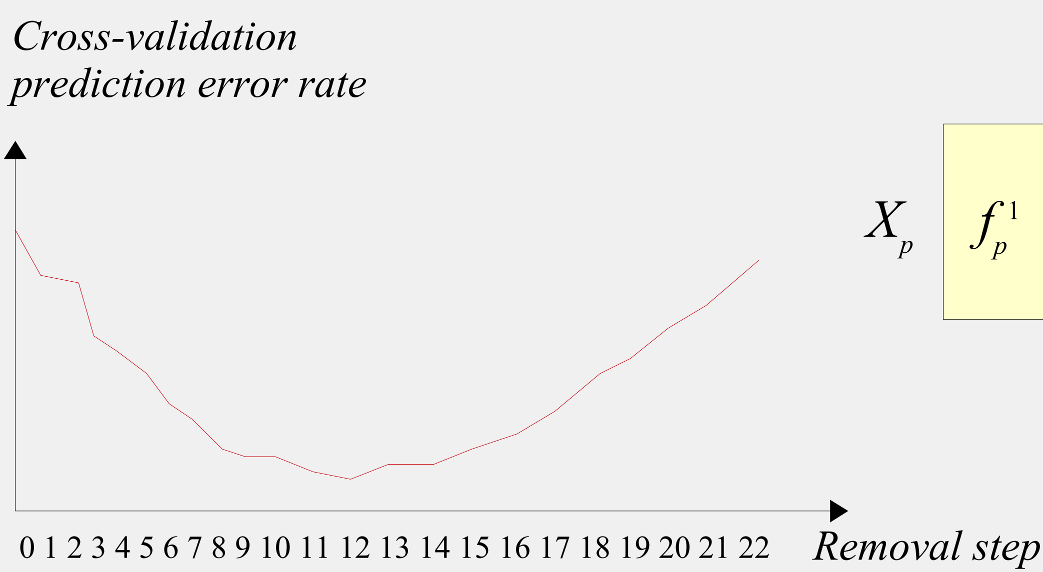

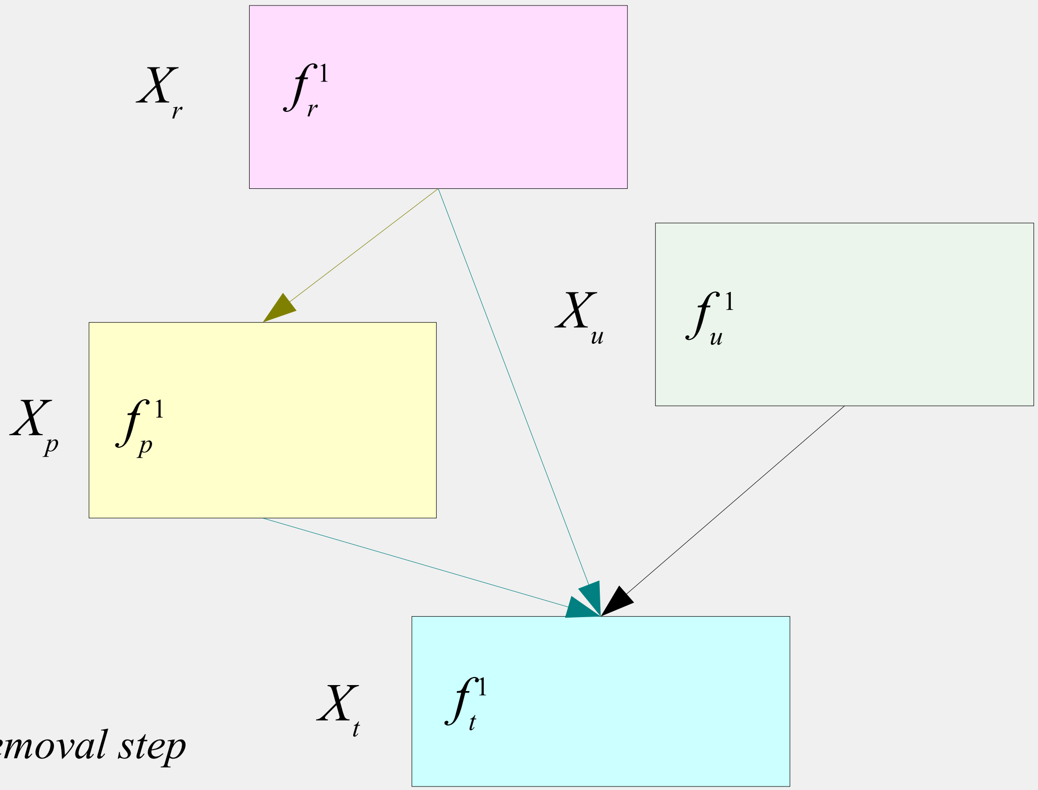

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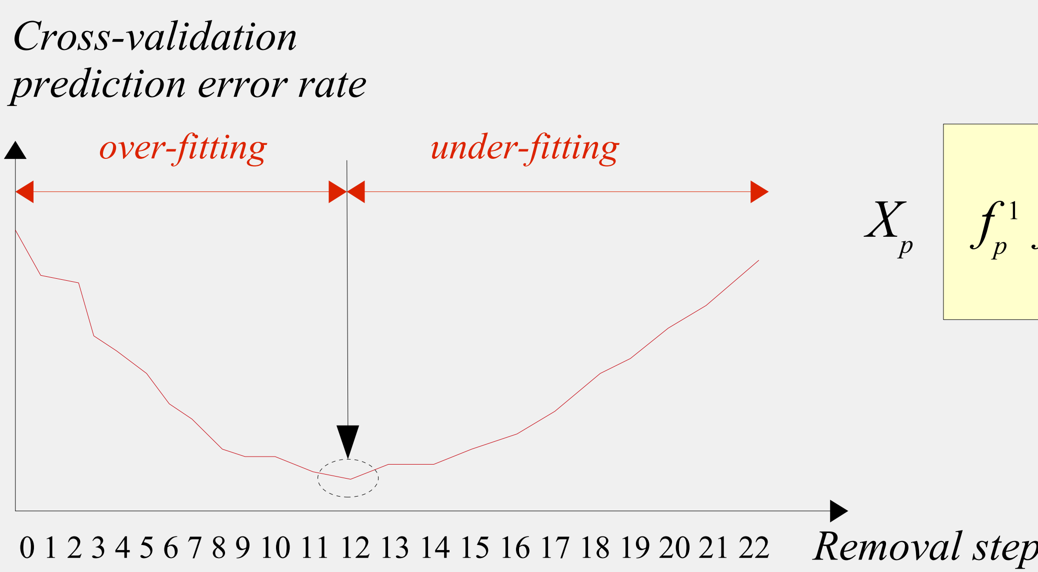
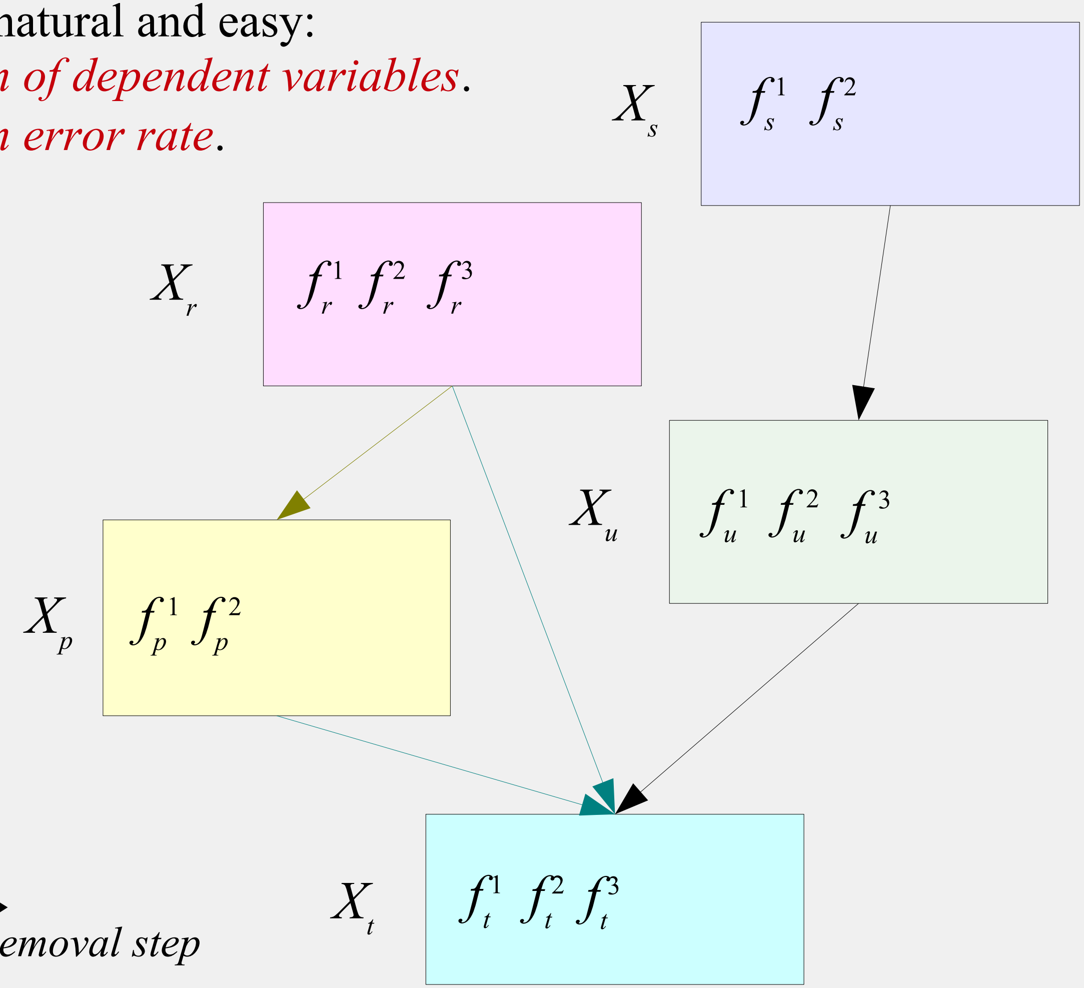




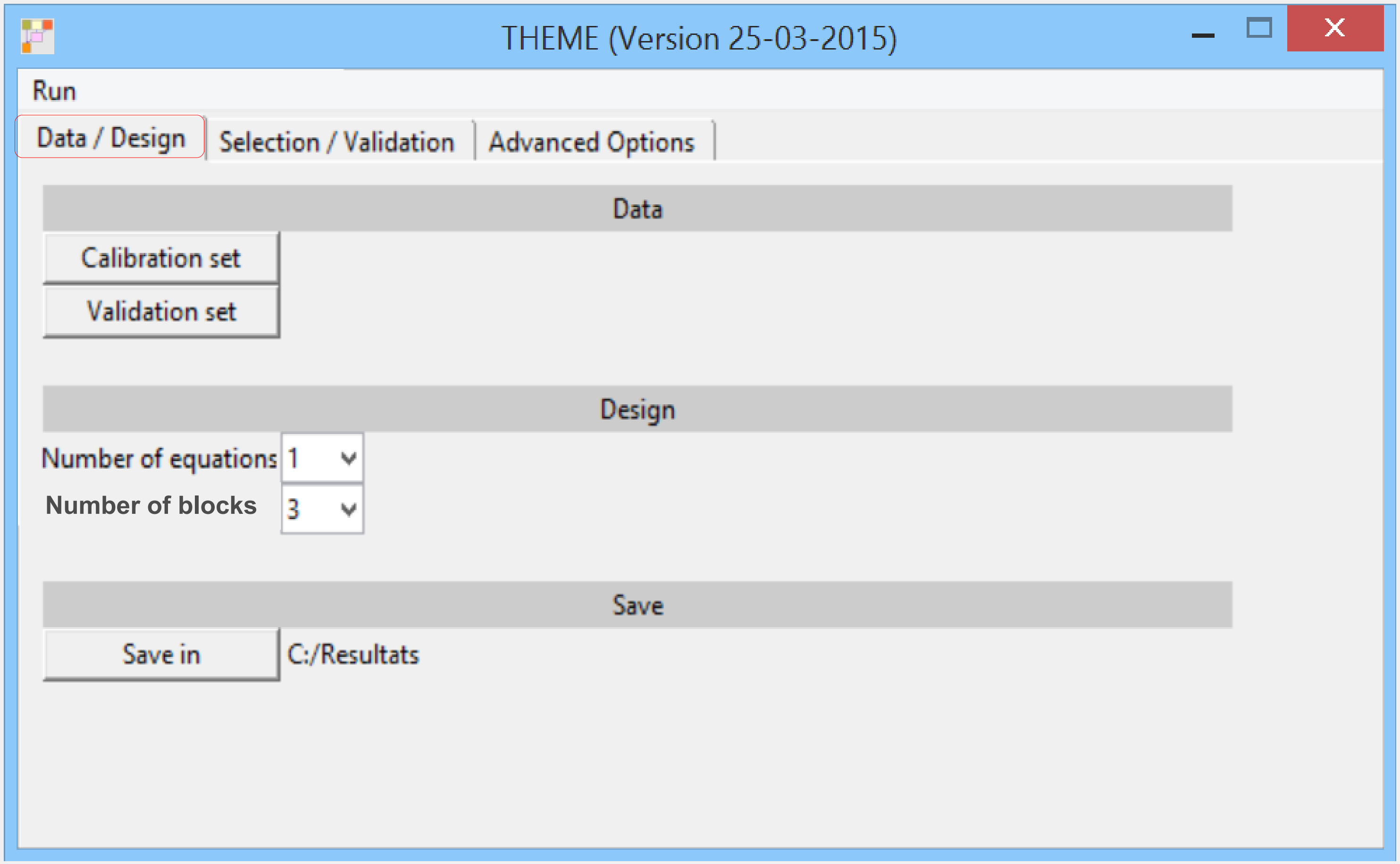
How to operate the THEME R-software?

1. The main window

Sample selection

Model design

Output

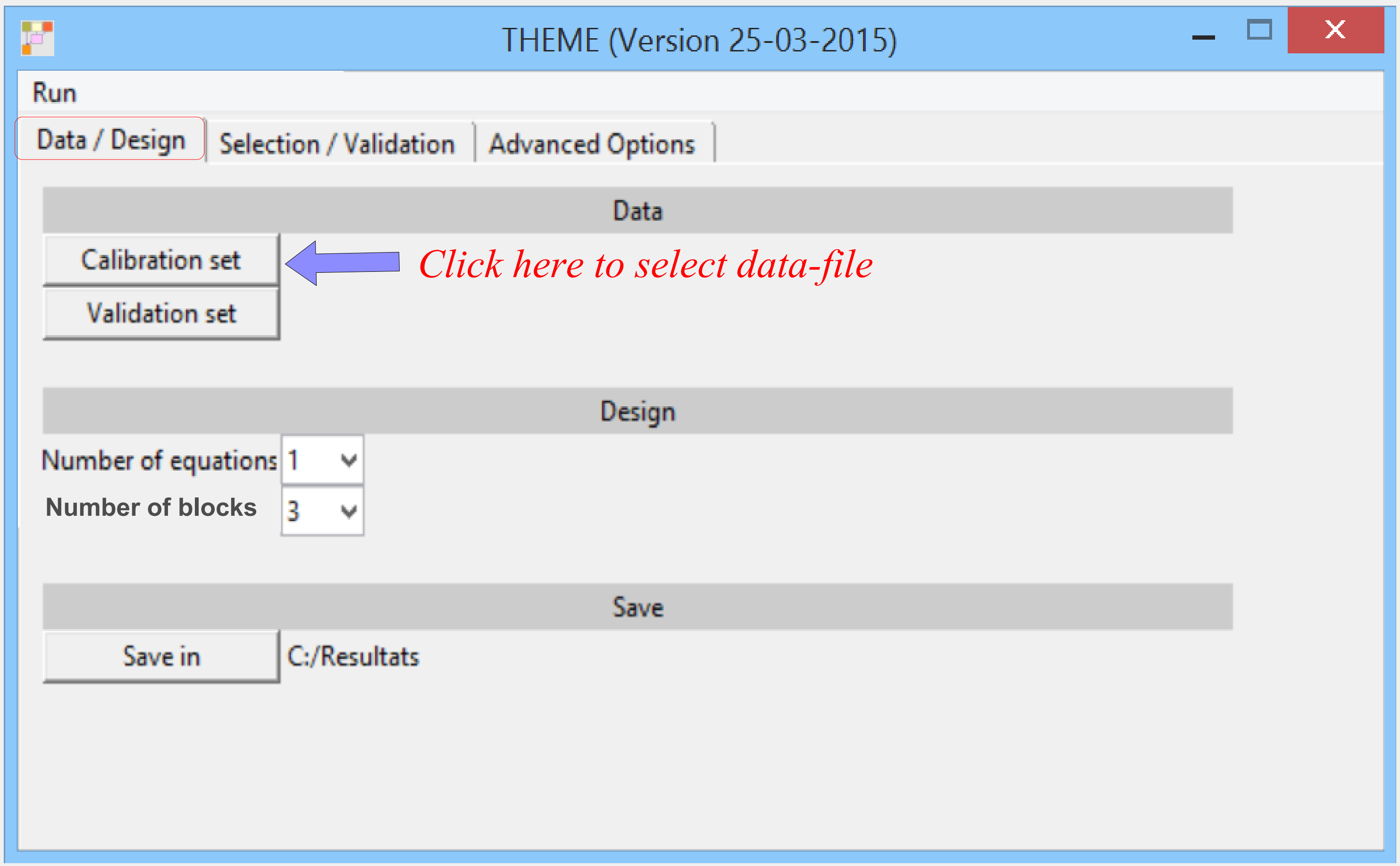


How to operate the THEME R-software?

1. The main window

Data Input

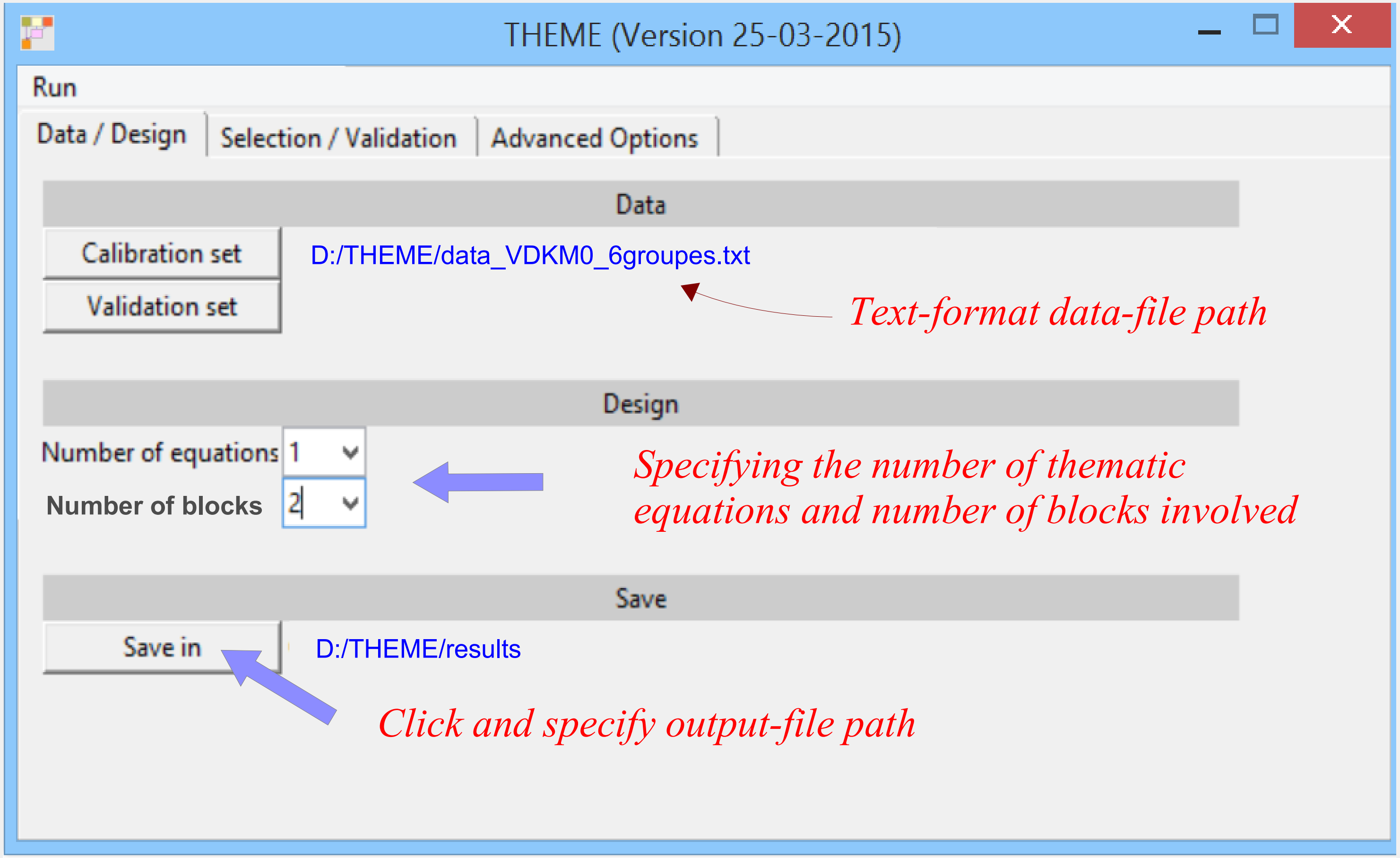
Output



Click here to select data-file

How to operate the THEME R-software?

1. The main window



How to operate the THEME R-software?

2. From raw data to Thematic Model

- ***Data file =*** ASCII-file with tab separator: data_VDKM0_6groupes.txt

Variables

Obs.

SAMPLE_NAME	code	Tchem_1	Tchem_2	Tchem_3	Tchem_4	Tchem_5	Tchem_6
cig1	6	1.54	0.67	1.85	42.38	3.56	89
cig2	2	0.4	0.92	1.95	42.18	2.31	66
cig3	1	0.56	0.75	1.8	43.23	2.74	123
cig4	5	0.97	0.96	1.83	41.27	2.79	96
cig5	5	0.66	0.85	1.47	41.37	2.29	119
cig6	1	0.89	0.77	2.03	42.2	2.88	142
…	…	…	…	…	…	…	…
cig29	4	0.87	0.77	1.89	40.72	2.75	177

How to operate the THEME R-software?

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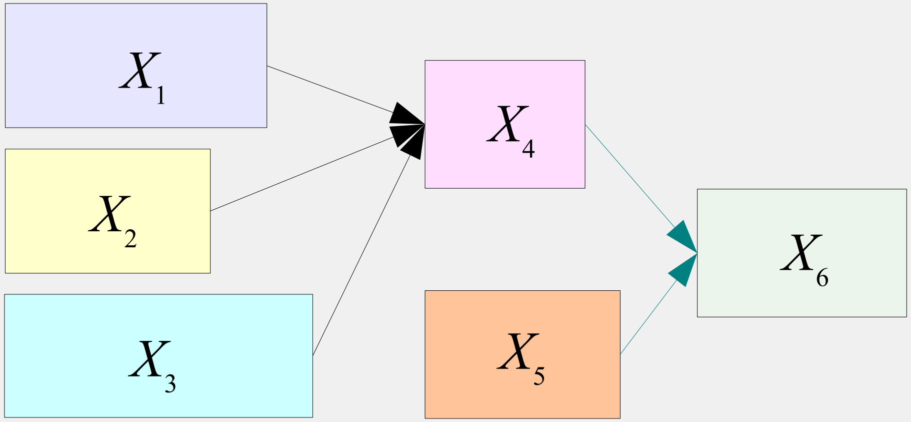
- ***Design of the thematic model:***



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…	…	…	…	…	…	…	…
cig29	4	0.87	0.77	1.89	40.72	2.75	177
TGC	cci	1	3	1	3	1	1

Thematic Group Coding
(0 = *variable not used*)

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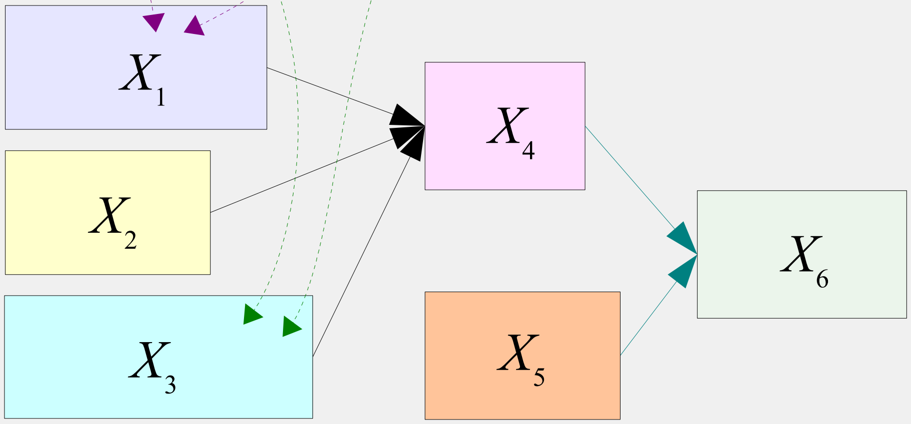
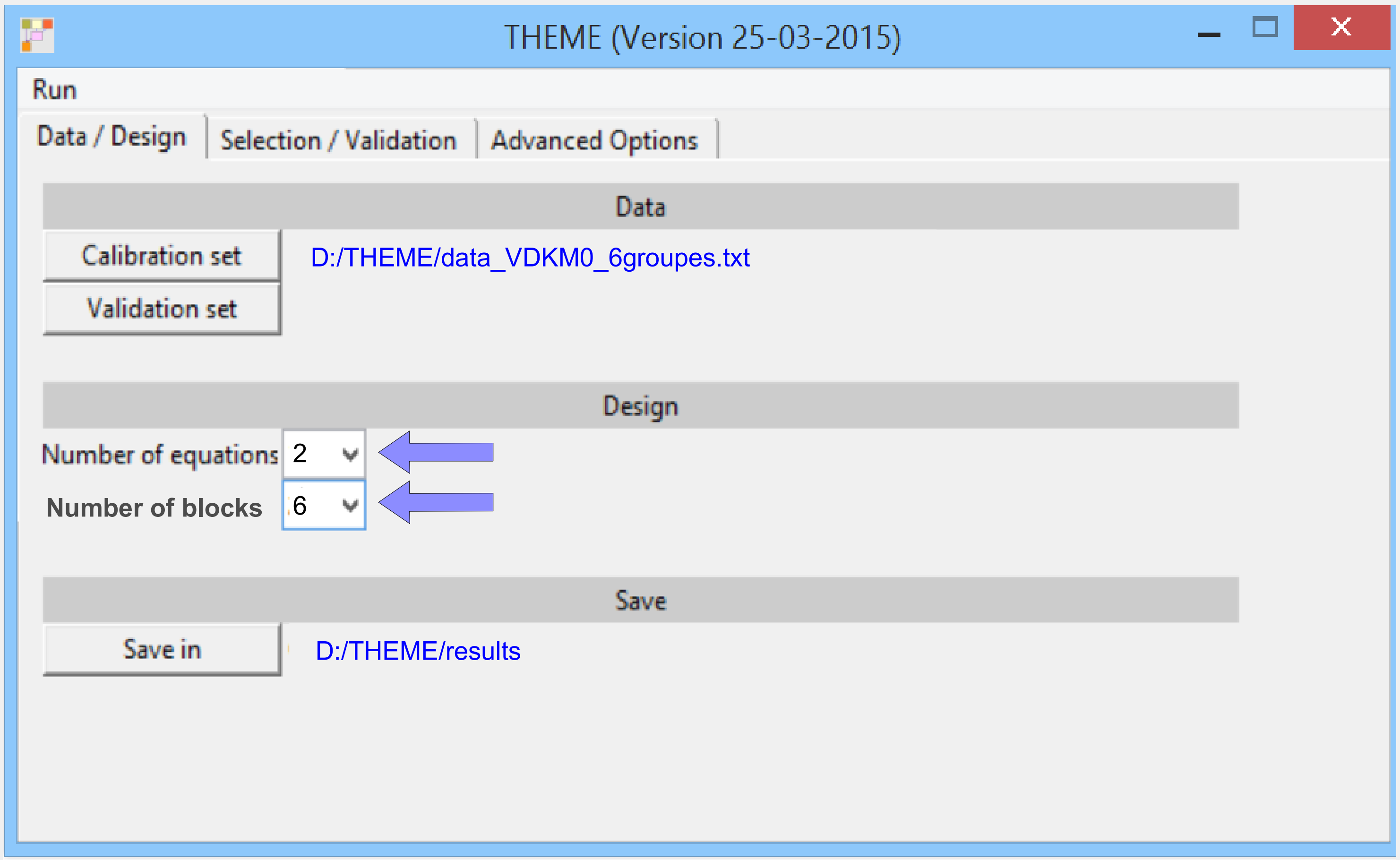


How to operate the THEME R-software?

2. From raw data to Thematic Model

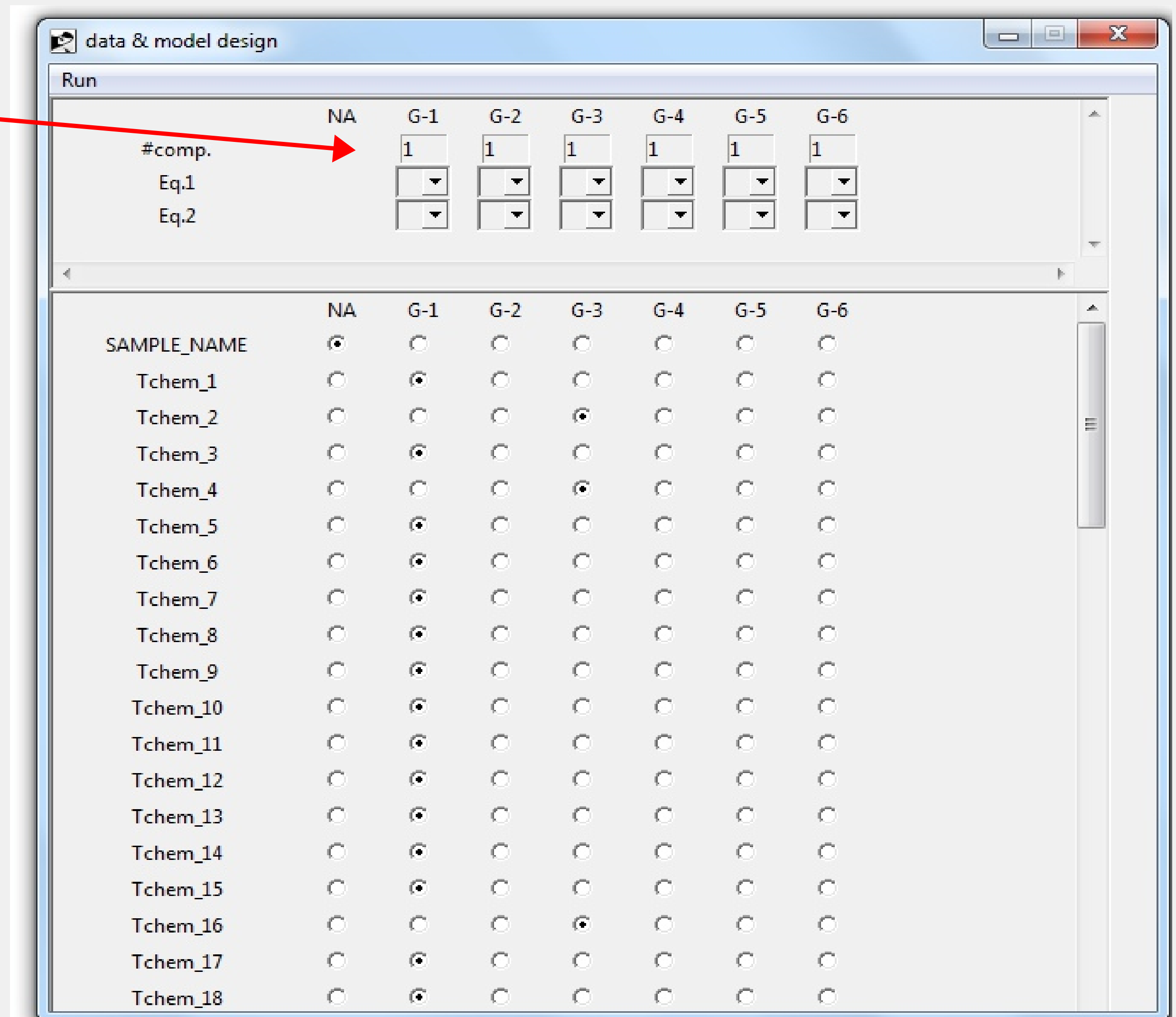
Model design



How to operate the THEME R-software?

2. From raw data to Thematic Model

Number of components in groups

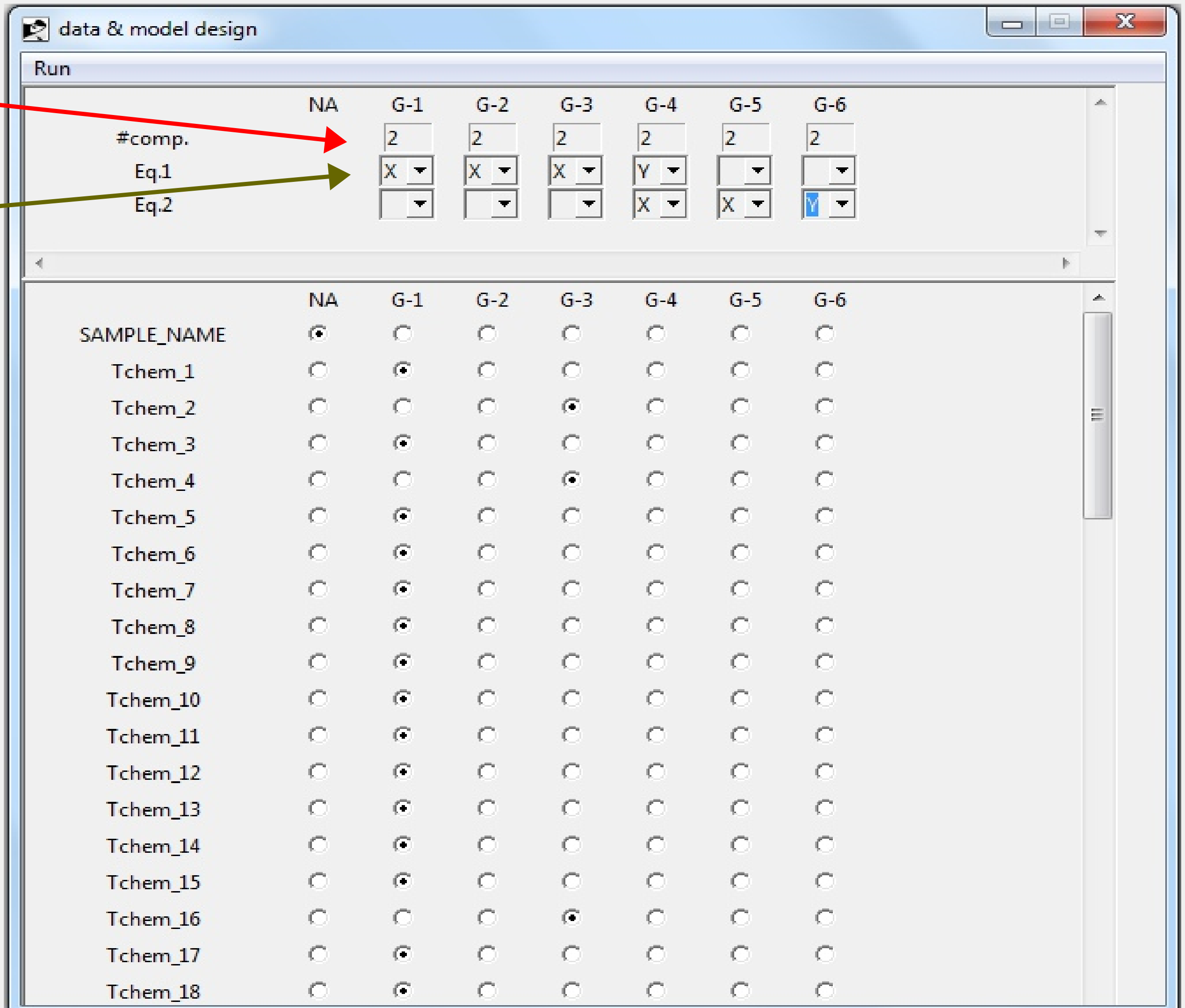


How to operate the THEME R-software?

2. From raw data to Thematic Model

Number of components in groups

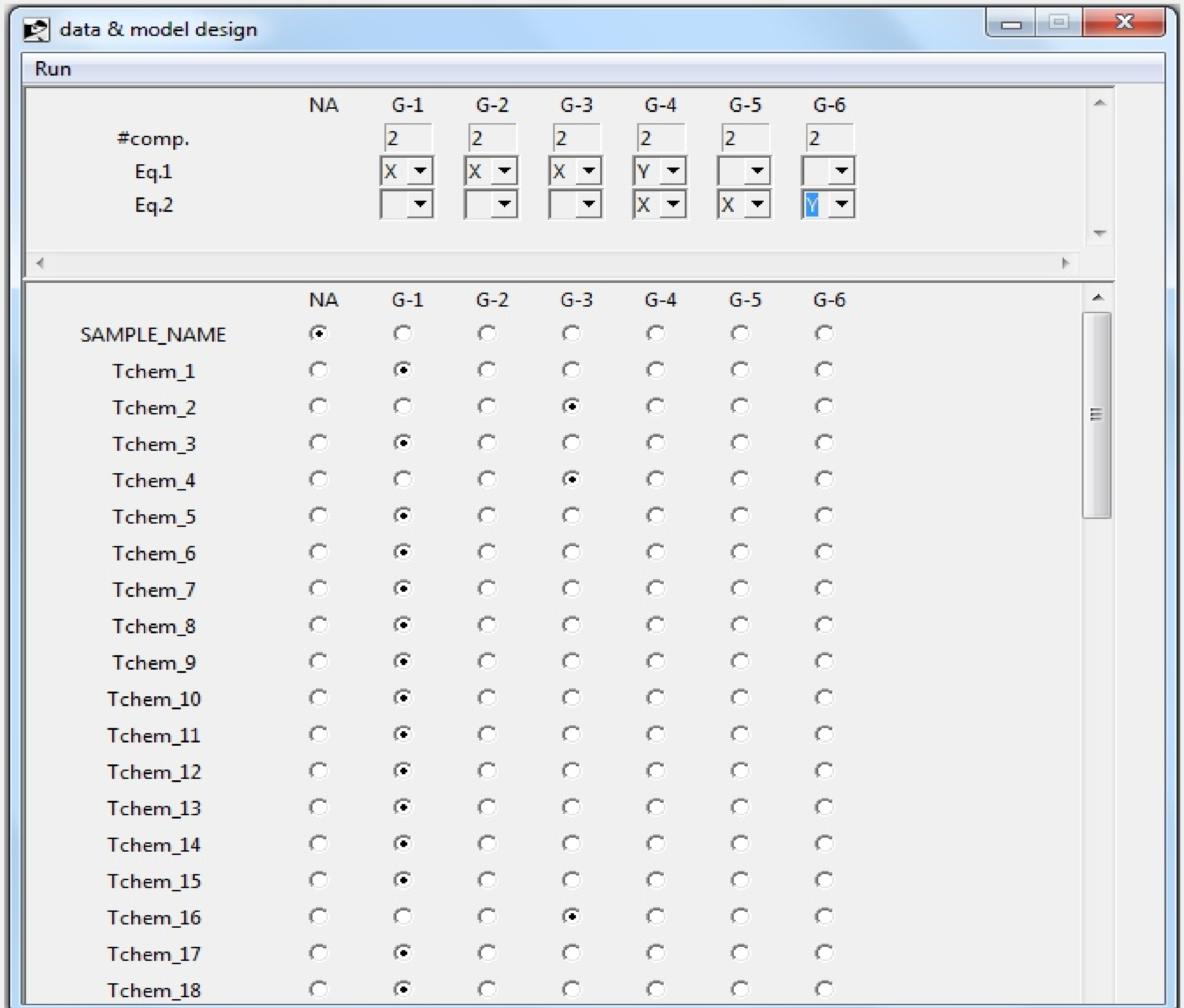
Role of groups in equation (explanatory=X, dependent =Y)



How to operate the THEME R-software?

2. From raw data to Thematic Model

If TGC line in datafile, pre-filled.
Else, design by click:

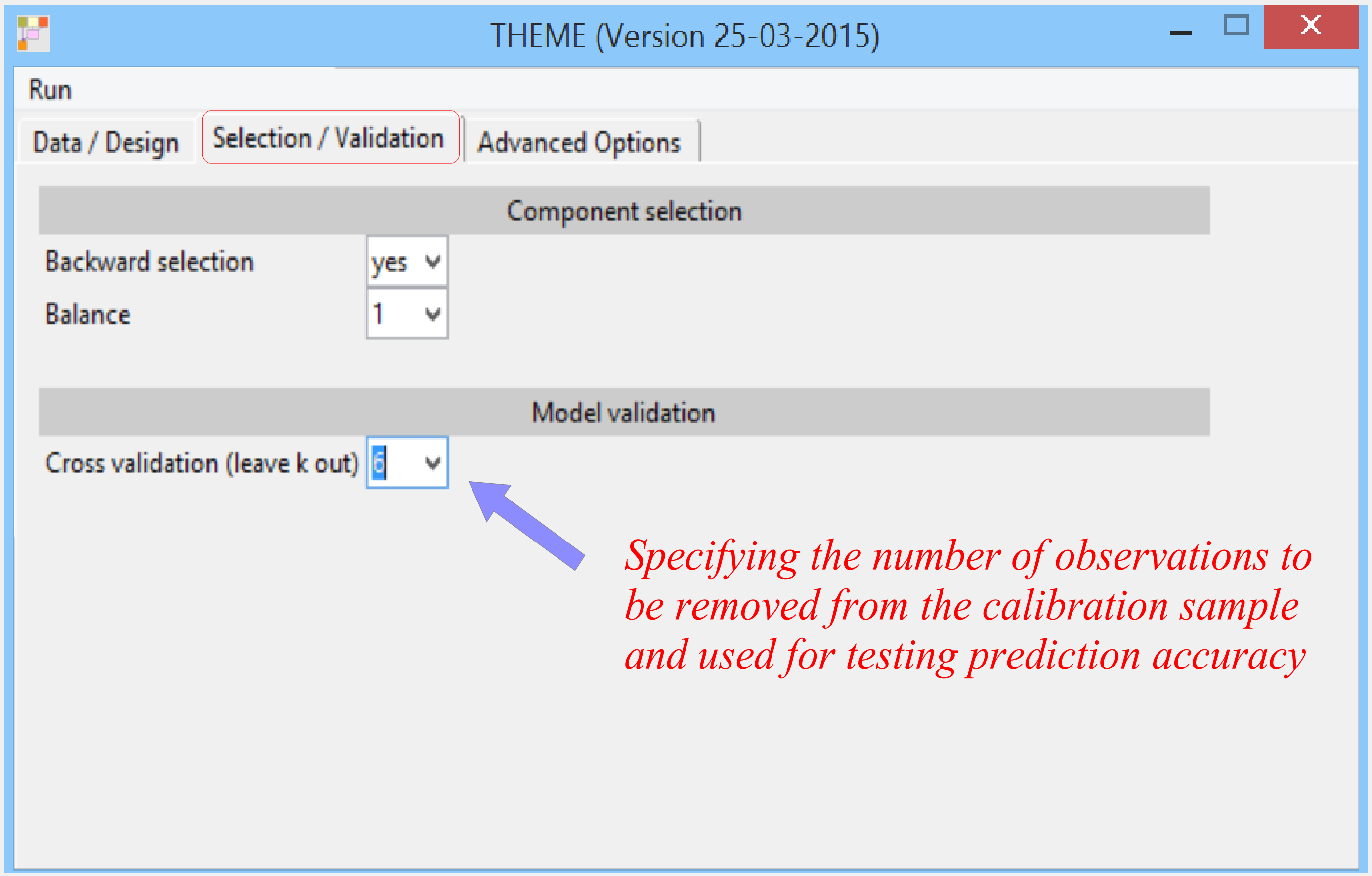


How to operate the THEME R-software?

3. Setting the selection & validation parameters

Component selection

Model cross-validation

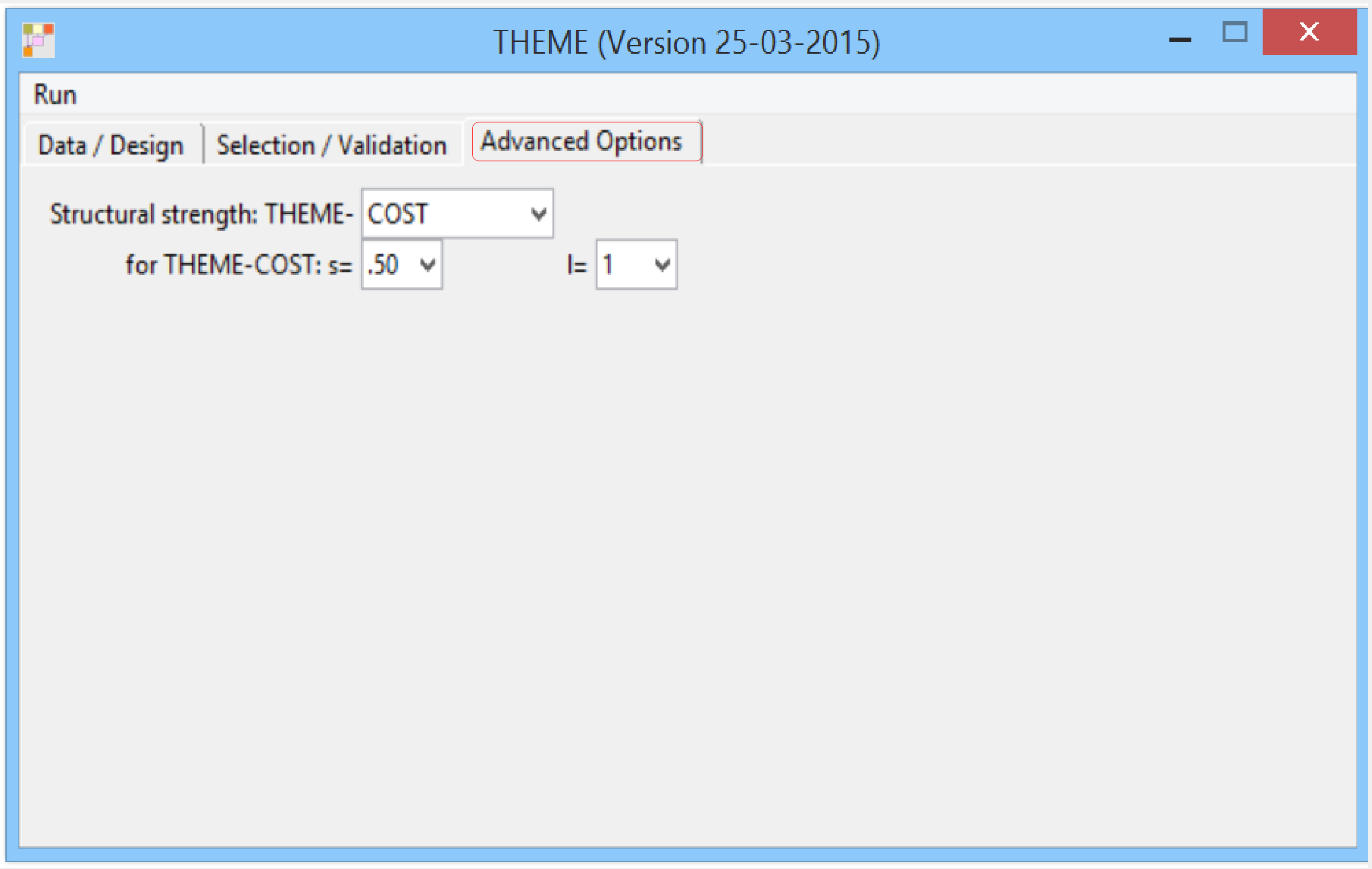


Specifying the number of observations to be removed from the calibration sample and used for testing prediction accuracy

How to operate the THEME R-software?

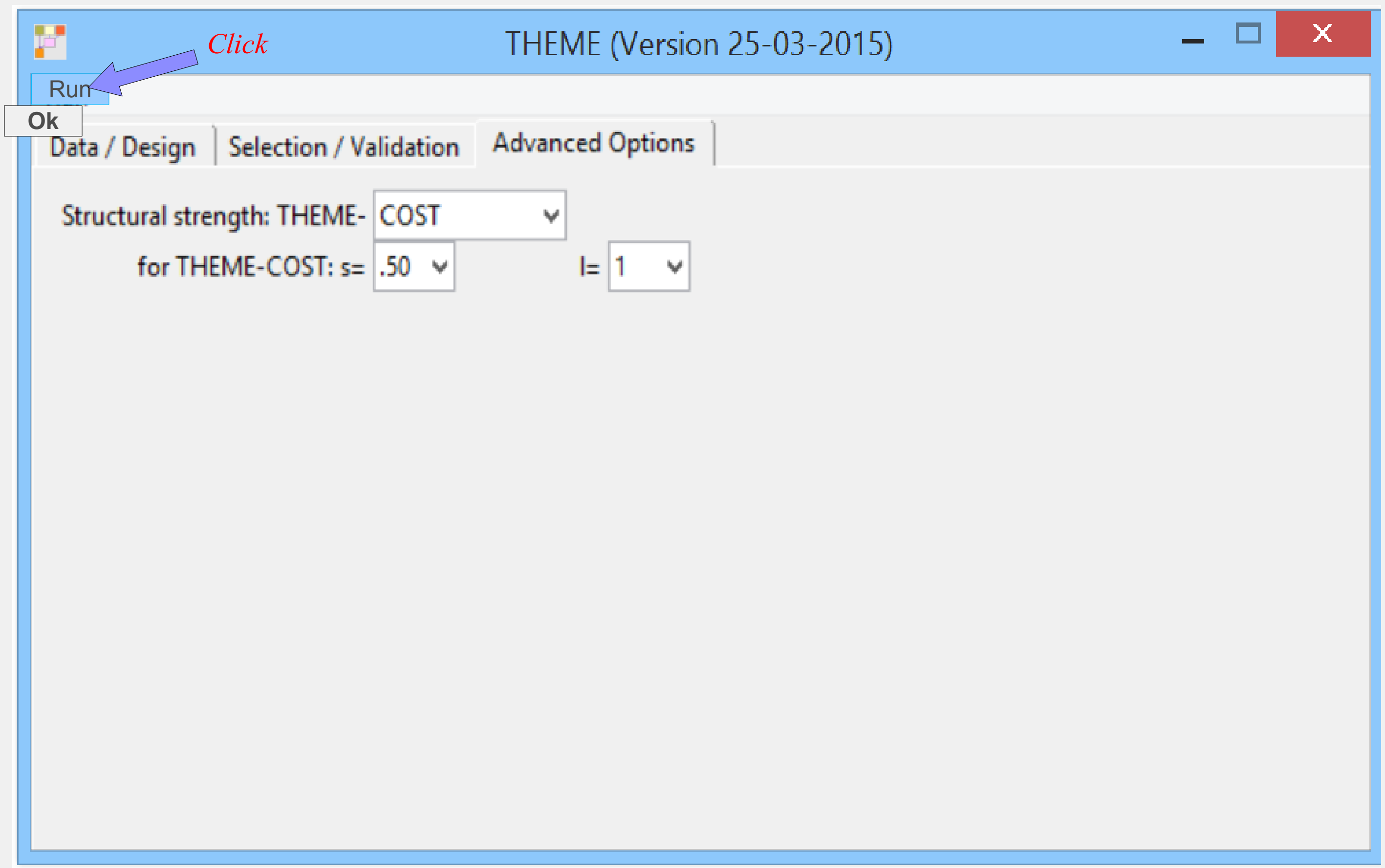
4. Setting the structural strength parameters

Structural strength parameters



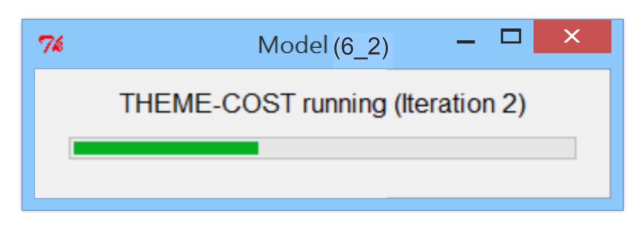
How to operate the THEME R-software?

5. Launching estimation



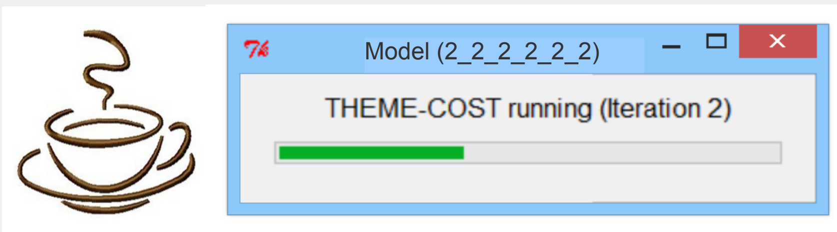
How to operate the THEME R-software?

6. Waiting for results

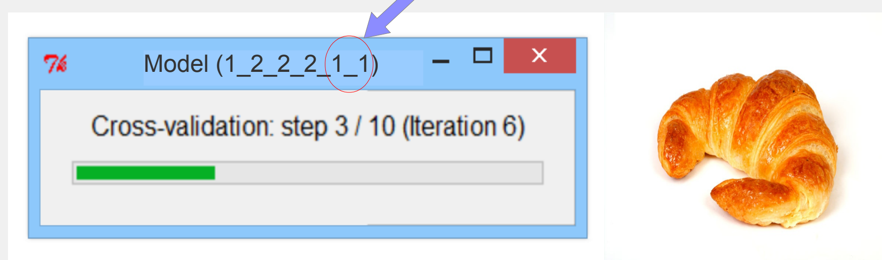


How to operate the THEME R-software?

6. Waiting for results



Number of components decreasing



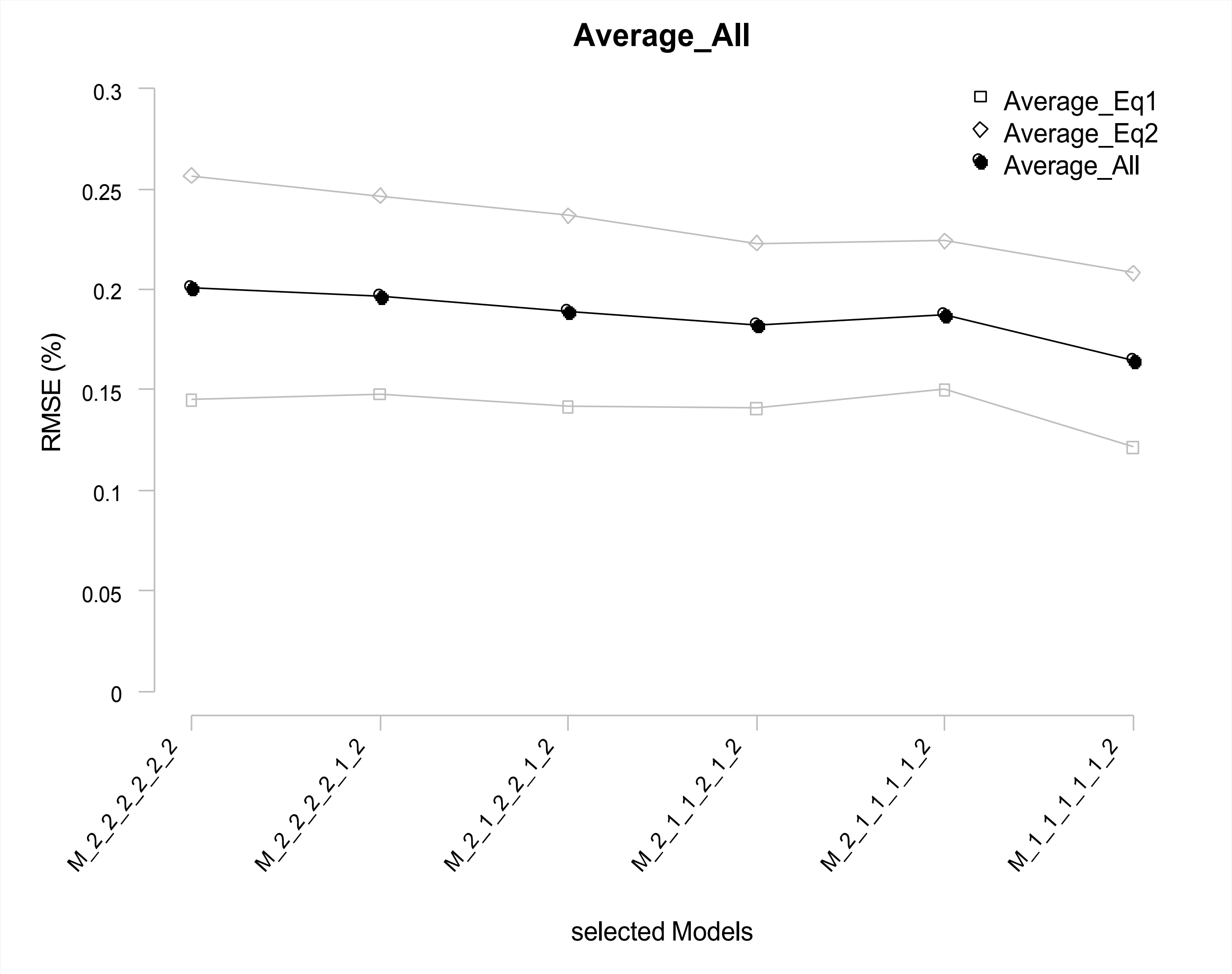
How to operate the THEME R-software?

6. Waiting for results

How to operate the THEME R-software?

7. Reaping results

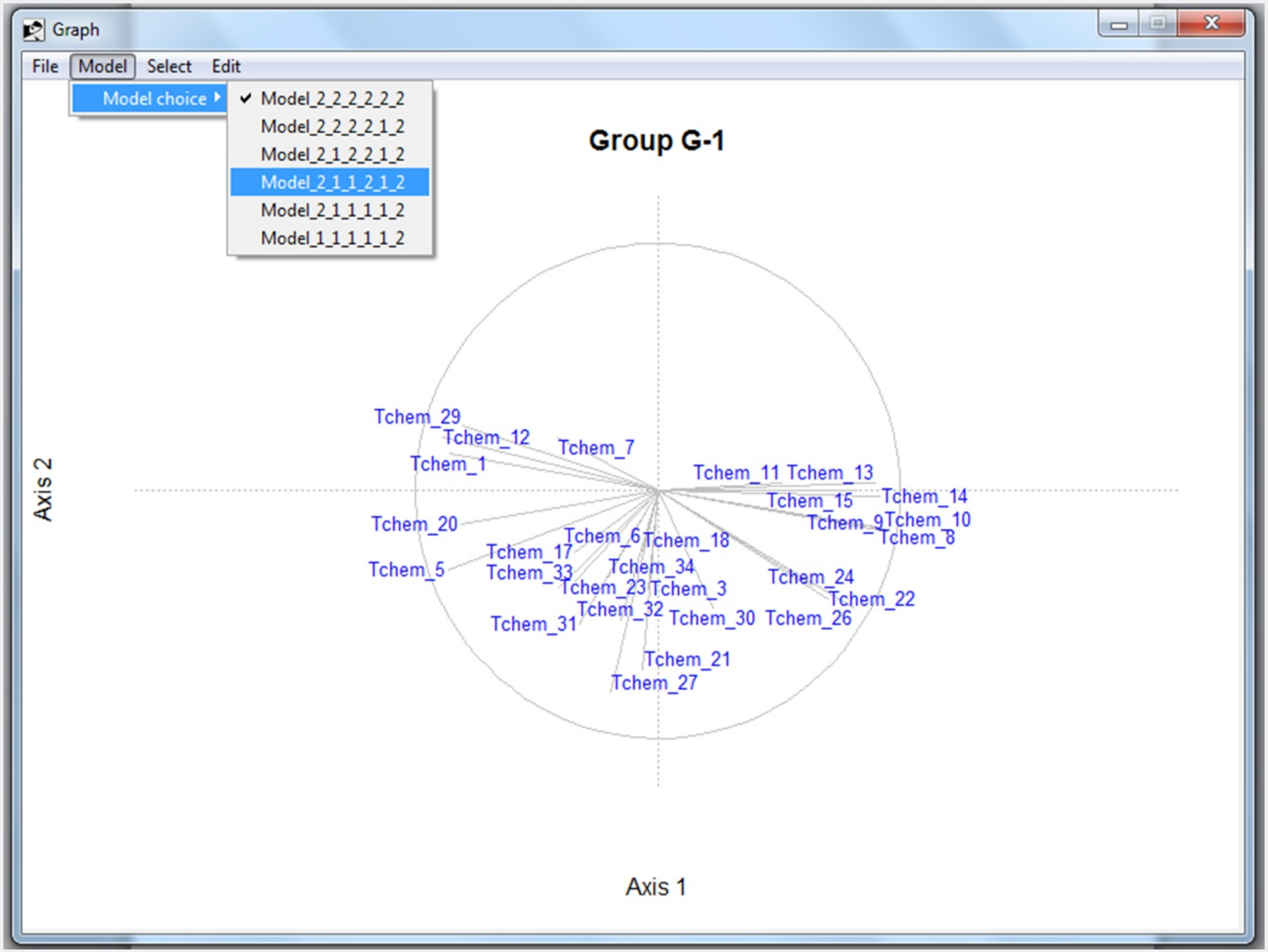
Model-selection



How to operate the THEME R-software?

7. Reaping results

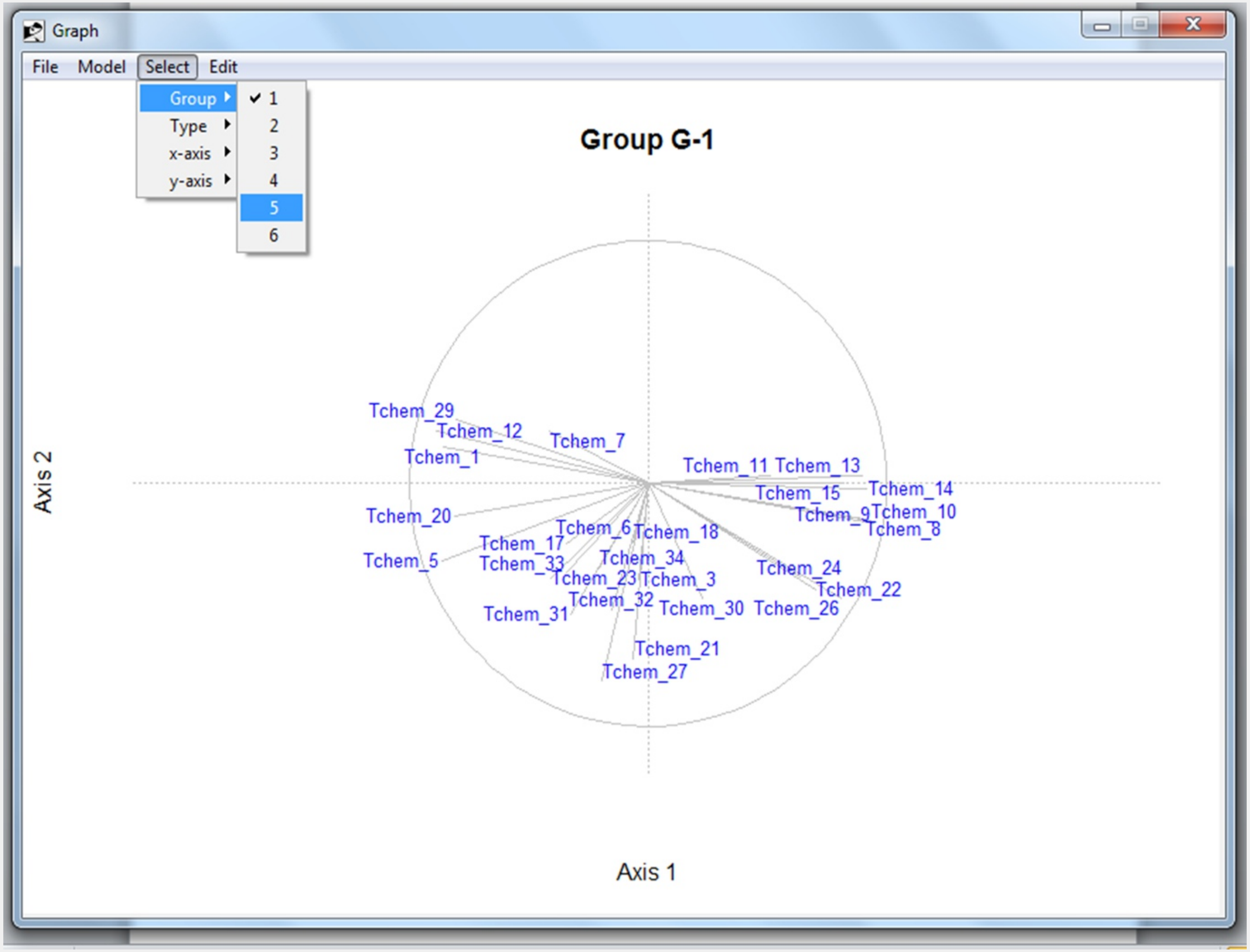
Model-selection* → *Graphing variables



How to operate the THEME R-software?

7. Reaping results

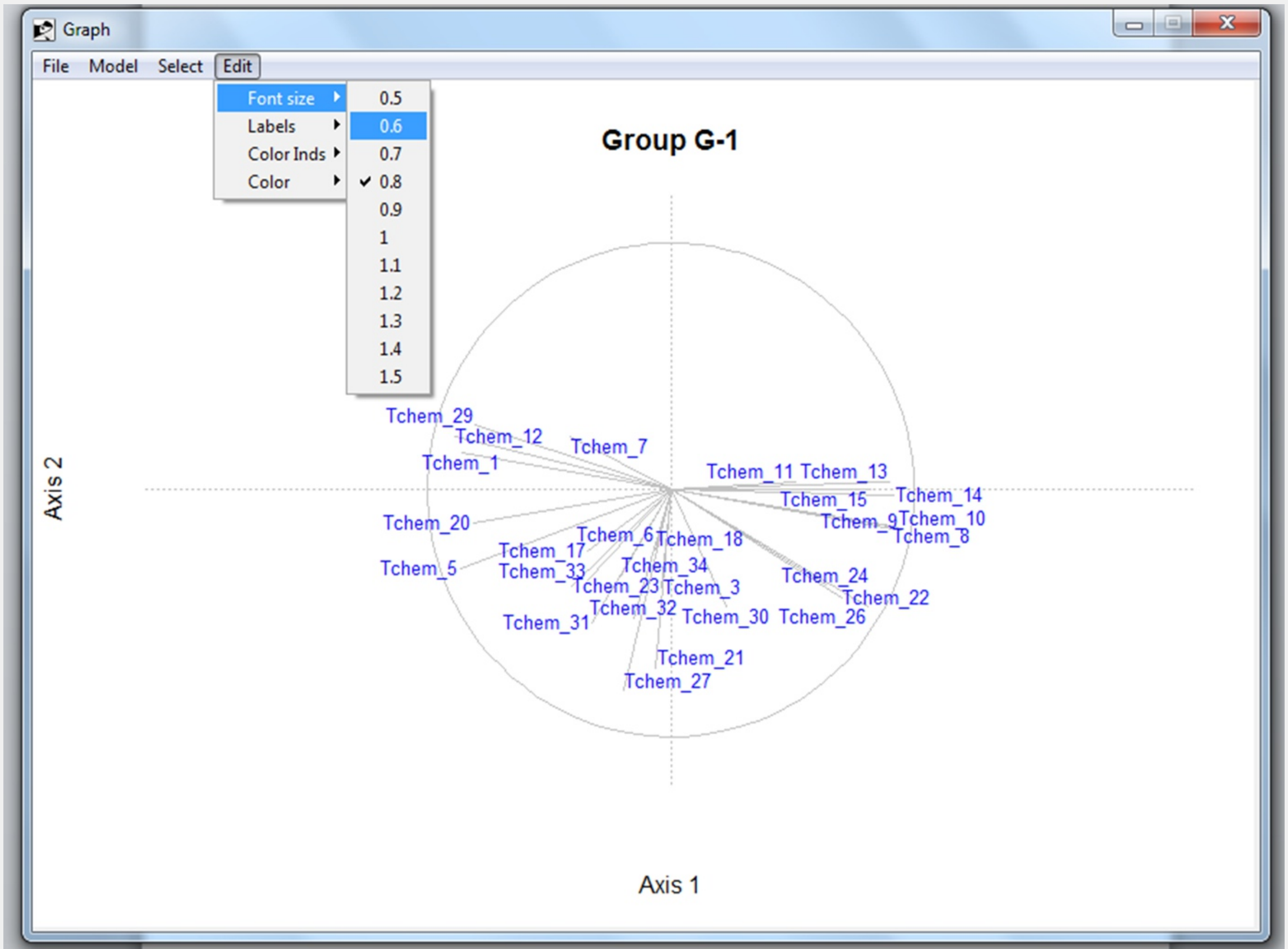
Graphing variables



How to operate the THEME R-software?

7. Reaping results

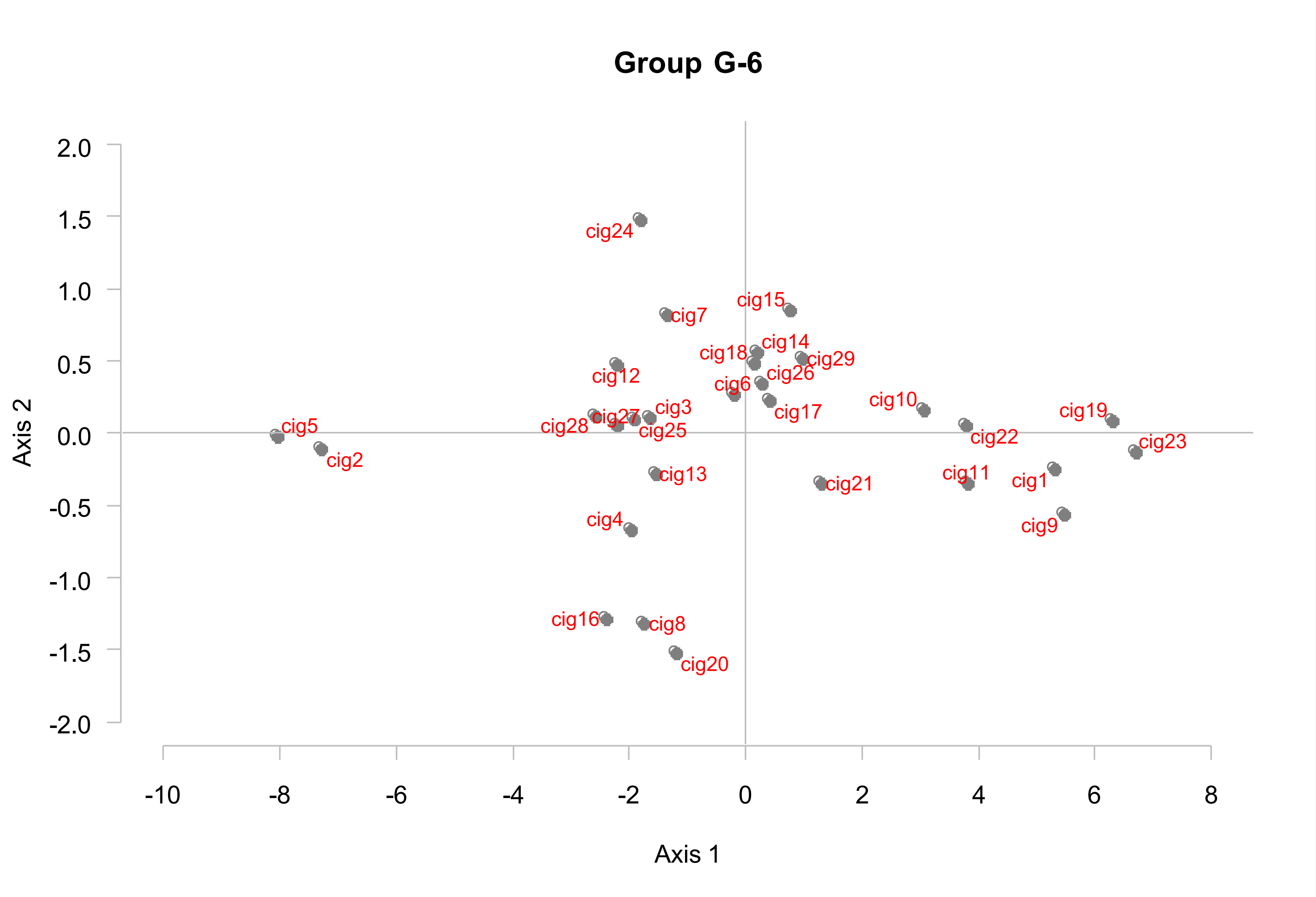
Graphing variables



How to operate the THEME R-software?

7. Reaping results

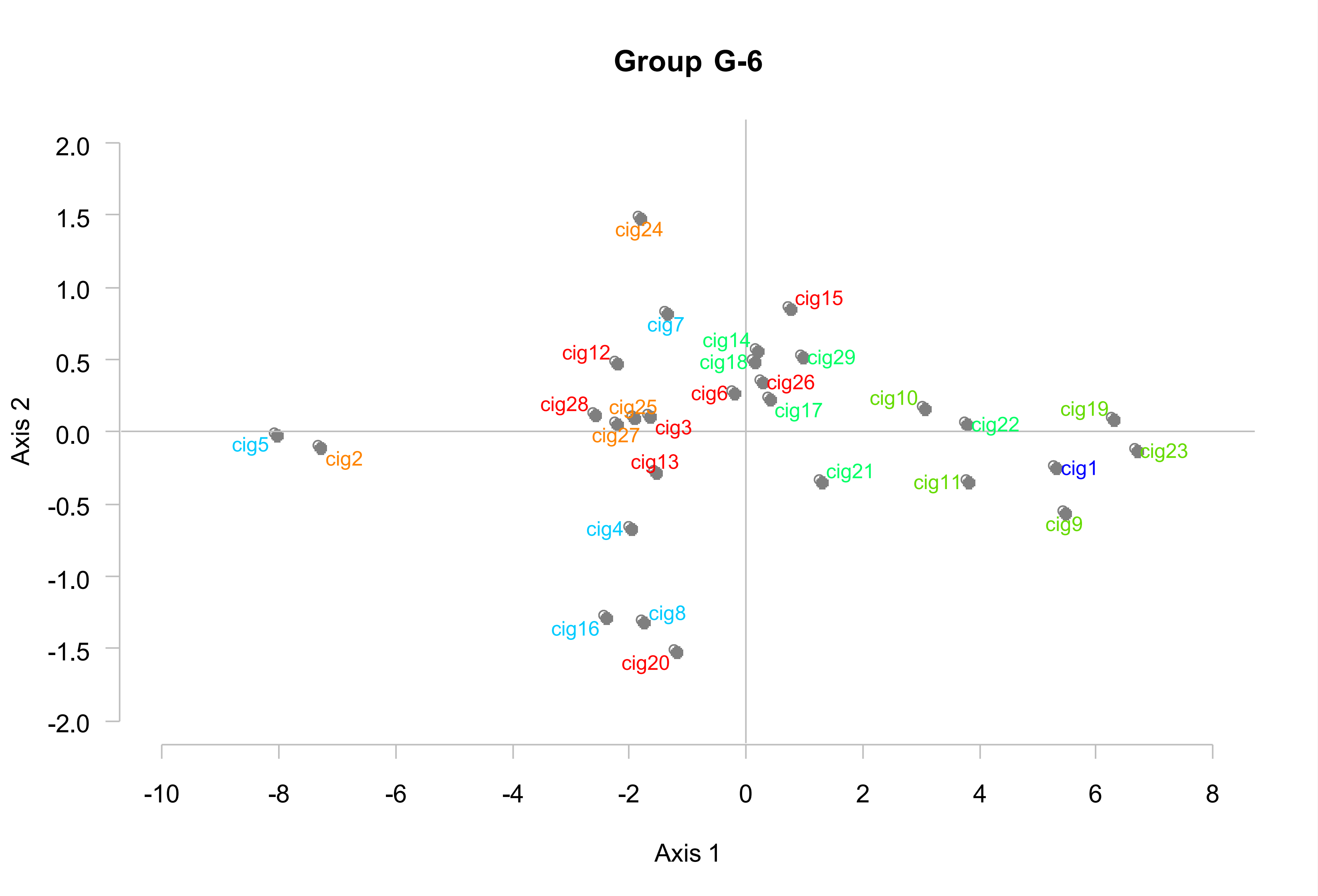
Graphing observations



How to operate the THEME R-software?

7. Reaping results

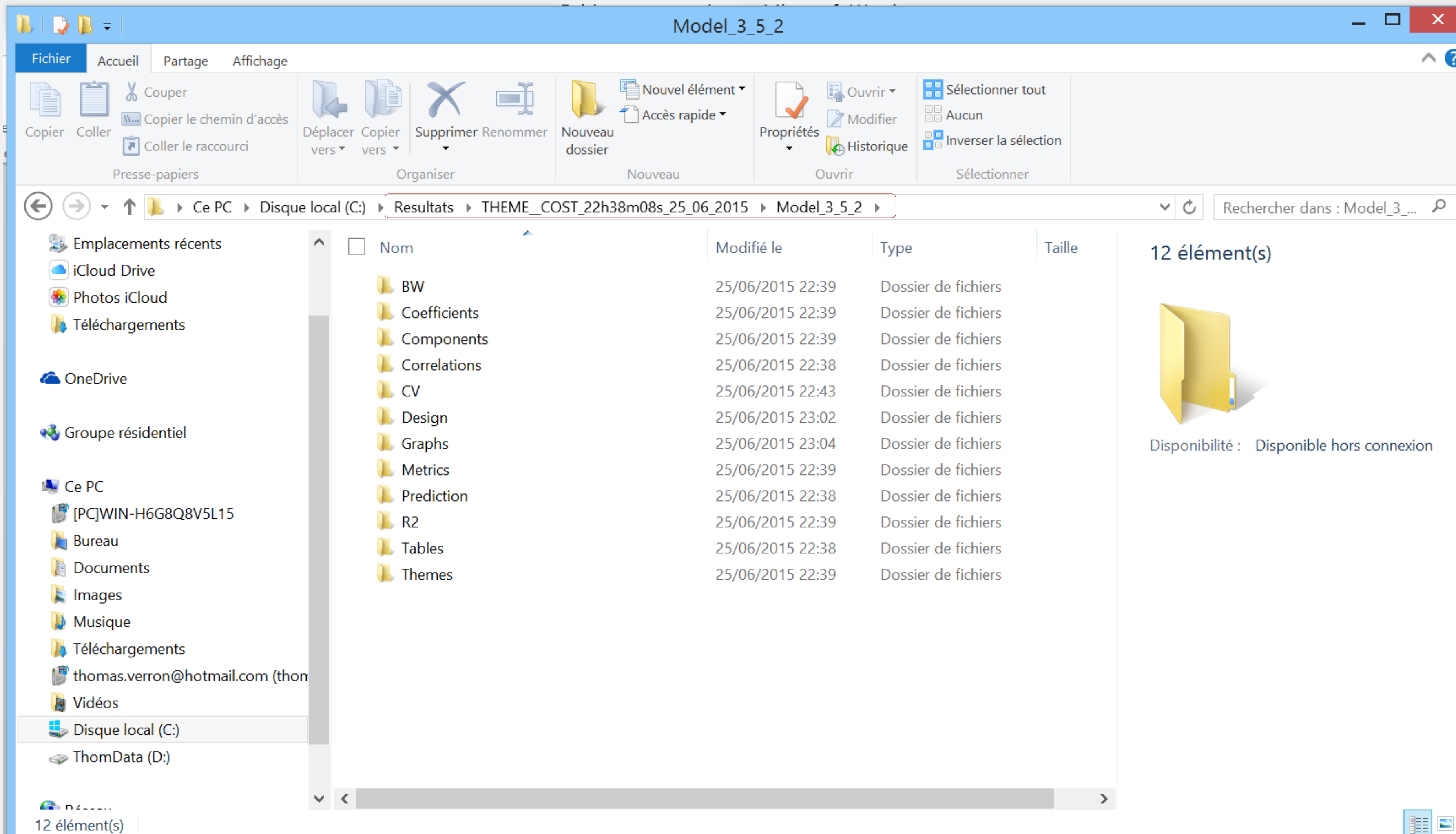
Graphing observations



How to operate the THEME R-software?

7. *Reaping results*

Getting ALL the results in sub-folders:



How to operate the THEME R-software?

7. Reaping results

Equation 1

.	*	**	***

Dependent variables

		NFDPM	Nicotine	CO	Acetaldehyde	Acrolein	Formaldehyde	BaP	NNK	NNN
Group 1	F1	0,03	-0,09	0,24	0,13	0,21	0,28	0,02	-0,40	-0,32
	F2	-0,22	-0,64	0,34	0,26	0,48	0,00	-0,53	-0,21	0,06
Group 2	F1	-0,19	-0,28	0,09	-0,06	-0,06	-0,10	-0,27	-0,47	-0,07
Group 3	F1	0,30	0,40	0,16	0,13	-0,03	0,17	0,41	0,19	0,05
	F2	0,06	0,06	-0,12	0,02	0,02	0,03	0,15	-0,18	0,38
Group 4	F1	-0,67	-1,02	0,10	-0,12	0,11	-0,09	-0,74	-0,95	-0,46
	F2	0,17	0,10	0,24	0,22	0,10	0,18	0,23	0,25	-0,34

Equation 2

		NFDPM	Nicotine	CO	Acetaldehyde	Acrolein	Formaldehyde	BaP	NNK	NNN
Group 7	F1	-0,13	-0,13	-0,08	-0,11	-0,10	-0,04	-0,22	-0,38	0,13
	F2	-0,12	-0,20	0,01	0,02	0,02	0,17	-0,07	-0,37	-0,48
	F3	0,06	0,22	-0,15	0,06	0,13	0,18	0,12	0,14	-0,60
Group 5	F1	0,50	0,43	0,60	0,50	0,51	0,51	0,33	-0,04	0,61
	F2	-0,01	-0,05	-0,04	0,08	0,08	0,25	0,00	0,01	-0,57

How to operate the THEME R-software?

7. Reaping results

Equation 1 . * ** *** *Dependent variables*

		NFDPM	Nicotine	CO	Acetaldehyde	Acrolein	Formaldehyde	BaP	NNK	NNN
Group 1	F1	0,03	-0,09	0,24	0,13	0,21	0,28	0,02	-0,40	-0,32
	F2	-0,22	-0,64	0,34	0,26	0,48	0,00	-0,53	-0,21	0,06
Group 2	F1	-0,19	-0,28	0,09	-0,06	-0,06	-0,10	-0,27	-0,47	-0,07
Group 3	F1	0,30	0,40	0,16	0,13	-0,03	0,17	0,41	0,19	0,05
	F2	0,06	0,06	-0,12	0,02	0,02	0,03	0,15	-0,18	0,38
Group 4	F1	-0,67	-1,02	0,10	-0,12	0,11	-0,09	-0,74	-0,95	-0,46
	F2	0,17	0,10	0,24	0,22	0,10	0,18	0,23	0,25	-0,34

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	F2	-0,12	-0,20	0,01	0,02	0,02	0,17	-0,07	-0,37	-0,48
	F3	0,06	0,22	-0,15	0,06	0,13	0,18	0,12	0,14	-0,60
Group 5	F1	0,50	0,43	0,60	0,50	0,51	0,51	0,33	-0,04	0,61
	F2	-0,01	-0,05	-0,04	0,08	0,08	0,25	0,00	0,01	-0,57

Equation 1 . * ** *** *Dependent variables*

		NFDPM	Nicotine	CO	Acetaldehyde	Acrolein	Formaldehyde	BaP	NNK	NNN
Group 1	F1	0,03	-0,09	0,24	0,13	0,21	0,28	0,02	-0,40	-0,32
	F2	-0,22	-0,64	0,34	0,26	0,48	0,00	-0,53	-0,21	0,06
	C_TO	0,99	0,25	-1,02	-37,51	-6,55	-1,60	1,71	6,58	1,14
	Mal_TO	-0,63	-0,18	0,88	30,60	5,23	3,03	-1,14	-7,07	-7,91
	N_TO	0,19	0,13	-1,11	-33,58	-5,43	-8,17	0,51	12,52	28,28
	PP_TO	0,92	0,16	-0,07	-9,60	-2,10	6,05	1,42	-4,67	-25,84
	MV_TO	0,00	0,00	0,00	0,14	0,02	0,00	-0,01	-0,02	0,01
	Asp_TO	2,50	0,84	-4,91	-162,08	-27,19	-24,08	4,80	45,33	74,36
	Cit_TO	-0,25	-0,01	-0,34	-7,62	-1,04	-4,74	-0,32	5,68	18,09
	NO3_TO	-2,53	-0,53	1,31	58,58	10,86	-7,11	-4,13	-0,82	37,11
	Alka_TO	1,67	0,46	-2,15	-75,58	-13,00	-6,33	2,98	16,32	14,87
	GFS_TO	0,05	0,00	0,09	2,14	0,31	1,10	0,05	-1,36	-4,13
	NH3_TO	-4,76	-0,64	-1,70	-10,28	1,39	-49,24	-6,92	49,83	197,75
	NAB_TO	-3,71	0,52	-12,94	-342,77	-51,81	-138,27	-3,06	181,82	510,65
	NAT_TO	-0,29	-0,01	-0,38	-8,56	-1,17	-5,36	-0,37	6,42	20,47
	NNK_TO	-2,83	-0,56	1,05	53,45	10,24	-11,55	-4,53	4,23	54,31
	NNN_TO	-0,06	0,02	-0,32	-8,88	-1,37	-3,20	-0,02	4,33	11,66
Group 2	F1	-0,19	-0,28	0,09	-0,06	-0,06	-0,10	-0,27	-0,47	-0,07
	Cit_PA	-1,80	-0,22	0,48	-16,81	-1,59	-4,72	-1,84	-20,54	-10,52
	PO4_PA	8,20	0,98	-2,18	76,34	7,22	21,43	8,34	93,27	47,77
	Acet_PA	-2,09	-0,25	0,56	-19,45	-1,84	-5,46	-2,12	-23,76	-12,17
	CaCO3_PA	-0,38	-0,05	0,10	-3,58	-0,34	-1,00	-0,39	-4,37	-2,24
	PERM1_SOD	-0,02	0,00	0,00	-0,16	-0,02	-0,04	-0,02	-0,19	-0,10
Group 3	F1	0,30	0,40	0,16	0,13	-0,03	0,17	0,41	0,19	0,05
	F2	0,06	0,06	-0,12	0,02	0,02	0,03	0,15	-0,18	0,38
	Mg_Ca_pc	0,06	0,01	0,01	0,79	-0,01	0,18	0,07	0,11	0,65
	Cl_TO	4,00	0,41	-1,05	46,02	1,11	10,30	5,15	-14,62	170,04
	PO4_TO	-2,85	-0,42	-6,40	-47,85	5,96	-10,45	0,17	-73,63	383,50
	K_pc_TO	4,34	0,47	0,63	53,63	-0,46	11,93	4,63	4,98	59,30
	Hg_TO	0,21	0,02	0,09	2,69	-0,08	0,60	0,19	0,97	-1,60
	Pb_TO	0,80	0,09	0,49	10,71	-0,44	2,37	0,65	5,34	-15,58
	Cd_TO	1,43	0,16	0,26	17,83	-0,20	3,97	1,50	2,28	15,76
	NO3_TO.1	2,70	0,31	1,00	34,67	-0,86	7,69	2,56	10,21	-5,76
Group 4	F1	-0,67	-1,02	0,10	-0,12	0,11	-0,09	-0,74	-0,95	-0,46
	F2	0,17	0,10	0,24	0,22	0,10	0,18	0,23	0,25	-0,34
	FDENSC	0,16	0,02	0,00	1,34	-0,04	0,19	0,13	1,06	1,01
	HC_BIN	-0,01	0,01	-0,09	-3,26	-0,20	-0,47	-0,03	-0,11	4,16
	PDEF	-0,07	-0,01	0,01	-0,36	0,03	-0,05	-0,06	-0,48	-0,80

Equation 2

		NFDPM	Nicotine	CO	Acetaldehyde	Acrolein	Formaldehyde	BaP	NNK	NNN
Group 7	F1	-0,13	-0,13	-0,08	-0,11	-0,10	-0,04	-0,22	-0,38	0,13
	F2	-0,12	-0,20	0,01	0,02	0,02	0,17	-0,07	-0,37	-0,48
	F3	0,06	0,22	-0,15	0,06	0,13	0,18	0,12	0,14	-0,60
	TAR	0,05	0,01	0,01	2,17	0,24	0,07	0,05	0,55	-0,77
	NICO	0,78	0,13	-0,47	32,32	4,77	2,55	0,79	8,61	-25,48
	CO	0,00	-0,01	0,12	0,87	-0,16	-0,24	0,00	0,02	2,37
	Acetal_MS	0,00	0,00	0,00	0,03	0,00	0,00	0,00	0,01	0,04
	Acro_MS	0,00	0,00	0,02	0,32	-0,01	-0,03	0,00	0,04	0,32
	Fo_MS	0,00	0,00	0,00	0,46	0,05	0,05	0,01	0,02	-0,44
	BaP_MS	0,07	0,01	-0,03	3,70	0,50	0,32	0,08	0,73	-3,05
	NNK_MS	0,01	0,00	0,00	0,05	0,00	-0,07	0,01	0,16	0,52
	NNN_MS	0,00	0,00	0,00	-0,07	-0,01	-0,03	0,00	0,04	0,24
Group 5	F1	0,50	0,43	0,60	0,50	0,51	0,51	0,33	-0,04	0,61
	F2	-0,01	-0,05	-0,04	0,08	0,08	0,25	0,00	0,01	-0,57
	FV	-0,06	0,00	-0,07	-3,45	-0,36	-0,25	-0,03	0,02	-0,92
	PD	0,05	0,00	0,05	4,65	0,49	0,58	0,02	0,00	-1,45
	PDFNE	-0,09	-0,01	-0,11	-4,60	-0,48	-0,26	-0,04	0,03	-2,02

How to get the THEME R-software?

Beta-version available for free, with quick guide.

Conclusion

Some differences with SEM estimation

***SEM* :**	***THEME* :**

Conclusion

Some differences with SEM estimation

SEM :	***THEME :***
Constraints on Latent Variables (LV): ➢ Distribution asumption (classically normal). ➢ One LV per theme. ➢ Regression-models relating LV's. ➢ Regression-models relating each LV to *all* observed variables in its theme (even the least useful for modelling!).	➢ Components belong to the observed space of their theme. No distribution assumption. ➢ Possibly several LV's per theme. Number found out. Hence full exploitation of theme dimensionality. ➢ Regression-models relating LV's. ➢ Bonus to flexible structural relevance (SR), apt to relate a component to the useful variables mostly.

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Estimation strategy: ➢ Plain likelihood maximization (MLE). No tuning parameters. Influence of theme-size. ➢ Estimation of *regression coefficients* based on the MLE of a constrained covariance matrix of the observed variables, or the EM algorithm. ➢ Possible estimation of expected values of LV's conditional on the data (through EM only) ➢ Problems with small samples.	➢ Tunable maximisation of trade-off criterion between GOF and SR. ➢ Calculation of component-values. ➢ Estimation of regression coefficients of all dependent variables (latent or observed). ➢ Cross-validation and assessment of model(s). ➢ Small samples OK.

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Prediction:	
➢ No prediction/regularisation performed.	➢ Regularised prediction of all dependent variables.

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Prediction:	
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Exploratory power:	
➢ Weak.	➢ High.

THE END

Thank you, all

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