

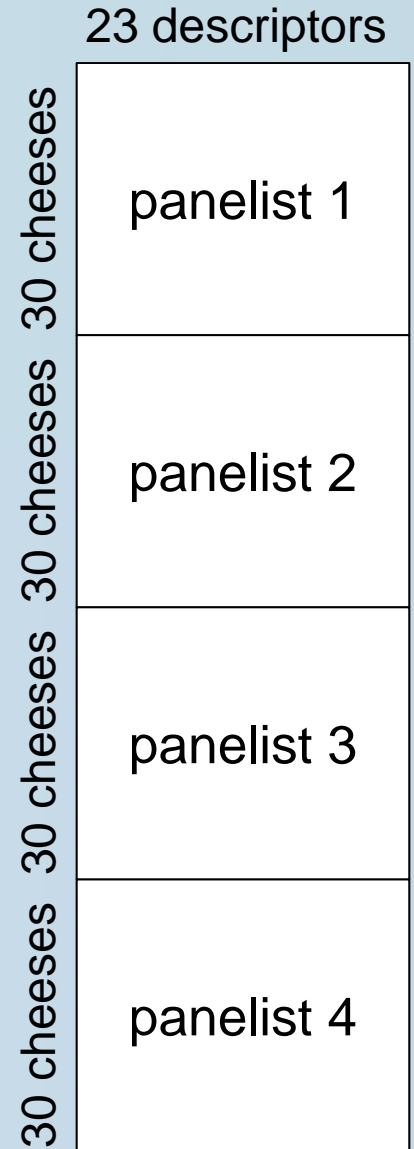


The CHull procedure for selecting among multilevel component solutions

Eva Ceulemans, K.U.Leuven
Marieke E. Timmerman, R.U.Groningen
Henk A.L. Kiers, R.U.Groningen

1. Class of multilevel component models

- two-level multivariate data
 - example: sensory profiling study
 - 8 panelists were asked to rate samples of 30 cream cheeses on 23 descriptors



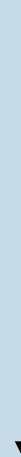
1. Class of multilevel component models

- similar to ANOVA, data are split up in two parts:

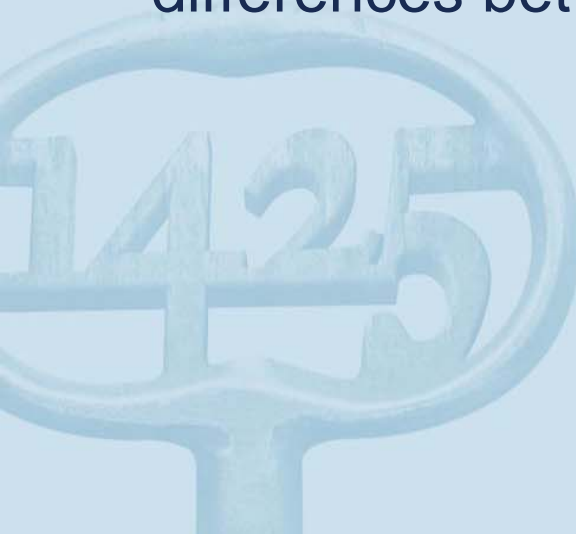
$$\text{DATA } (\mathbf{X}) = \text{BETWEEN PART } (\mathbf{X}^b) + \text{WITHIN PART } (\mathbf{X}^w)$$



mean values of each panelist
differences between-panelists

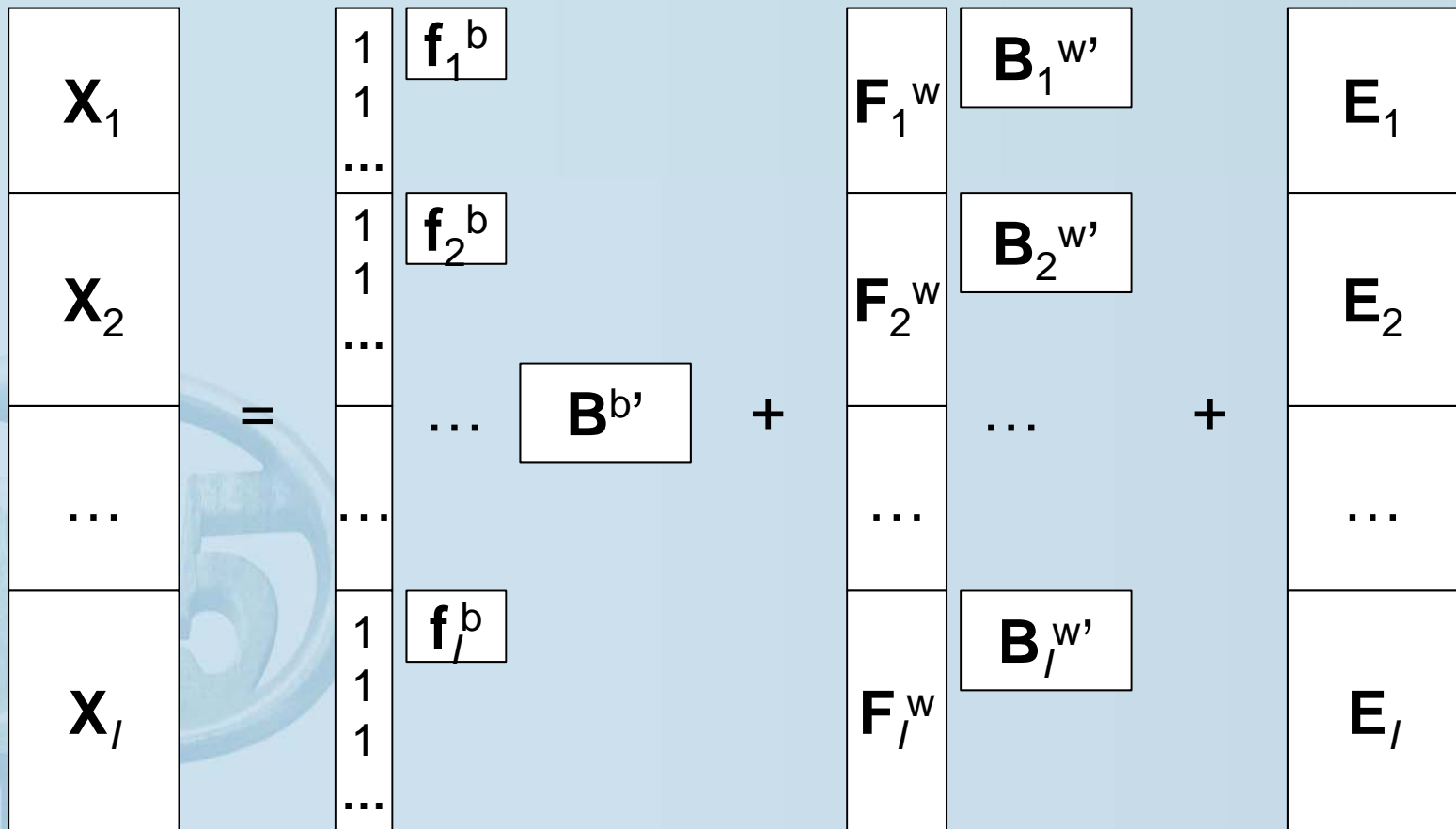


deviations from mean values per panelist
differences within-panelists



1. Class of multilevel component models

$$\begin{aligned} \mathbf{X}_i &= \mathbf{X}_i^b + \mathbf{X}_i^w \\ &= \mathbf{1}_{K_i} \mathbf{f}_i^b \mathbf{B}^{b'} + \mathbf{F}_i^w \mathbf{B}_i^{w'} + \mathbf{E}_i \end{aligned}$$



1. Class of multilevel component models

$$\mathbf{X}_i = 1_{K_i} \mathbf{f}_i^b \mathbf{B}^b + \mathbf{F}_i^w \mathbf{B}_i^w + \mathbf{E}_i$$

variant	Within-Loadings \mathbf{B}_i^w	Correlations \mathbf{F}_i^w	Variances \mathbf{F}_i^w
MLCA	Free	-	-
MLSCA-P	Equal for all i	Free	Free
MLSCA-PF2	Equal for all i	Equal for all i	Free
MLSCA-IND	Equal for all i	Equal to 0	Free
MLSCA-ECP	Equal for all i	Equal for all i	Equal for all i

1. Class of multilevel component models

$$\begin{array}{c}
 \boxed{\mathbf{x}_1} \\
 \boxed{\mathbf{x}_2} \\
 \dots \\
 \boxed{\mathbf{x}_l}
 \end{array}
 =
 \begin{array}{c}
 1 \\
 1 \\
 \dots \\
 1 \\
 1 \\
 \dots \\
 1 \\
 1 \\
 1 \\
 \dots
 \end{array}
 \begin{array}{c}
 \boxed{\mathbf{f}_1^b} \\
 \boxed{\mathbf{f}_2^b} \\
 \dots \\
 \boxed{\mathbf{f}_l^b}
 \end{array}
 \boxed{\mathbf{B}^{b'}}
 +
 \begin{array}{c}
 \boxed{\mathbf{F}_1^w} \\
 \boxed{\mathbf{F}_2^w} \\
 \dots \\
 \boxed{\mathbf{F}_l^w}
 \end{array}
 \boxed{\mathbf{B}^{w'}}
 +
 \begin{array}{c}
 \boxed{\mathbf{E}_1} \\
 \boxed{\mathbf{E}_2} \\
 \dots \\
 \boxed{\mathbf{E}_l}
 \end{array}$$

2. CHull heuristic

- between-model selection problem
 - number of between-components?
- within-model selection problem
 - variant? number of within-components?
- formal rule which assesses complexity of different solutions by considering number of free parameters (Ceulemans & Kiers, 2006)



2. CHull heuristic: within-part

$$\mathbf{X}_i^w \approx \mathbf{F}_i^w \mathbf{B}_i^w$$

component scores + # loadings - Q_w^2 - Q_w



transformation freedom



mean within-component score of each panelist = 0

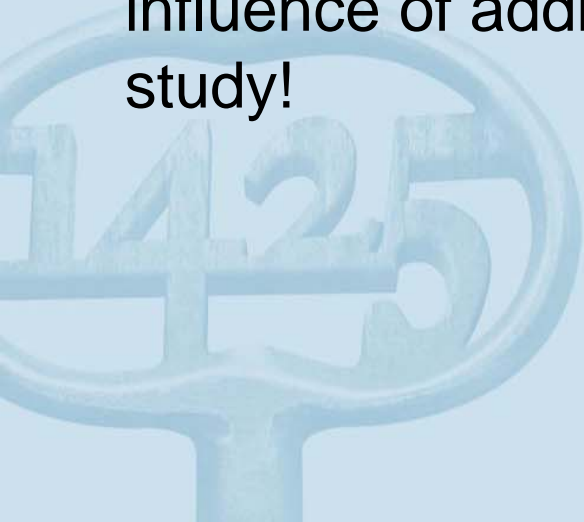


2. CHull heuristic: within-part

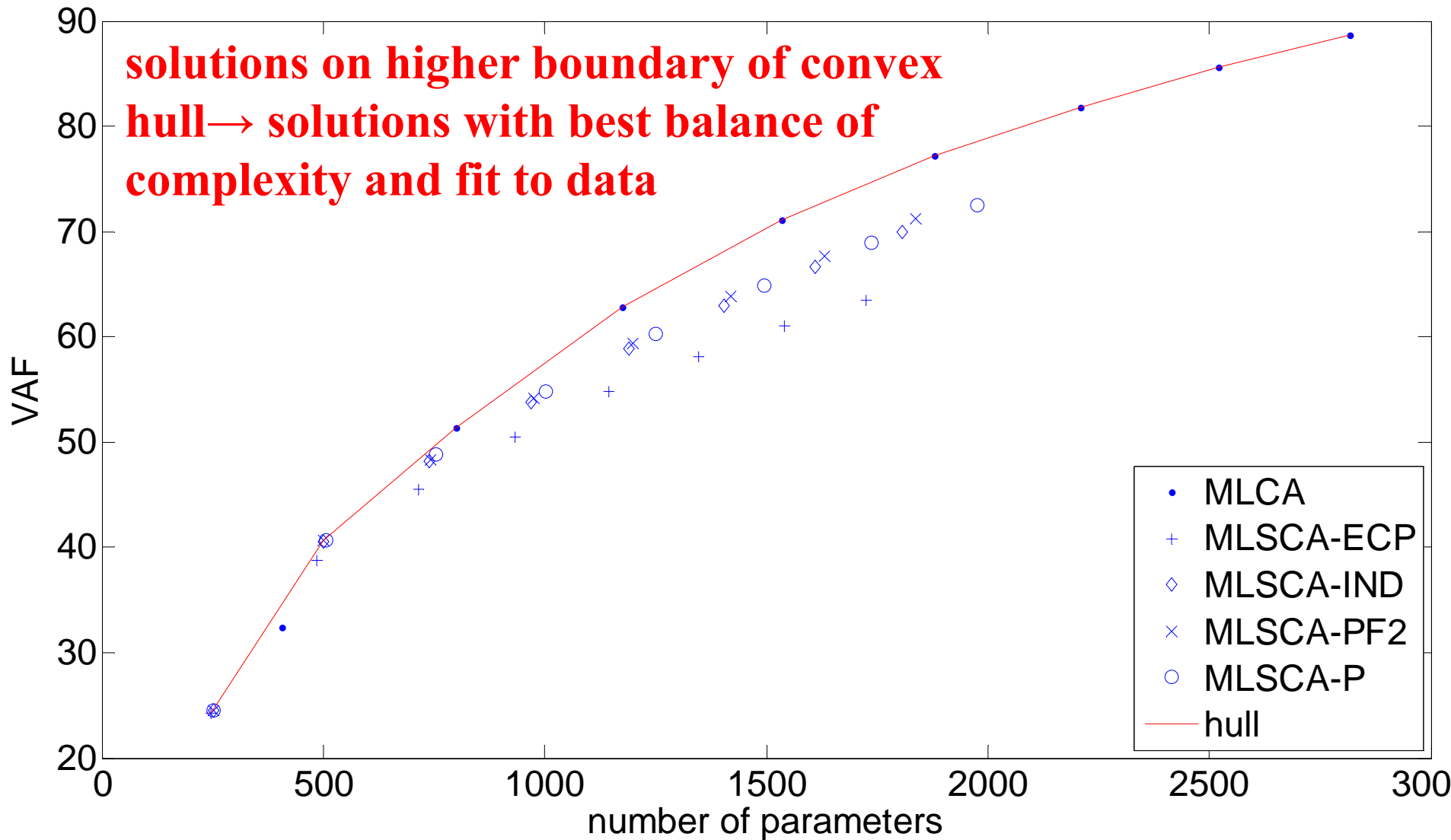
$$\mathbf{X}_i^w \approx \mathbf{F}_i^w \mathbf{B}_i^w$$

component scores + # loadings – $Q_w^2 - Q_w$

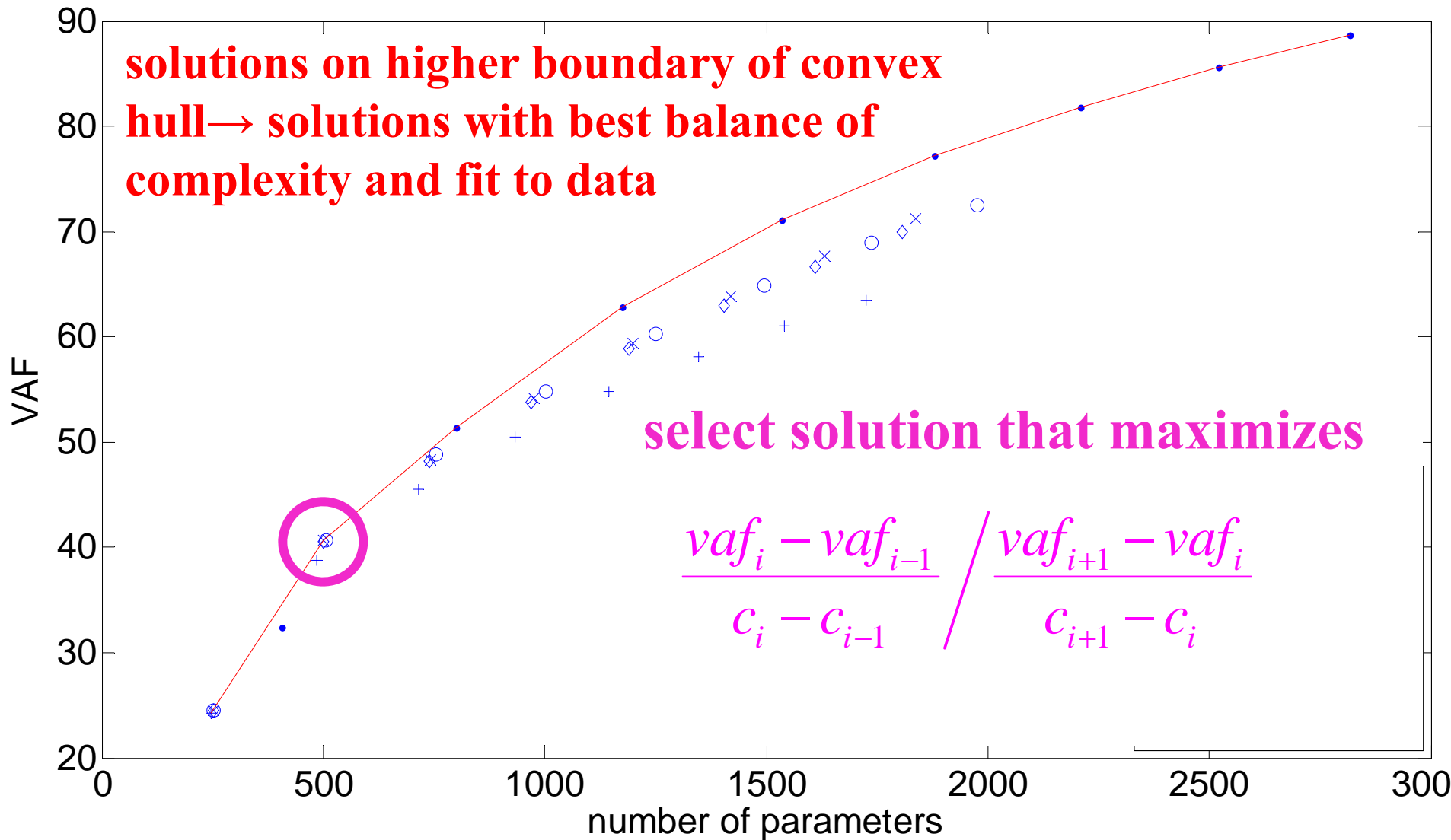
- #cheeses* Q_w : if #cheeses increases, term becomes too large
- $\min(\text{\#cheeses}, \ln(\text{\#cheeses}) * \text{\#variables}) * Q_w$: mitigates influence of additional cheeses -> works well in simulation study!



2. CHull heuristic: within-part



2. CHull heuristic: within-part



3. Simulation study: 84240 data sets

- assessing the number of between-components: easy (98.8%)
- determining the number of within-components: easy (91.4%)
- tracing the underlying within-model variant (60.71%):
 - differences in within-loadings: easy
 - differences in variances of within-components: easy
 - differences in correlational structure of within-components: difficult (procedure often indicates that correlations differ, whereas they do not)

4. Discussion

- CHull heuristic is a useful tool
- more fundamental problem remains: how to determine number of free parameters in component analysis?



References

- Ceulemans, E., & Kiers, H.A.L. (2006). Selecting among three-mode principal component models of different types and complexities: A numerical convex hull based method. *British Journal of Mathematical and Statistical Psychology*, 59, 133-150.
- Ceulemans, E., Timmerman, M.E., & Kiers, H.A.L. (in press). The CHULL procedure for selecting among multilevel component solutions. *Chemometrics and Intelligent Laboratory Systems*.
- Timmerman, M.E. (2006). Multilevel component analysis. *British Journal of Mathematical and Statistical Psychology*, 59, 301–320.