Bayesian Methods for Tensor Decompositions



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BIT50 June 19, 2010

A common problem encountered in Modern Massive Datasets (MMDS)

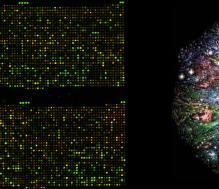
1) Multiple comparisons 2)What is the true number of independent tests (data highly correlated) 3) Data extremely noisy, i.e. low SNR rendering tests insignificant.

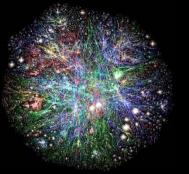


 \mathbf{X}^{Gene} seq.×Samples

 $\mathbf{X}^{Webpages imes Webpages} \quad \mathbf{X}^{Term imes Document}$

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Neurol nformatics

BioInformatics ComplexNetworks WebDataMining

Unsupervised Learning attempts to find the hidden causes and underlying structure in the data. (Multivariate exploratory analysis – driving hypotheses)



Goal of unsupervised Learning (Ghahramani & Roweis, 1999)

- Perform dimensionality reduction
- Build topographic maps
- Find the hidden causes or sources of the data
- Model the data density
- Cluster data

Purpose of unsupervised learning (Hinton and Sejnowski, 1999)



Extract an efficient internal representation of the statistical structure implicit in the inputs





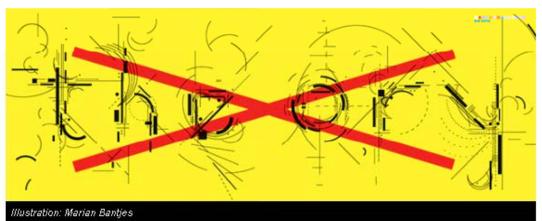
WIRED MAGAZINE: 16.07

2008

SCIENCE : DISCOVERIES 题

The End of Theory: The Data Deluge Makes the Scientific Method Obsolete

By Chris Anderson 🖂 👘 06.23.08



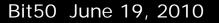
THE PETABYTE AGE:

Sensors everywhere. Infinite storage. Clouds of processors. Our ability to capture, warehouse, and understand massive amounts of data is changing science, medicine, business, and technology. As our collection of facts and figures grows, so will the opportunity to find answers to fundamental questions. Because in the

"All models are wrong, but some are useful."

So proclaimed statistician George Box 30 years ago, and he was right. But what choice did we have? Only models, from cosmological equations to theories of human behavior, seemed to be able to consistently, if imperfectly, explain the world around us. Until now. Today companies like Google, which have grown up in an era of massively abundant data, don't

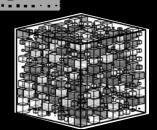
Analysis of massive amounts of data will be the main driving force of all sciences in the future!!



Vector: 1-way array/ 1st order tensor,

Matrix: 2-way array/ 2nd order tensor,

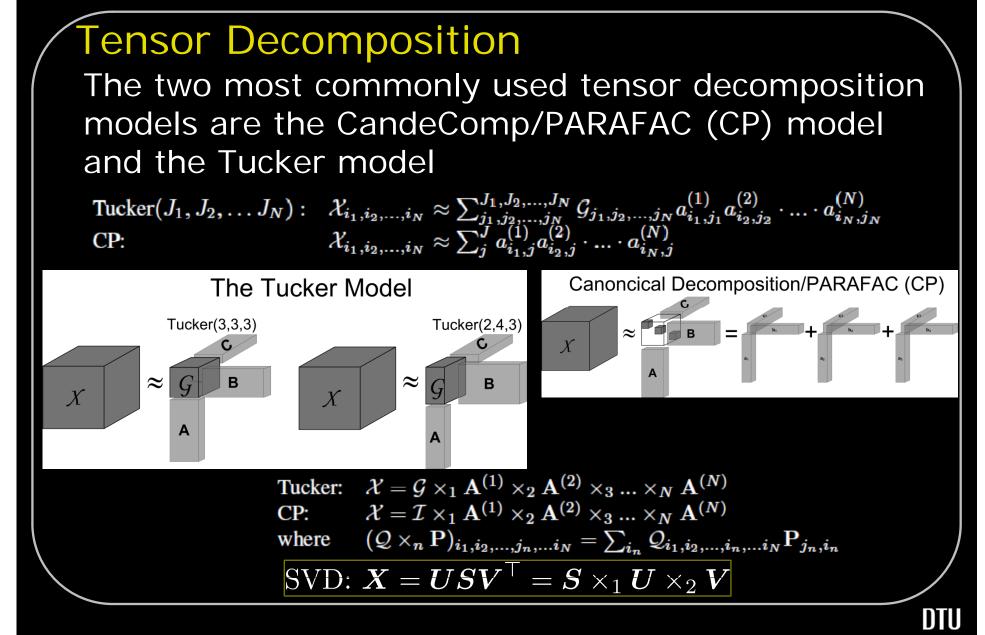
3-way array/3rd order tensor



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Multi-way modeling has become an important tool for **Unsupervised Learning** and are in frequent use today in a variety of fields including

- Psychometrics (Subject x Task x Time)
- **Chemometrics** (Sample x Emission x Absorption)
- Neurolmaging (Channel x Time x Trial)
 - Textmining (User x Query x Webpage or Webpage x Webpage X Anchor text)
 - Signal Processing (ICA, i.e. diagonalization of Cummulants)



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Important Question:

What constitutes an adequate number of components?

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i.e. determining J for CP and $J_1, J_2, ..., J_N$ for Tucker, is an open problem, particularly difficult for the Tucker model as the number of components are specified for each modality separately

Notice:

CP-model unique

 $\mathcal{X} \approx (\mathcal{D} \times_1 \mathbf{Q} \times_2 \mathbf{R} \times_3 \mathbf{S}) \times_1 (\mathbf{A}\mathbf{Q}^{-1}) \times_2 (\mathbf{B}\mathbf{R}^{-1}) \times_3 (\mathbf{C}\mathbf{S}^{-1}) = \widetilde{\mathcal{D}} \times_1 \widetilde{\mathbf{A}} \times_2 \widetilde{\mathbf{B}} \times_3 \widetilde{\mathbf{C}}.$

Tucker model not unique

 $\mathcal{X} \approx (\mathcal{G} \times_1 \mathbf{Q} \times_2 \mathbf{R} \times_3 \mathbf{S}) \times_1 (\mathbf{A}\mathbf{Q}^{-1}) \times_2 (\mathbf{B}\mathbf{R}^{-1}) \times_3 (\mathbf{C}\mathbf{S}^{-1}) = \widetilde{\mathcal{G}} \times_1 \widetilde{\mathbf{A}} \times_2 \widetilde{\mathbf{B}} \times_3 \widetilde{\mathbf{C}}.$ However, contrary to SVD neither of the two models are nested, i.e., factors for the smaller models not in general contained in larger model!







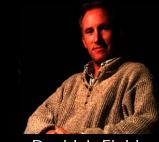
Bruno A. Olshausen

Nature, 1996

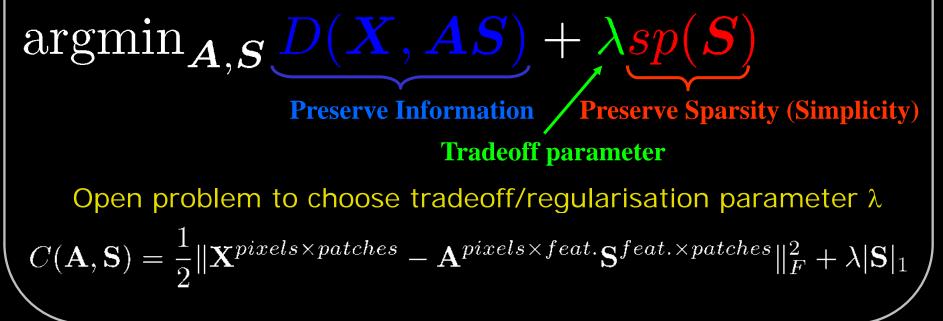
Emergence of simple-cell receptive field properties by learning a sparse code for natural images

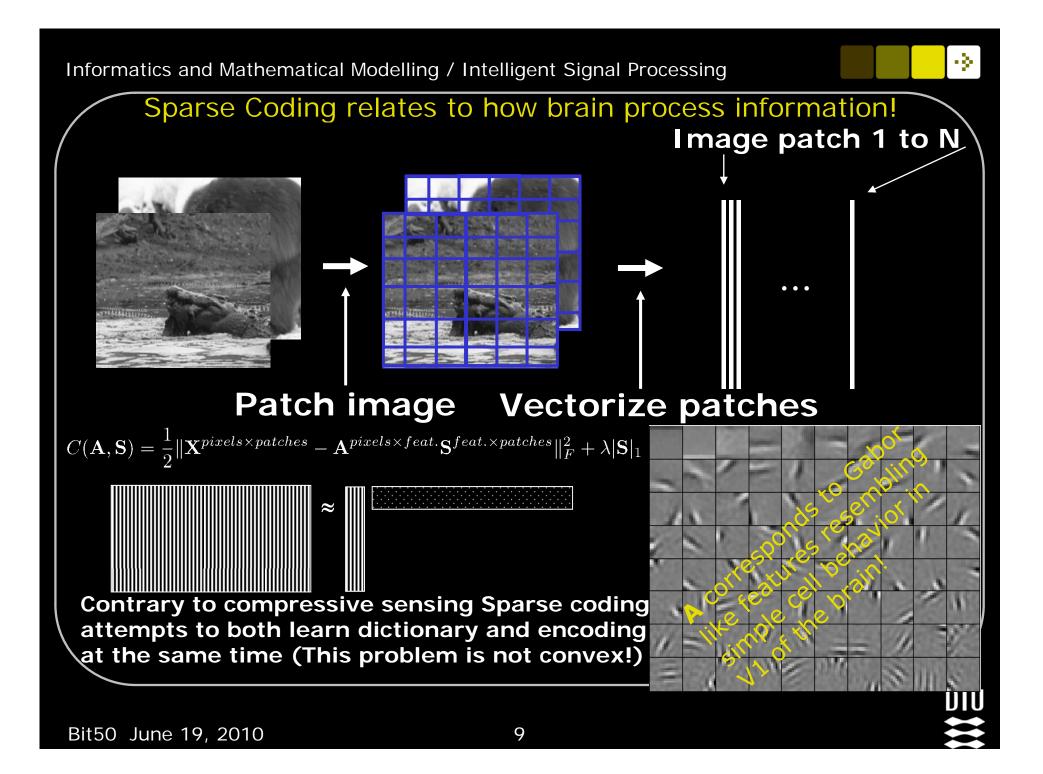
Bruno A. Olshausen* & David J. Field

Department of Psychology, Uris Hall, Cornell University, Ithaca, New York 14853, USA



David J. Field

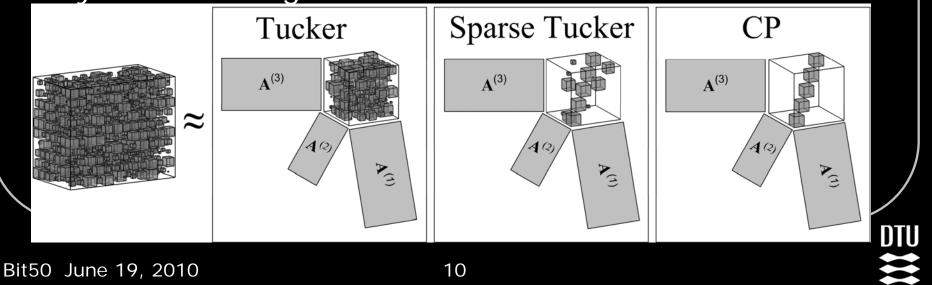






Agenda

- To use sparse coding to Simplify the Tucker core forming a unique representation as well as enable interpolation between the Tucker (full core) and CP (diagonal core) model.
- To use sparse coding to turn off excess components in the CP and Tucker model and thereby select the model order.
 - To tune the pruning/regularization strength from data by Automatic Relevance Determination (ARD) based on Bayesian learning.



Bayesian Learning and the Principle of Parsimony

The explanation of any phenomenon should make as few assumptions as possible, eliminating those that make no difference in the observable predictions of the explanatory hypothesis or theory.

William of Ockham

To get the posterior probability distribution, multiply the prior probability distribution by the likelihood function and then normalize

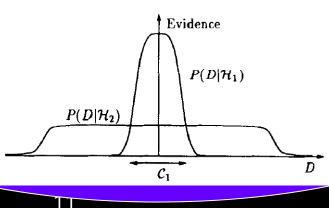


Thomas Bayes

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Bayesian learning embodies Occam's razor, i.e. Complex models are penalized.

David J.C. MacKay





Many inference paradigms in Bayesian Learning

- Maximum a posteriori estimation (MAP) seeks optimal solution (admit standard optimization) however, the approach does not take parameter uncertainty into account
- Sampling methods Marcov Chain Monte Carlo (MCMC)
 - Variational methods (VB) and Belief Propagation (BP) Approximate likelihood P(θ) by factorized form Q(θ) that is tractable VB: minimize the Kulback Leibler divergence KL(P(θ)|Q(θ)) BP: minimize the Kulback Leibler divergence KL(Q(θ)|P(θ))

(Notice: Bayesian Learning based on MAP admits direct use of all your favorite standard optimization tools)

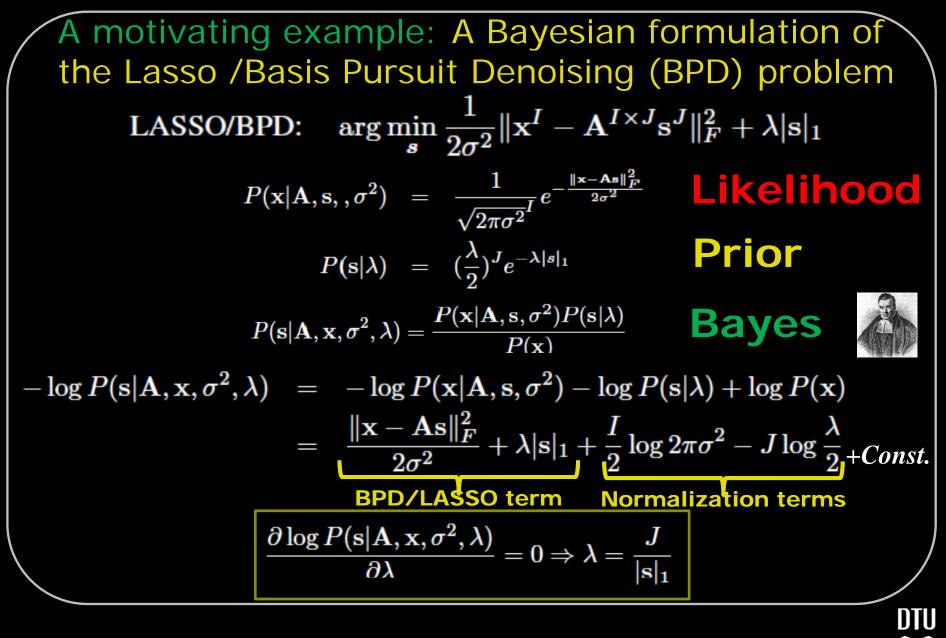
Automatic Relevance Determination (ARD)

- Automatic Relevance Determination (ARD) is a hierarchical Bayesian approach widely used for model selection
- In ARD hyper-parameters explicitly represents the relevance of different features by defining their range of variation.

(i.e., Range of variation $\rightarrow 0 \Rightarrow$ Feature removed)



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ARD in reality a l_0 -norm optimization scheme. As such ARD based on Laplace prior corresponds to

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 ℓ_0 -norm optimization by re-weighted ℓ_1 -norm

In particular if we define λ for each entry in s, i.e.

$$\frac{1}{2\sigma^2} \|\mathbf{x}^I - \mathbf{A}^{I \times J} \mathbf{s}^J\|_F^2 + \sum_j \lambda_j |\mathbf{s}_j|$$

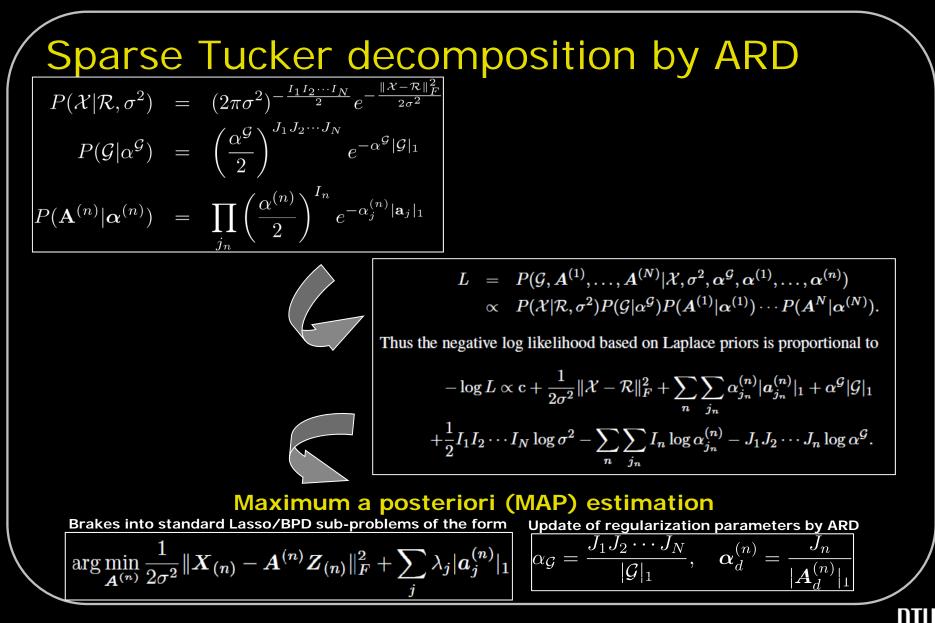
Corresponding to the Laplace prior $P(\mathbf{s}|\boldsymbol{\lambda}) = \prod_{j \geq 2} e^{-\lambda_j |s_j|}$ optimizing for λ_j gives $\lambda_j = \frac{1}{|s_j|}$ such that

$$\frac{1}{2\sigma^2} \|\mathbf{x}^I - \mathbf{A}^{I \times J} \mathbf{s}^J\|_F^2 + \sum_j \frac{|\mathbf{s}_j|}{|\mathbf{\widetilde{s}}_j|}$$

 ℓ_0 norm by re-weighted ℓ_2 follows by imposing Gaussian prior instead of Laplace

Notice that we are all the time monotonically decreasing

 $-\log P(\mathbf{s}|\mathbf{A},\mathbf{x},\sigma^2,\lambda)$



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Solving efficiently the Lasso/BPD sub-problems

Algorithm 1 Gradient Based Sparse Coding (GBSC): $A = \text{GBSC}(X, Z, \lambda)$, solves $\arg \min_{A} \frac{1}{2} ||X - AZ||_{F}^{2} + \sum_{j} \lambda_{j} |a_{j}|_{1}$

1: repeat

2: Take gradient step according to LS-objective

$$A^{new} \leftarrow A^{old} - \mu(AZ - X)Z$$

4: Take gradient step according to l_1 -regularization

5: if
$$|a_{i,j}^{new}| < \mu \lambda_j$$
 then

$$a_{i,j}^{new} = 0$$

7: else

$$a_{i,j}^{new} = a_{i,j}^{new} - \mu \lambda_j \operatorname{sign}(a_{i,j}^{new})$$

- 9: end if
- 10: Estimate μ by line-search
- 11: until Convergence

	100 imes256	256 imes 256	1000 imes 256	2500 imes256
SIGNSEARCH	0.0750 ± 0.0359	$\textbf{0.1984} \pm \textbf{0.1342}$	0.3734 ± 0.1759	$\textbf{1.6969} \pm \textbf{0.6441}$
CONJUGATE GRADIENT	0.4172 ± 0.0651	1.1219 ± 0.2560	9.0297 ± 1.8055	45.6297 ± 12.0142
LARS	0.0453 ± 0.0226	0.1313 ± 0.0787	0.4313 ± 0.1477	1.9813 ± 0.6342
NNQP	0.5703 ± 0.0696	0.9313 ± 0.0748	2.8719 ± 0.1389	15.5047 ± 0.7882
GBSC	0.0125 ± 0.0066	0.3172 ± 0.2121	2.0688 ± 1.0760	22.8828 ± 12.2846

Notice, in general the alternating sub-problems for Tucker estimation have J<I!

The Tucker ARD Algorithm

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Algorithm 2 Sparse Tucker estimation based on Automatic Relevance Determination (ARD)

- 1: set J_1, J_2, \ldots, J_n large enough to encompass all potential models, $\sigma^2 = \|\mathcal{X}\|_F^2/(I_1I_2\cdots I_n(1+10^{\text{SNR}/10}))$, set $\alpha_{\mathcal{G}} = 0$, $\alpha^{(n)} = 0$ and initialize by random $A^{(n)}$ for $n = 1, 2, \ldots, N$
- 2: repeat
- 3: $Q = A^{(1)} \otimes A^{(2)} \otimes \ldots \otimes A^{(N)}, \operatorname{vec}(\mathcal{G}) \leftarrow \operatorname{gbsc}(\operatorname{vec}(\mathcal{X}), Q, \sigma^2 \alpha_{\mathcal{G}}),$ 4: $\alpha_{\mathcal{G}} = \min\{\frac{J_1 J_2 \cdots J_N}{1}, \frac{1}{2}\}$

5:
$$\mathcal{R} = \mathcal{G} \times_1 A^{(1)} \times_2 A^{(2)} \times_3 \ldots \times_N A^{(N)}$$

- 6: **for** n=1:N **do**
- 7: $Z_{(n)} = (\mathcal{R} \times_n A^{(n)^{\dagger}})_{(n)}, A^{(n)} \leftarrow \operatorname{gbsc}(X_{(n)}, Z_{(n)}, \sigma^2 \alpha^{(n)}), \alpha_d^{(n)} = \min\{\frac{J_n}{|A_{\ell}^{(n)}|_1}, \frac{1}{\epsilon}\}$

8: If
$$\alpha_{j_n}^{(n)} = \frac{1}{\epsilon}$$
 then $J_n = J_n - 1$, $A^{(n)} = A^{(n)}_{\backslash j_n}$, $\mathcal{G} = \mathcal{G}_{\backslash j_n}$,

9:
$$\alpha^{(n)} = \alpha^{(n)}_{\setminus j_n}$$
 end

10:
$$R_{(n)} = A^{(n)} Z_{(n)}$$

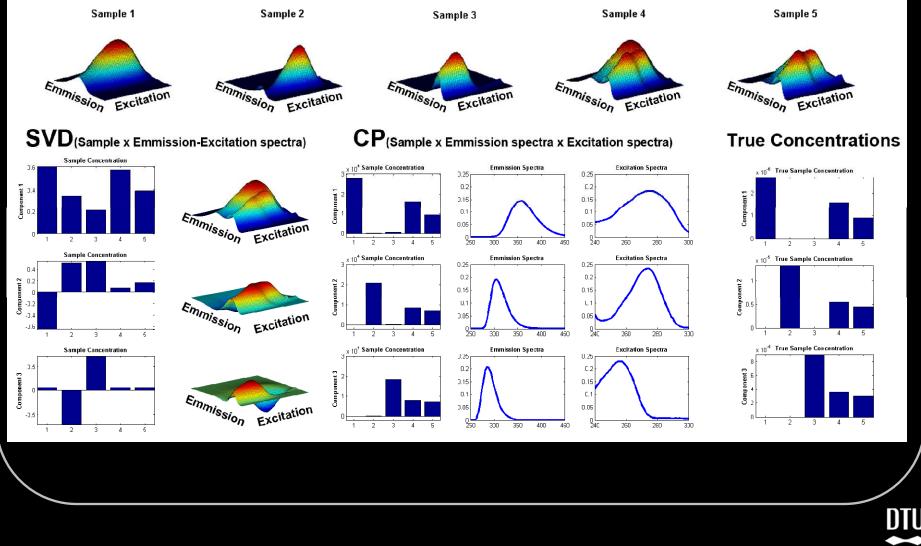
11: end for

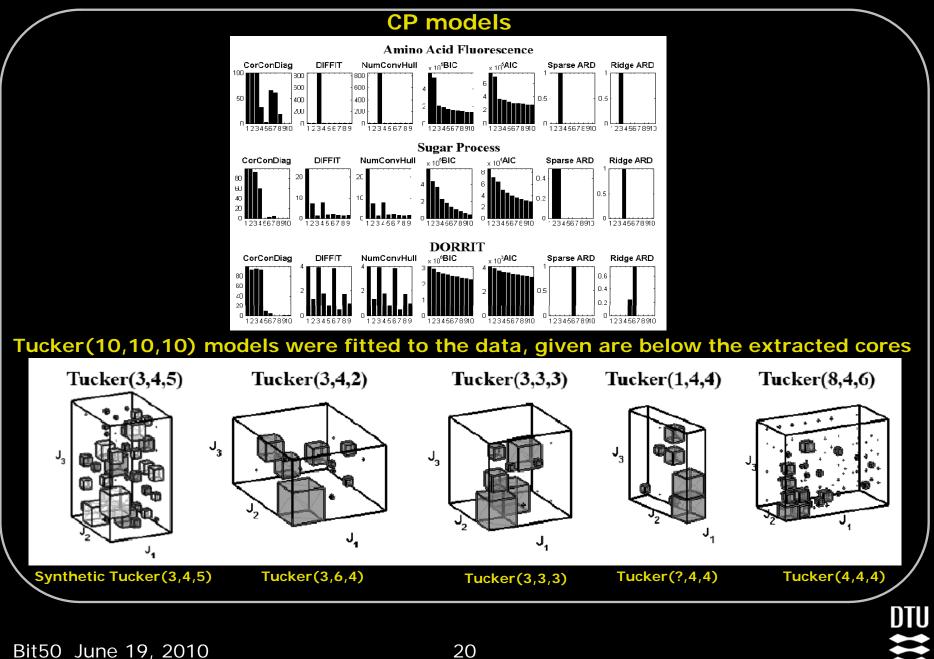
12: **until** convergence

CP follows setting G=IEstimating the number of components comes at the same cost as fitting one conventional model!

Results on Fluorscence spectroscopy data

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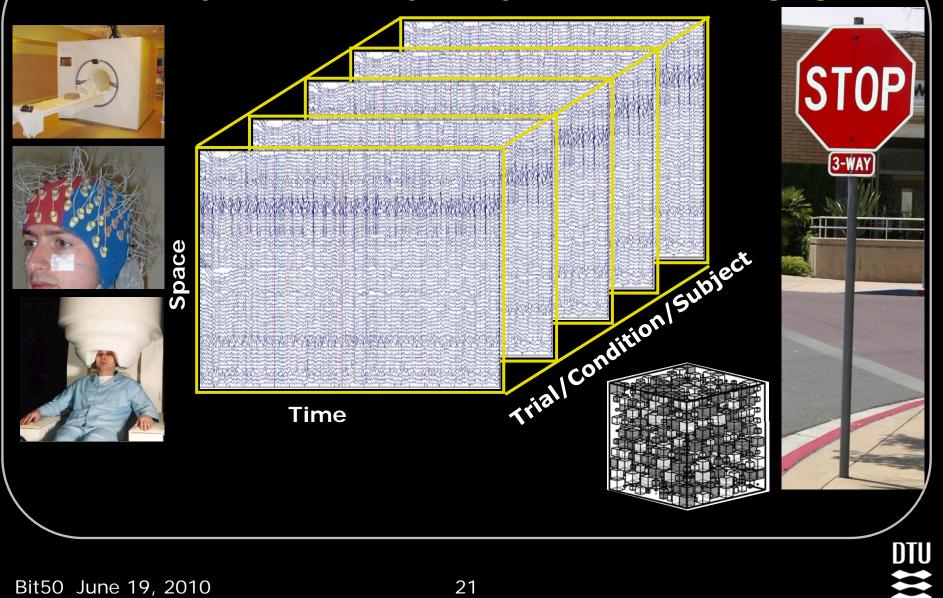


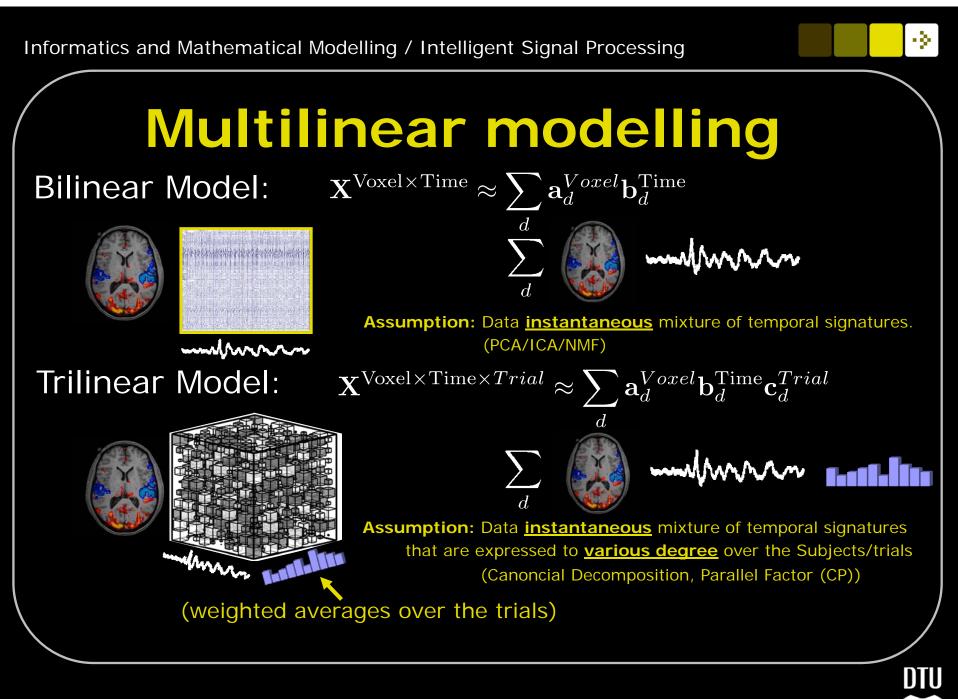


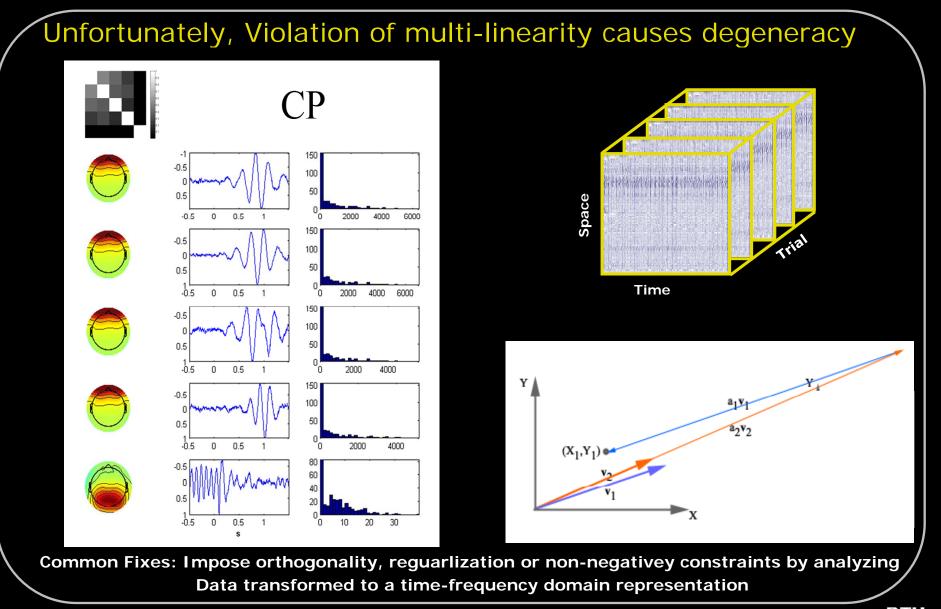
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From 2-way to multi-way analysis of Neurolmaging data

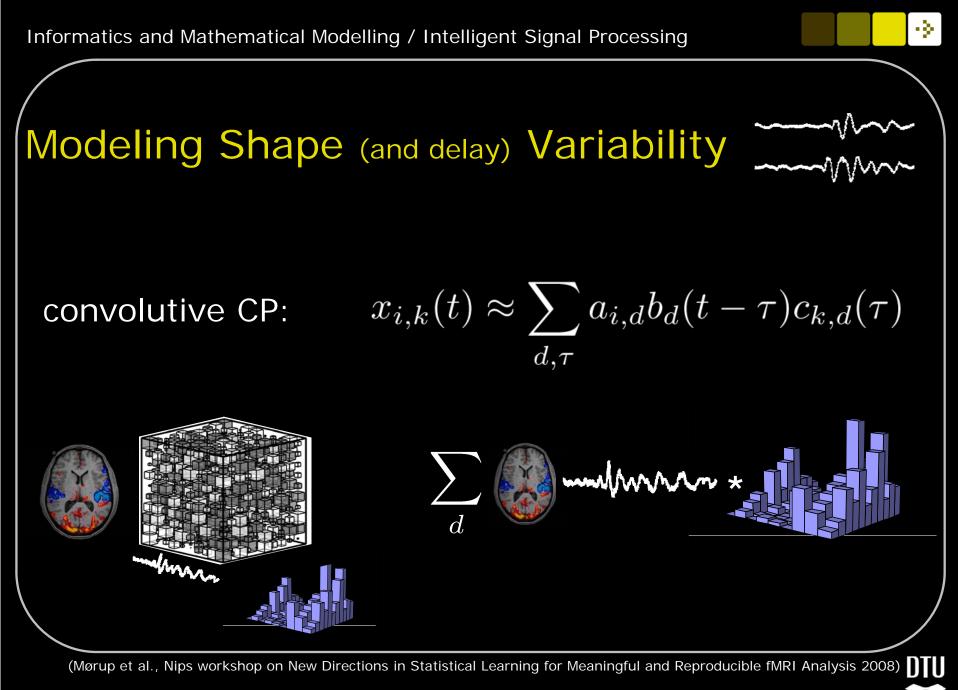
÷2.





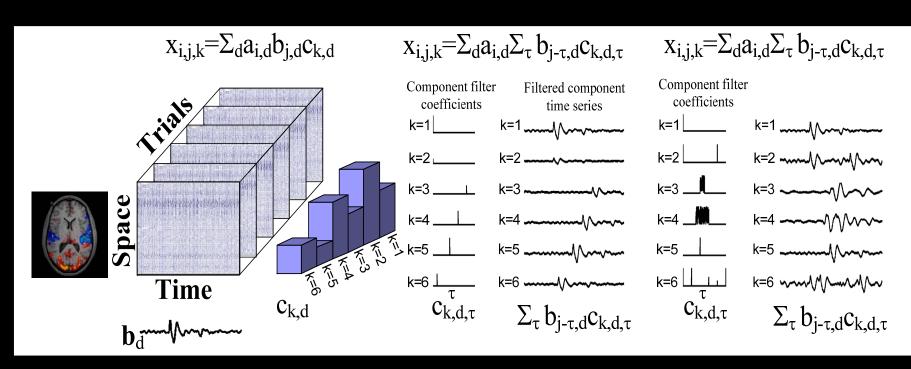


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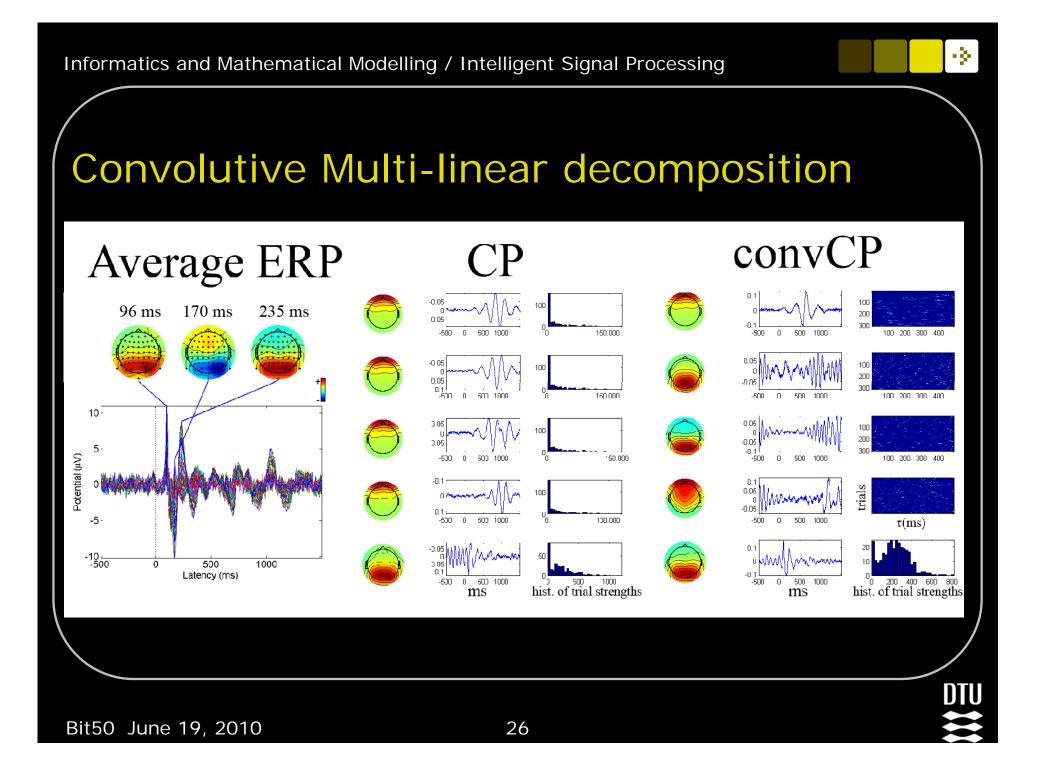


CP, ShiftCP and ConvCP

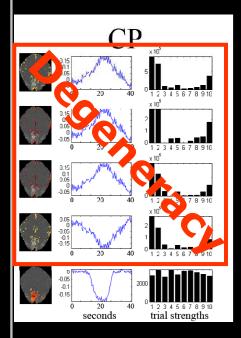


ConvCP: Can model arbitrary number of component delays within the trials and account for shape variation within the convolutional model representation. Redundancy between what is coded in C and B resolved by imposing sparsity on C. Number of components and sparsity cegularisation identifed through ARD.

(Mørup et al., Nips workshop on New Directions in Statistical Learning for Meaningful and Reproducible fMRI Analysis 2008)





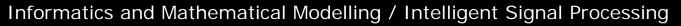


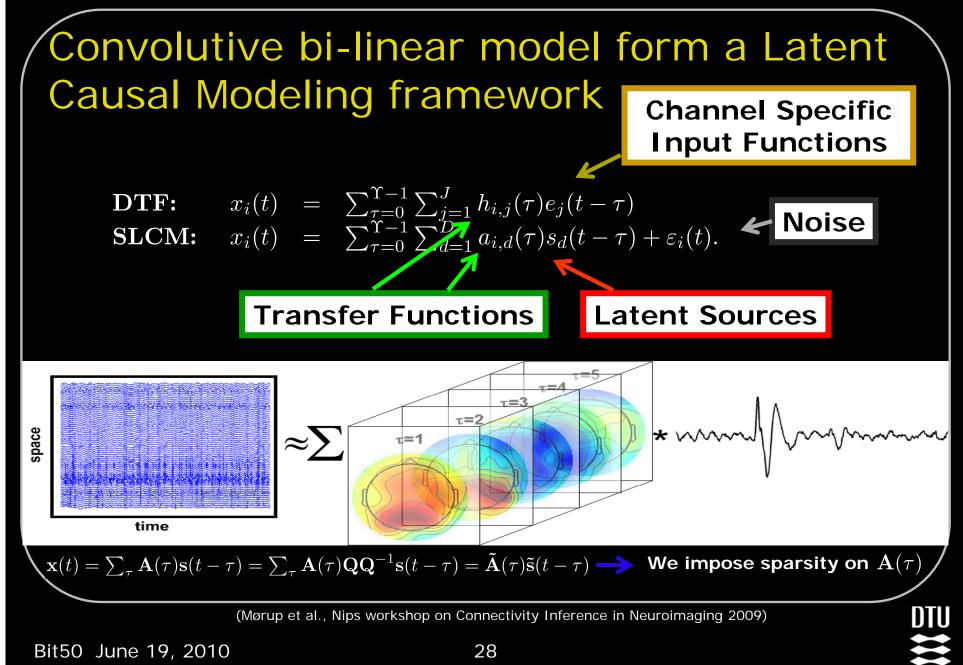
Each trial consists of a visual stimulus delivered as an annular full-field checkerboard reversing at 8 Hz.

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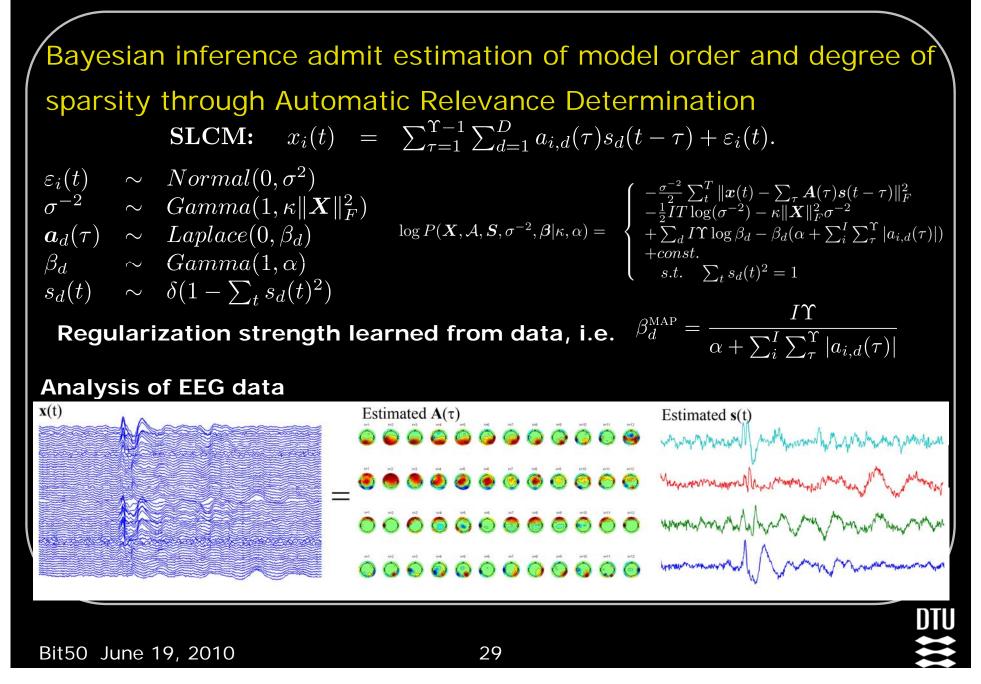
λ' is ℓ_1 sparsity regularization imposed on third mode

(Mørup et al., Nips workshop on New Directions in Statistical Learning for Meaningful and Reproducible fMRI Analysis 2008)





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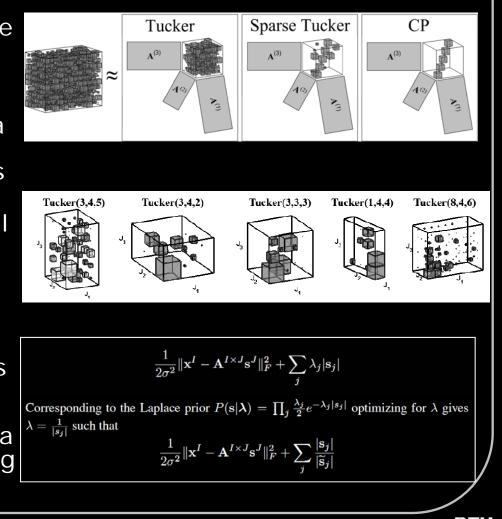


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Conclusion

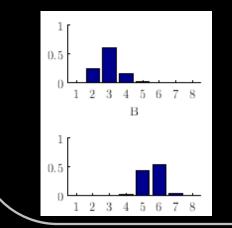
- Imposing sparseness on the core enable to interpolate between Tucker and CP model
- ARD from Bayesian learning based on MAP estimation form a simple framework to tune the pruning in sparse coding models giving the model order.
- ARD framework especially useful for the Tucker model where the order is specified for each mode separately which makes exhaustive evaluation of all potential models expensive.
- ARD-estimation based on MAP is closely related to ℓ_0 norm estimation based on reweighted ℓ_1 and ℓ_2 norm. Thus, ARD form a principled framework for learning the sparsity pattern.

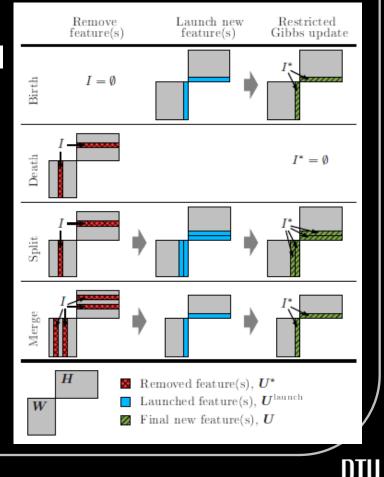


Current research

Non-parametric efficient sampling approaches for model order estimation based on reversible jump MCMC for the described models.

(See also Schmidt and Mørup, Infinite Non-negative Matrix Factorization, to appear EUSIPCO 2010)





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References

- M. Mørup, Applications of tensor (multi-way array) factorizations and decompositions in data mining, to appear Wiley DMKD 2010.
- M. N. Schmidt, M Mørup, Infinite Non-negative Matrix Factorization, to appear Eusipco 2010
- M. Mørup, L.K. Hansen, Automatic Relevance, Determination for multi-way models, Journal of Chemometrics, 2009
- M. Mørup, Kristoffer H. Madsen, L.K. Hansen, Latent Causal Modeling of Neuroimaging Data, NIPS workshop on Connectivity inference in Neuroimaging data, 2009
- M. Mørup, L.K. Hansen, S.M. Arnfred, L.-K. Lim, K.M. Madsen, Shift Invariant Multilinear Decomposition of Neuroimaging Data, NeuroImage vol. 42(4), pp.1439-50, 2008
- M. Mørup, Kristoffer H. Madsen, L.K. Hansen Modeling trial based neuroimaging data, Nips workshop on New Directions in Statistical Learning for Meaningful and Reproducible fMRI Analysis, 2008



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