Thursday, September 26, 2019 Explainable AI and dimensionality reduction | AI Village learning session #2



Explainable AI, Cognitive Science and Culture:

Towards a transparent, democratic and secular AI

Harald Martens

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Explainable AI, Cognitive Science and Culture:

Towards a transparent, democratic and secular AI

PCA and bi-linear data modelling A toolbox for discovering the real world

Outline:

- 30 min:
 - What is soft modelling?
 - What is PCA, and how can it be used
- 10 min break
- 30 min
 - Explainable AI
 - Bilinear PCA extensions
- Discussion

Vårt fargesyn er bra, men begrenset



Vår hørsel er bra, men begrenset





Trad. instruments: 1 channel



Trad. instruments: 1 channel

2 channels

Utvid sansene				
Trad. instruments: 1 channel	2 channels	A guitar: 6 string	12 strings	

Utvid sansene				<image/>
Trad. instruments: 1 channel	2 channels	A guitar: 6 string	12 strings	A grand piano : Lots of keys

Utvid sansene				<image/>
Trad. instruments: 1 channel	2 channels	A guitar: 6 string	12 strings	A grand piano : Lots of keys



A band: 7 instruments



A band: 7 instruments

A symphony orchestra: 100 instruments



Further compressed into chords only



Further compressed into chords only







A cacophony of sounds









A cacophony of sounds









Human Perception

and

Interpretation

Data







Human Perception

and

Interpretation

Data













5 2 2.5 Time (s)



(+ «random» noise)

Ordinate:

Amplitude:

How strong

Two types of info in data from any instrument:



Abscissa: Pitch: Which tone? Which rotation rate of machinery?

The Math Gap



The Math Gap



The Math Gap



A two-way bridge across the math gap



Source of knowledge at any given moment



Two roads from question to answer in science and technology



Two roads from question to answer in science and technology



Two roads from question to answerIn science and technology

machine learning



Two roads from question to answer in science and technology



Two roads from question to answer



Two roads from question to answer in science and technology



Verden har mønstre – finn dem

Big Data Cybernetics: Combining advanced process control and chemometrics



Dept. Engineering Cybernetics, NTNU Trondheim 2018/2019:

5 +1 professors, lots of students:

«How to discover the real world»





SYKEHUSET ØSTFOLD



+ banks, metallurgy & other industry ...

Big Data Cybernetics: Combining advanced process control and chemometrics

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5 +1 professors, lots of students: **«How to discover the real world**»







• SYKEHUSET ØSTFOLD



+ banks, metallurgy & other industry ...








idletechs Analytics



idletechs Application



A causal phenomenon's time-dependent development







A causal phenomenon's Its multi-channel property profile time-dependent development







A causal phenomenon's time-dependent development

Its multi-channel property profile





Vector algebra First: Caspar Wessel from Vestby, 1797

600







CAUSAL MATH MODEL: $A_{obs} = B \times C + D$



How Quantitative Big Data are NOT analyzed





How Quantitative Big Data are sometimes analyzed today





How Quantitative Big Data may be analyzed

Multivariate analysis:



Naturens rytmer og harmonier (eller mangel på sådan)

Fem ulike forskningsgruppers estimat av jordklodens gjennomsnitts-temperatur

1880-2014

(New Scientist August 2015)



The earth's average temperature from 1880 till 2014, as estimated by five different laboratories (from New Scientist 2015)









(New Scientist August 2015

Data driven multivariate modelling by PCA will reveal *expected patterns* and *unexpected patterns*



Data driven multivariate modelling by PCA will reveal *expected patterns* and *unexpected patterns*



Three of the 5 (or e.g. 50 000?) available variables



Mean centering:



First principal component:



Multivariate soft data-modelling gives fewer, but more sensitive alarms, for three different types of abnormalities:



Data driven multivariate modelling by PCA will reveal *expected patterns* and *unexpected patterns*



Data driven multivariate modelling by PCA will reveal *expected patterns* and *unexpected patterns*



Data driven multivariate modelling will also reveal *unexpected patterns*



b)

Data driven multivariate modelling will also reveal *unexpected patterns*



b)

Find patterns in a data set, e.g. consumer' purchase of products by PCA



The bilinear data-model as numbers, vectors and matrices:

Simple but mighty math

Principal Component Analysis illustrated

• 21 = 3×7 a = b × c

- 21 = 3×7 a = b × c
- $21.1 = 3 \times 7 + 0.1$

 $a = b \times c + d$

- 21 = 3×7 a = b × c
- $21.1 = 3 \times 7 + 0.1$ $a = b \times c + d$
- 41.1 = $3 \times 7 + 2 \times 10 + 0.1$ $a = b_1 \times c_1 + b_2 \times c_2 + d = \mathbf{b} \times \mathbf{c} + d$

Vector-algebra, published av Caspar Wessel 1797

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Vector-algebra, published av Caspar Wessel 1797



 $A = B \times C + D$

Matrix-algebra, published 1835

BIG DATA Rhythms

From data-table **A**, discover the unknown causal structure **B** \times **C** and noise **D**

- 21 = 3×7 $a = b \times c$
- $21.1 = 3 \times 7 + 0.1$ $a = b \times c + d$
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 $A = B \times C + D$ Matrix-algebra, published 1835

Rhythms **BIG DATA**

From data-table **A**, discover the unknown causal structure **B** \times **C** and noise **D**

Principal component-analyse (PCA or SVD): All multivariate methods' mother!

Automatic modelling of "ever-lasting" data streams

From raw streams of data, systematic patterns and relationships are automatically discovered and modelled. The data is stored in a highly compressed format:



Raffaele Vitale, Anna Zhyrova, João F. Fortuna, Onno E. de Noord, Alberto Ferrer, Harald Martens: On-The-Fly Processing of continuous high-dimensional data streams Chemometrics and Intelligent Laboratory Systems 161 (2017) 118–129 Idletechs AS provides new software tools for

automatic modelling & compression and for human interpretation,

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of multidimensional, dynamic data.

Utvid sansene

Vårt fargesyn er bra, men begrenset



Looking at art



Photographed in 3 colours (R,G,B)



Else Tronstad, Leksvika

Photographed in 3 colours (R,G,B)



Else Tronstad, Leksvika

Photographed in 3 colours (R,G,B)



Photographed in several hundred «colours» (wavelength channels in vis. & NIR) Courtesy of NMBU (Ingunn Burud)



Photographed in 3

colours (R,G,B)

Photographed in several hundred «colours» (wavelength channels in vis. & NIR) Courtesy of NMBU (Ingunn Burud)



Else Tronstad, Leksvika

Photographed in 3 colours (R,G,B)

Photographed in several hundred «colours» (wavelength channels in vis. & NIR) Courtesy of NMBU (Ingunn Burud)
Giving surgeons molecular view!

Multi-channel spectroscopy («Hyperspectral imaging») of muscle tissue in the Near-infrared wavelength range.

Hyperspectral NIR measurements of post-rigor porcine *l.dorsi* :

(Ingunn Burud, NMBU/Joao Fortuna NTNU)



Composite molecular image

10 min BREAK

Finn sam-variasjonsmønstre i en data-tabell



PCA, MCR, ICA osv

Data driven multivariate modelling will also reveal *unexpected patterns*



b)

Towards a transparent, democratic and secular Al

Artificial Intelligence (AI): A new « religion » ?

Automatically building mathematical models from BIG DATA

 \approx Machine learning

Previously ANN with sigmoid relations, now often CNN with piecewise linear relations For classification of images, language translation, forecasting in time, autonomous cars,...

Powerful methods. But slow, and difficult to optimize: Need LOTS of GOOD DATA.

Serious problems: Black box, and not always reliable predictions.

Towards a transparent, democratic and secular AI

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• Explainable AI (XAI):

 \approx *Interpretable* Machine Learning: CNN and hybrid modelling

• Several levels of interpretation:

«Outer level»: Explain why an AI system has made a certain decision, e.g. after an accident
«Inner level»: Discover and interpret new, systematic patterns in data

Towards a transparent, democratic and secular AI

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• My personal research agenda since 1972: Democratic, «secular» data modelling methods: Not mystical! Simple, open to surprise, interpretable in light of prior knowledge



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of multidimensional, dynamic data.

Thermal camera



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Purpose	Monitor furnace temperatures, e.g. outer surface, electrode or tap hole area,
	to detect anomalities and unexpected trends



Related example:



Continuous monitoring of wood ovens: Heating efficiency experiment at SINTEF 2018

Making quantitative data understandable for ordinary people: e.g. XAI for thermal analysis of high-power electrical equipment



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Making quantitative data understandable for ordinary people: e.g. XAI for thermal analysis of high-power electrical equipment



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Demo example (non-commercial ③): idletechs Home appliance equipment

Experiment setup:

- Instruments:
 - waffle iron
 - burger grill
 - curling iron
 - clothes iron
- Disturbances:
 - water bottle
 - tea cup
 - hair dryer
 - human interf
 - timers



Discovered State variable: Hamburger grill

- Trends of two timers
 - Built-in thermostat in equipment
 - 30min timer on equipment
 - Deviation in end, probable mistake in experiment





Discovered State variable: Heat dissipation hamburger grill

- Same timer trends as hamburger grill
- Small phase offset from heat source, suggests heat dissipation





Discovered State variable: Waffle iron

- Trends of two timers
 - Built-in thermostat in equipment
 - 30min timer on equipment





Discovered State variable : Heat dissipation waffle iron

- Same timer trends as waffle iron
- Small phase offset from heat source, suggests heat dissipation





Discovered State variable : Clothes iron



Discovered State variable : Curling iron

- Trends of two timers
 - Built-in thermostat in equipment
 - 30min timer on equipment
 - Manual timers in end of day
- Deviation around lunch
 - User paused equipment due to potential fire hazard

After all "natural" variations discovered, modelled and subtracted: Small but systematic Residuals

→ Fewer, more sensitive outlier warnings:

Finn sam-variasjonsmønstre i en data-tabell

PCA, MCR, ICA osv

Finn sam-variasjonsmønstre mellom to data-tabeller

PCR, PLSR, RR osv

Finn sam-variasjonsmønstre mellom to data-tabeller

PCR, PLSR, RR osv

Harald Martens, Kristin Tøndel, Gunnar Cedersund, Lars M. Munck (2017)

Nils K. Skjærvold, Helge Brovold, Hodjat Rahmati, Harald Martens, Kristin Tøndel, Gunnar Cedersund, Lars M. Munck (2017)

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How to teach mathematics to all types of scientists?

Matematikk uten tårer

Psykolog Helge Brovold, PhD: Fire veier inn i matematikken. Data fra 2200 jobbsøkere i Norge:

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Finn sam-variasjonsmønstre mellom to data-tabeller, bruk modell til prediksjon

PCR, PLSR, RR osv

Instrumentation example: Multivariate calibration of multi-wavelength NIR absorbance process spectroscopy

850 854 858 862 866 870 874 878 882 886 890 894 898 902 906 910 914 918 922 926 930 934 938 942 946 950 954 958 962 966 970 974 978 982 986 990 994 998 1002 1008 1014 1020 1026 1032 1038 104

Chemical mixtures of protein and starch powders, measured under different physical conditions Wavelength, nm 100 channels

«Best» channel: useless calibration Playing the piano with only one finger

Many complex samples similar to gas/oil/water/sand

Playing the same piano with two fingers

Playing the same piano with two fingers





Measure more than you need, for math is cheaper than physics



Measure more than you need, for math is cheaper than physics

Play your instrument with more than one finger at a time



Measure more than you need, for math is cheaper than physics

Play your instrument with more than one finger at a time

Don't use a black box if you can avoid it







What is CHEMOMETRICS ? A particular science culture & tool box for «soft multivariate data modelling»: interpretable machine learning





Success story: Multivariate calibration of high-speed nonselective instruments







Knowledge- & data-driven subspace modelling





idletechs Deshadowing via Informative Converse model: Separating illumination / ground properties in HSI

Data Model

In order to apply the described method, it is useful to first define a model for the measured data in each pixel:

 $\mathbf{Y} = \mathbf{C} \mathbf{S}^{\mathsf{T}} + \mathbf{D} \mathbf{Z}^{\mathsf{T}} + \mathbf{F}$

With:

 $\begin{cases} \mathbf{Z} = \mathbf{A}^{\mathsf{T}} \mathbf{S}^{\mathsf{T}} + \mathbf{Z}_{\perp \mathbf{S}}^{\mathsf{T}} \\ \mathbf{C} = \mathbf{D} \mathbf{B} + \mathbf{C}_{\perp \mathbf{D}} \end{cases}$

Where:

• Y is absorbance data obtained by sensor

- \bullet CST is the contribution of partially known effects (e.g. illumination variations, "shadows")
- $\bullet\, DZ^{\intercal}$ is the contribution of unknown effects (e.g. ground geology/biology variations)
- F is measurement noise, assumed normal
- $\cdot\,A$ captures the non-orthogonality between Z and S
- B captures the non-orthogonality between C and D

Assumptions

- Illumination effects are multiplicative in Reflectance
- Y data is given in Absorbance $(-\log_{10}(R))$
- Spectra of different illumination sources **S** are known

Earth Observing-1

Data from the Hyperion instrument onboard the EO-1 Satellite. Data contains 200 bands in the VIS-NIR region.



Input data Y, in RGB



Deshadowed image, in RGB



"Shadow" (illumination change) image, \widehat{CS}^{\intercal} , in RGB

J.F. Fortuna and H. Martens, *J. Spectral Imaging* **6**, a2 (2017)

Multivariate data modelling for de-shadowing of airborne hyperspectral imaging

Input HSI image, in RGB



How much trees and grass? Healthy trees?

Hybrid multivariate modelling of causalities in HSI spectra:

Example from arial surveillance of biological resources by NEO HYSPEX camera

How much trees and grass?

Healthy trees?

Input HSI image, in RGB



Hybrid multivariate modelling of causalities in HSI spectra:

Example from arial surveillance of biological resources by NEO HYSPEX camera



Input HSI image, in RGB



Shadow image

Input HSI image, in RGB

Deshadowed image

Shadow image















Industrial Big Data: new opportunities!





D DATES



























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Point temperatures / Cooling water temperatures



Making quantitative data understandable for ordinary people: e.g. XAI for thermal analysis of high-power electrical equipment



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Thermal camera



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Example of hybrid modelling:

Hyperspectral monitoring of the drying of wood



Hyperspectral video analysis: Hyperspectral image data streams interpreted by modeling known and unknown variations

Authors: P. Stefansson^a, J. Fortuna^{b, c}, H. Rahmati^b, I. Burud^a, T. Konevskikh^a, H. Martens^{b, c}

Eaculty of Science and Technology, Norwegian University of Life Sciences NMBU, <u>Drøbakveien</u> 31, 1430 Ås Udletechs AS, <u>Havnegata</u> 9, 7010 Trondheim Norway Department of Engineering Cybernetics, Norwegian University of Science and Technology NTNU, 7034 Trondheim Norway

a)



(2200 x 1070)

wavelengths

× 150 time points.

pixels

×159

Figure 2.12.1. The experiment. a) Illustration of experimental setup used to measure the spectral reflectance and weight of a drying wood sample. b) RGB rendering of wood sample in wet state (drying time = 0 hours). c) RGB rendering of wood sample in dry state (drying time = 21 hours).

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What are the

wood drying ?

* Spectra?

causes that control

* Spatial patterns?

* Time dynamics?



Figure 2.12.1. The experiment. a) Illustration of experimental setup used to measure the spectral reflectance and weight of a drying wood sample. b) RGB rendering of wood sample in wet state (drying time = 0 hours). c) RGB rendering of wood sample in dry state (drying time = hours).





P. Stefansson, J. Fortuna, H. Rahmati, I. Burud, T. Konevskikh, H. Martens (2019): Hyperspectral video analysis: Hyperspectral image data streams interpreted by modeling known and unknown variations. *In press*.

« AI » :



« XAI » : Combine knowledge and data





« XAI » : Combine knowledge and data



« XAI » : Combine knowledge and data



« XAI » : Combine knowledge and data



« XAI » : Combine knowledge and data



« XAI » : Combine knowledge and data



Since the Enlightenment: Now, with BIG DATA: Understand more! Understand less?

BIG DATA: Keep humans in the loop!

We need more Mathematical Modelling, more Statistical Assessment and more Learning from Data, but less Macho Mathematics, less Gucci Statistics and less Blind Machine Learning

Thank you!

