







About: Marco Spruit 2003 × Information Retrieval • Ph.D researcher in Computational Linguistics, University of Amsterdam 2007 • Assistant \rightarrow Associate • Big Data system professor Information ALL SOLUTION Science, Utrecht University Applied Data Science Lab 22 2020 Т • Product software Professor Translational \mathbf{O} Data Science in Population 2 Health, LUMC/Leiden 4 University LLI. • PH Living Lab S • CAIRE Lab LLI. • SIG Health Data Science



degree of fundamental understanding

What main methodology are you using for your analytics, data mining, or data science projects ? [200 votes total]

2014 poll 2007 poll





https://www.kdnuggets.com/polls/2014/analytics-data-mining-data-science-methodology.html



degree of practical use consideration



Chapman, P. Clinton, J., Kerber, R., Khabaza, T., Reinartz, T., Shearer, C., and Wirth, R. (2000). CRISP-DM 1.0 Step-by-step Data Mining Guide (p.6). [online]



 Basic
 Translational

 data science
 Translational

 Taxonomic
 Applied

 studies
 Applied

 data science
 data science

Business Understanding	Data Understanding	Data Preparation	Modeling	Evaluation	Deployment
Determine Business Objectives Background Business Objectives Business Objectives Business Success Criteria Assess Situation Inventory of Resources Requirements, Assumptions, and Constraints Risks and Constraints Risks and Constraints Risks and Constraints Risks and Constraints Determine Data Mining Goals Data Mining Goals Data Mining Success Criteria Produce Project Plan Project Plan Initial Assessment of Tools and Techniques	Collect Initial Data Initial Data Collection Report Describe Data Data Description Report Explore Data Data Exploration Report Verify Data Quality Data Quality Report	Select Data Rationale for Inclusion/ Exclusion Clean Data Data Cleaning Report Construct Data Derived Attributes Generated Records Integrate Data Merged Data Format Data Reformatted Data Dataset Dataset Description	Select Modeling Techniques Modeling Technique Modeling Assumptions Generate Test Design Build Model Parameter Settings Models Model Descriptions Assess Model Model Assessment Revised Parameter Settings	Evaluate Results Assessment of Data Mining Results w.r.t. Business Success Criteria Approved Models Review Process Review of Process Determine Next Steps List of Possible Actions Decision	Plan Deployment Deployment Plan Plan Monitoring and Maintenance Plan Produce Final Report Final Report Final Presentation Review Project Experience Documentation

Chapman, P. Clinton, J., Kerber, R., Khabaza, T., Reinartz, T., Shearer, C., and Wirth, R. (2000). *CRISP-DM* 1.0 Step-by-step Data Mining Guide (p.6). [online]



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Example: Understanding Long-term Care

- Portion of Dutch healthcare budget: 38% = 34B!
- Care Intensity Package (ZZP)
 - *ZZP1:* Extramural living with some guidance
 - ZZP8: Intramural living under full surveillance and 24/7 care
- 18 unstructured in-depth interviews
 - 8 (board of) directors experts
 - 7 management experts
 - 7 experts from stakeholders perspective (MinVWS, IGZ, Care insurer)
- 56 information needs derived (33Q, 23F) from 18 unstructured in-depth interviews with 22 experts

Spruit, M., Vroon, R., & Batenburg, R. (2014). Towards healthcare business intelligence in long-term care: an explorative case study in the Netherlands. *Computers in Human Behavior, 30,* 698–707. [online]

Technology selection for process analysis to improve performance	<i>Translational</i> data science
Taxonomic studies	How can Dutch long- term care institutions be supported with data?

Example: Understanding Long-term Care

• Score = $\sum_{Expert \ level} \frac{Times \ mentioned}{Number \ of \ interviews} \times Valuation$				
#	Туре	Information need	Score	
1	Q	Customer experience	16.6	
2	F	Staffing with respect to ZZP-mix	14.8	
3	F	ZZP-mix per business unit	13.6	
4	F	ZZP-mix prognoses	13.6	
5	F	Staffing with respect to operations	13.5	
6	Q	Number of incidents occured	13.5	
7	Q	Types of incidents occured	13.5	
8	Q	Causes of occured incidents	13.5	
9	F	Operations per ZZP	13.0	

Production information (planned,

realized, declared)

13.0

F

10



Example: Understanding Long-term Care					
Information needs	Data mining goals				
 Number of occured incidents Types of occured incidents Causes of the occured incidents Patterns in occured incidents 	 Identify patterns in incidents^[1] 				
 Number of clients at an increased risk Types of risk the clients run 	 Identify relationships in risk assessment 				
 Progress of care-related measures 	 Identify patterns in care- related measures 				
 Treatment goals (obtained & not-obtained) Care plan information 	 Identify patterns in obtained and not-obtained treatment goals 				
 Number of clients per demand for care ZZP-mix ZZP-mix prognosis 	• Identify & predict the ZZP mix ^[2]				

Example: Understanding Long-term Care













Example: Exploring Mental Healthcare

- **CRISP-IDM: Cross Industry Standard Process for** *Interactive* Data Mining
- "Big data" approach: not hypothesis-driven

Торіс	Theme	Priority
What are relations between the different ROM scores, and can they predict treatment length?	ROM	1
Do medication prescription and change in medication influence the length of admission and the likeliness of readmission?	Medication	2
Can aggression incidents in inpatients be predicted?	Aggression	3
In what way are patients referred between, for example, general practitioners, secondary care institutions, and the UMCU?	Patient referrals	4

Menger, V., Spruit, M., Hagoort, K., & Scheepers, F. (2016). Transitioning to a data driven mental health practice: collaborative expert sessions for knowledge and hypothesis finding. Computational and *Mathematical Methods in Medicine*, Article ID 9089321, 11. [online]



Example: Exploring Mental Healthcare

• Data descr.: EHR, Incident report system, External

			Records
(1) Diagnosis	Categoric	Structured	5,800
(2) Treatment plan	Categoric, textual	Both	6,500
(3) Medication prescriptions	Categoric, numeric	Structured	22,000
(4) Routine Outcome Monitoring	Numeric, textual	Both	13,000
(5) Admission information	Categoric	Structured	5,400
(6) Daily reports	Textual	Unstructured	150,000
(7) Aggression incident reports	Categoric, textual	Both	1,200
(8) Census data	Numeric	Structured	21,000
(9) Geographic data	Numeric	Structured	5,000

degree of fundamental understanding for more collaborative and interdisciplinary EDA? Taxonomic studies

degree of practical use consideration

Translational

data science

How to uncover nonhypothesis driven topics in mental healthcare?

Example: Exploring Mental Healthcare

• 26 Weekly interactive data visualization explorations!





Example: Exploring Mental Healthcare

Finding: Domain experts indicated that the lack of variation does not justify scoring the Kennedy Axis V (a ROM on Well-being) on a regular basis.



degree of practical use consideration



Example: Exploring Mental Healthcare

• *Finding:* A peak in aggression incidents occurs at day five, esp. in adult patients (dark)?





degree of practical use consideration

Example: Exploring Mental Healt	hcare
 Finding: 24/29 hypotheses are new due to 	CRISP-IDM!
Top-5 hypotheses	Theme
There exists a positive relation between season of admission and length of admission (longer admissions during winter)	Admission
A peak in aggression incidents occurs on the <mark>fifth</mark> day of admission	Aggression
There exists a relation between aggression incidents and wearing of medication effects in patients diagnosed with ADHD	Aggression, medication
There is an absence of a relation between amount of green space in patient environment and likelihood of developing a disorder	Context factors
There is a negative relation between economic status of living environment and length of admission	Admission, context factors

Evenue Los Eveloring Montal Hoaltheare





degree of fundamental understanding

degree of fundamental understanding



degree of practical use consideration

Example: Extracting Lifestyle Characteristics with NLP

Muizelaar, H., Haas, M., Putten, P. v.d., & Spruit, M. (submitted).

Example text data	Smoking	Alcohol	Drugs	
Patient smokes, does not drink or use drugs	Current user	Non-user	Non-user	
Patient used to smoke, drinks 1 beer a day	Former user	Current user	Unknown	
Patient used to smoke, uses marihuana daily	Former user	Unknown	Current user	
Model	Smoking	Alcohol	Drugs	
String Matching	0.84	0.74	0.68	
Machine Learning (SGD)	0.85	0.71	0.60	
HAGALBERT	0.66	0.54	0.43	
RobBERT-HAGA	0.87	0.71	0.63	
belabBERT-HAGA	0.48	0.64	0.57	
MedRoBERTa.nl-HAGA	<mark>0.93</mark>	0.79	<mark>0.77</mark>	
BioBERT (translated)	0.91	0.72	0.52	
ClinicalBERT (translated)	0.92	<mark>0.80</mark>	0.61	





How to

extract

mation for

Example: Extracting Lifestyle Characteristics with NLP

tSNE visualisation of MedRoBERTa.nl-HAGA sentence embeddings •











with

Example 1: Automated Machine Learning in Healthcare

*Question: "*How can we support the knowledge • discovery process of domain experts in healthcare using automated machine learning?"



Ooms, R., & Spruit, M. (2020). Self-Service Data Science in Healthcare with Automated Machine Learning. Applied Sciences, 10(9), Medical Artificial Intelligence, 2992. [online]



Example: Automated Machine Learning in Healthcare

 Data: All medical datasets suited for binary classification problems (4) in OpenML-CC18 opensource benchmark suite (Gijsbers *et al.*, 2019)

Dataset	Data points	Missing data	Predictive features	Class variable
Breast cancer	699	-	9	458/241
Diabetes	768	-	8	500/268
Indian Liver Patients	583	-	10	416/167
Sick	3772	6064	29	3541/231

• All AutoML methods receive 1 hour in a 10-fold crossvalidation set-up to create the best pipeline on these datasets



 Benchmarkina AutoML Translational technique characteristics data science and performances How can we empower researcherphysicians with AutoML?

degree of practical use consideration

Example: Automated Machine Learning in Healthcare

- Decision tree and constant predictor as baseline •
- Hyperopt performs worst; TPOT and Auto-Sklearn best <1-hour budget>





Translational

data science

How can we empower researcher-

physicians

with AutoML?

Example: Automated Machine Learning in Healthcare

 When benchmarking with 4 hour budget, again, TPOT and Auto-Sklearn perform best <4-hour budget>





Example: Automated Machine Learning in Healthcare

Evaluation: Webapp vs Notebook deployment ۲



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PS: PyCaret for Self-Service Data Science?

best = compare models(sort='R2')

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE	TT (Sec)
rf	Random Forest Regressor	2342.1429	22959433.7357	4762.0337	0.8351	0.4097	0.2091	0.2360
gbr	Gradient Boosting Regressor	2275.4641	22815428.3119	4750.1089	0.8350	0.3858	0.1874	0.0740
ada	AdaBoost Regressor	3257.2171	23279230.3521	4807.0257	0.8339	0.4770	0.4264	0.0330
lightgbm	Light Gradient Boosting Machine	2491.6919	24030584.9610	4865.2118	0.8272	0.4153	0.2118	0.4180
et	Extra Trees Regressor	2364.4206	25237906.1980	4999.4284	0.8167	0.4283	0.2116	0.2060
catboost	CatBoost Regressor	2530.8745	25732627.8903	5042.4862	0.8134	0.4088	0.2020	1.0060
xgboost	Extreme Gradient Boosting	2931.6919	31946244.2000	5615.7612	0.7678	0.4551	0.2602	0.3410
dt	Decision Tree Regressor	3031.4152	42283353.7664	6468.0098	0.6936	0.5132	0.3181	0.0240
omp	Orthogonal Matching Pursuit	5645.3004	59119654.4986	7679.3606	0.5758	0.6831	0.6880	0.0190
ridge	Ridge Regression	4066.3599	61583179.6000	7714.4257	0.5583	0.4400	0.2707	0.0150
br	Bayesian Ridge	4072.9367	61948316.9816	7735.3075	0.5556	0.4399	0.2705	0.0210
Ir	Linear Regression	4081.2541	62419186.8000	7762.5140	0.5521	0.4399	0.2702	0.6810
lar	Least Angle Regression	4081.2284	62418429.6714	7762.4664	0.5521	0.4399	0.2702	0.0210
knn	K Neighbors Regressor	4590.2544	70154126.3724	8271.6145	0.5162	0.5252	0.3131	0.0260
huber	Huber Regressor	4211.3096	80449305.4129	8799.2293	0.4214	0.4535	0.2076	0.0240
par	Passive Aggressive Regressor	5841.9890	94762106.9683	9607.9039	0.2863	0.6406	0.4609	0.0260
en	Elastic Net	8222.6689	160918301.6000	12608.0390	-0.1206	0.9079	0.9707	0.0200
lasso	Lasso Regression	8249.2145	161224220.8000	12619.7366	-0.1227	0.9107	0.9777	0.0150
llar	Lasso Least Angle Regression	8249.2145	161224210.7582	12619.7361	-0.1227	0.9107	0.9777	0.0190


degree of practical use consideration

0.3 -0.2 -

0.1 -0.0 - all and and and and and

<mark>ABM</mark> approach (Ammar Faiq)	CGAN approach (Jim Achterberg)				
 Synthea-based dataset An ELAN 'digital twin' is already being used in the PHM Fundamentals master course to let students analyse COVID outbreaks in The Hague region (see below) Joint research with Statistics Netherlands (CBS) & Syntho Workshop 'Guidance Ethics': many stakeholders, 50+ effects 	 <u>Thesis</u> Evaluation Framework for synthetic EHR data (supporting heterogeneous types, time series, unpredictable quality) tSNE extension two-sample GoF test evaluation metric for privacy risk through AiAs Horizon Europe, NWO OSF 				
Covid 19 0.7- 0.6- 0.5- 0.4-	Cases in %				







degree of practical use consideration

Example: Discovering Bias in Mental Health

 Effects and mitigation of gender fairness bias on a model trained to predict the future administration of benzodiazepines to psychiatric patients (AI Fairness 360)



Mosteiro, P., Kuiper, J., Masthoff, J., Scheepers, F., & Spruit, M. (2022). Bias Discovery in Machine Learning Models for Mental Health. *Information*, *13*(5), Advances in Explainable Artificial Intelligence, 237. [online] degree of fundamental understanding

How much performance is sacrificed when applying bias mitigation? Taxonomic studies Gender bias in predicting benzodiazepines prescriptions in psychiatry?

degree of practical use consideration

Example: Discovering Bias in Mental Health

	Model				Performance (comp. to baseline)				
	Classifier			Aitigation strategy	∆ Balanced accuracy		Δ F1		
	0	egression Regression Regressi Regression Regression Regression Regression Regression Reg		Predudice remover	-0.040 ± 0.013		-0.041 ± 0.025		
	0			e-weighing	-0.003 ± 0.013		-0.005 ± 0.013		
_	Random fo			e-weighing	0.003 ± 0.002		0.005 ± 0.001		
	Model			Fairness metric (compared to baseline)					
	Classifier	Mitigation strategy		∆ Disparate impact	∆ Average odds difference	∆ Statistica parity difference		∆ Equal opportunity difference	
	Logistic regression	Predudice remover		0.092 ± 0.036	0.038 ± 0.021	0.05 0.0		0.018 ± 0.042	
	Logistic regression	Re- weighing		0.075 ± 0.021	0.043 ± 0.017	0.043 ± 0.014		0.042 ± 0.034	
	Random forest	Re- weighing		0.034 ± 0.013	0.014 ± 0.006	0.01 0.0		0.014 ± 0.011	





Feasibility of ML model deployment from within a highly secure sandbox env Taxonomic studies Make ELAN ML models available ondemand to GP practices

degree of practical use consideration

Example: Deploying Prediction Models for CDSS Lisanne Wallaard GitHub Thesis Demo Feature Selection Heart Disease Prediction Are you wondering about the condition of your heart? This app will help you to diagnose it! Did you know that machine learning models can help you predict heart disease pretty accurately? In this app, you can estimate your chance of heart disease (yes/no) in seconds! Here, a logistic regression model using an undersampling technique was

Here, a logistic regression model using an undersampling technique was constructed using survey data of over 300k US residents from the year 2020. This application is based on it because it has proven to be better than the random forest (it achieves an accuracy of about 80%, which is quite good).

To predict your heart disease status, simply follow the steps bellow:

- 1. Enter the parameters that best describe you;
- 2. Press the "Predict" button and wait for the result.

Keep in mind that this results is not equivalent to a medical diagnosis! This model would never be adopted by health care facilities because of its less than perfect accuracy, so if you have any problems, consult a human doctor.

Author: Kamil Pytlak (GitHub)

You can see the steps of building the model, evaluating it, and cleaning the data itself on my GitHub repo <u>here</u>.





Example: STRIP Assistant for Medication Reviews

- A 10-years running research programme with big funding (OPERAM, OPTICA, STRIMP)
- Basically lost the fight with UU biz developers: *no product*

Jungo,K., ..., Spruit,M., ..., Rodondi,N., Streit,S. (2023). Optimising prescribing in older adults with multimorbidity and polypharmacy in primary care (OPTICA): cluster randomised clinical trial. BMJ, 381. [online]









tdslab.nl

Translational Data Science LAB : former members *d.d.* 9-10-2023



data science

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