INDUSTRY / R&D

PREDICTION OF CONCRETE COMPRESSIVE STRENGTH

Benchmark vs. Random Forest, Boosted Trees & Neural Networks

Use Case 2023/03 (v1.1) • xtractis.ai

PROBLEM DEFINITION

PROBLEM

How to successfully predict the compressive strength of high-performance concrete, given the hyper-complexity of the phenomenon (strongly nonlinear function of age and ingredients)?

GOALS & BENEFITS

- ☑ Allow domain experts and civil engineers to understand the causal relationships between concrete parameters and its compressive strength.
- ☑ Find the really influential parameters to anticipate the compressive strength of the concrete and thus optimize its production.
- ☑ Create new custom-designed concretes for specific uses.

REFERENCE DATA

- ▶ **Observations**: 875 reference points for Training/Validation, and 155 points for External Test.
  Source: Prof. I-Cheng Yeh, Department of Information Management, Chung-Hua University, Hsin Chu, Taiwan Dataset: Dua, D. and Graff, C. (2019). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science
- ▶ **Predictive Variables**: 8 Potential Predictors characterizing each concrete trial batch [age, cement, blast furnace slag, fly ash, water, superplasticizer, coarse aggregate, fine aggregate].
- ▶ **Variable to Predict**: Compressive Strength ∈ [2.3 ; 81.8] MPa.

MODEL TYPE: **Regression** | Multinomial Classification | Binomial Classification | Scoring

XTRACTIS SOLUTION

PROCESS	Reference Data	INDUCTION + Reverse-Engineering[1]	XTRACTIS Top-Model	New Cases	DEDUCTION	Automated Decision (supporting experts' decision) Compressive Strength
SOFTWARE ROBOTS		XTRACTIS® GENERATE			XTRACTIS® PREDICT	+ PREDICTion Report (for decision explainability)

RESULTS

- ☑ **Intelligible Predictive Top-Model**: Decision system composed of 86 unchained gradual rules, each rule using some of the 8 variables that XTRACTIS confirmed as predictors.
- ☑ **Robust Predictive Top-Model**: Good Real Performance in External Test.
- ☑ **Operational Efficient System**: Real-time predictions up to 70,000 decisions/s., offline or online (API).

TOP-MODEL INDUCTION

INDUCTION PARAMETERS

We launch 1,000 inductive reasoning strategies; each strategy is applied to 40 different 5-fold-partitions of the Training/Validation dataset to get a reliable assessment of the descriptive and predictive performances. Each strategy thus generates 200 unitary models called **Individual Virtual Expert (IVE)**, whose decisions are aggregated with 3 possible operators into a **College of Virtual Experts (CVE)**. Among the 3,000 CVE, the top-CVE with the best predictive performance remains complex (8 predictors shared by 6,719 rules).

We then apply 2,000 induction strategies to the same single Training (34%)/Validation (33%)/Test (33%) partition of a synthetic dataset: 43,750 new cases simulated by deduction from the top-CVE, around the 875 cases but distinct from these original cases. This XTRACTIS Reverse-Engineering[1] process induces 2,000 IVE. The top-IVE selected is as efficient as the top-CVE, but more intelligible (8 predictors shared by 86 rules).

Total number of induced unitary models	Criterion for the induction optimization	Validation criterion for the top-model selection	Duration of the process (Induction Power FP64)
202,000 IVE	RMSE	RMSE	12 days (1 Tflops)

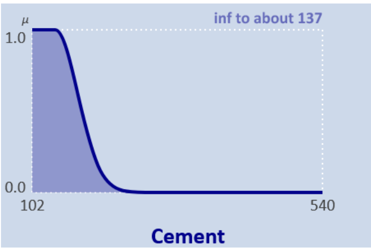
STRUCTURE

→ Intelligibility

The top-IVE model has a good intelligibility for a complex regression model as it combines the 8 predictors automatically selected by XTRACTIS into 86 rules, aggregated into 30 disjunctive rules. Its Structure Report reveals all the internal decision logic and ensures that the human expert understands the model. This decision system is a *white-box* model that can be audited by the domain expert and certified by the regulator before its deployment to end-users.

PREDICTORS

- 8 features out of 8
- Ranked by impact significance (2 strong signals, 2 medium signal, 4 weak signals): #1 Age /#2 Cement /#3 …
- Labeled by fuzzy classes. Example: **fuzzy interval** "*inferior to about 137*"



RULES

- 86 connective fuzzy rules without chaining (aggregated into 30 disjunctive fuzzy rules)
- 3 to 8 predictors per rule (on average, 6.7 predictors per rule)
- Example: **fuzzy rule R3** uses 4 predictors and concludes {8.1}. 85 other fuzzy rules complete this model.

IF	Cement (kg / m³)	IS	inferior to about 137
AND	Blast furnace slags (kg / m³)	IS	inferior to about 8.05
AND	Water (kg / m³)	IS	superior to about 189.81
AND	Age (d)	IS	inferior to about 15
THEN	Compressive Strength	IS	8.1

PERFORMANCE

→ Robustness

The top-IVE performances, measured in Training/Validation/Test on synthetic data, then in External Test on reference data, guarantee the model's predictive and real performances.

	Synthetic Data			Reference Data
Performance	DESCRIPTIVE	PREDICTIVE	REAL	REAL
Dataset	34% Training	33% Validation	33% Test	External Test
RMSE	0.8 (0.80%)	0.9 (0.87%)	0.9 (0.91%)	4.5 (4.55%)
Correlation	0.999	0.998	0.998	0.970

→ Xtractis Top-Model: Intelligible AND Good Predictive Capacity

EXPLAINED PREDICTIONS FOR 2 CASES FROM THE EXTERNAL TEST SET

CASE (not used in Training/Validation) | **DEDUCTIVE INFERENCE OF RULES** | **AUTOMATED DECISION**

Concrete #652
(actual value = 4.9 MPa *Low Compressive Strength*)

Cement	184
Blast furnace slags	122.6
Fly ashes*	0.00
Water	203.5
Superplasticizers*	0.0
Coarse aggregates	959.2
Fine aggregates	800
Age	3

→ Real Time

For this concrete, 17 rules are triggered to conclude to 9.9 MPa, a low compressive strength:

# Rule	Conclusion	Firing Degree
R1 →	8.1	0.953
R6 →	8.1	0.835
R5 →	8.1	0.807
R4 →	8.1	0.675
R2 →	8.1	0.378
R3 →	8.1	0.033
R8 →	10.5	0.040
R9 →	10.5	0.027
R11 →	13.3	0.153
R14 →	18.3	0.002
R18 →	20.4	0.008
R33 →	30.9	0.020
R40 →	32.5	0.005
R49 →	40.8	0.014
R51 →	40.8	0.006
R70 →	57.0	0.001
R68 →	55.6	6.54E-04
PREDICTION=	9.9	

NUMBER OF TRIGGERED RULES
17 / 86

FUZZY PREDICTION
{ 8.1 | 0.953,
13.3 | 0.153,
10.5 | 0.04,
30.9 | 0.02,
40.8 | 0.014,
20.4 | 0.008,
32.5 | 0.005,
18.3 | 0.002,
57.0 | 0.001,
55.6 | 6.54E-04 }

FINAL PREDICTION
{ 9.9 }

The system delivers a correct prediction compared to that given by laboratory measurements:

Low Compressive Strength

Concrete #182
(actual value = 82.6 MPa *High Compressive Strength*)

Cement	390
Blast furnace slags	189
Fly ashes*	0.0
Water	145.9
Superplasticizers	22
Coarse aggregates	944.7
Fine aggregates	755.8
Age	91

→ Real Time

For this concrete, 7 rules are triggered to conclude to 72.7 MPa, a high compressive strength:

# Rule	Conclusion	Firing Degree
R60 →	49.9	5.82E-04
R72 →	58.8	0.011
R73 →	64.2	0.025
R78 →	70.6	0.159
R81 →	71.9	0.275
R83 →	73.8	0.335
R85 →	73.8	0.818
PREDICTION=	72.7	

NUMBER OF TRIGGERED RULES
7 / 86

FUZZY PREDICTION
{ 73.8 | 0.818,
71.9 | 0.275,
70.6 | 0.159,
64.2 | 0.025,
58.8 | 0.011,
49.9 | 5.82E-04 }

FINAL PREDICTION
{ 72.7 }

The system delivers a correct prediction compared to that given by laboratory measurements:

High Compressive Strength

Predictor value is out of the variation Range of the model (<0.50 % OOR for case #652 and case #182) but inside the allowed extrapolation range. Xtractis will refuse to give a result for an extrapolation far from the allowed extrapolation range. It is one situation of the "Refusal" prediction.

TOP-IVE BENCHMARK

	XTRACTIS	RANDOM FOREST	BOOSTED TREES	NEURAL NETWORK
MODELS RELEASE	2023/01	2023/01	2023/01	2023/03
ALGO VERSION	XTRACTIS **GENERATE** 12.2.44127	Python 3.9, LightGBM 3.3.2	Python 3.9, LightGBM 3.3.2	Python 3.9, TensorFlow 2.10.0, Keras 2.10.0
CROSS-VALIDATION TECHNIQUE	40×5 folds for each CVE model Then 1-Split Validation for each IVE model (for the reverse engineering of top-CVE): 34% Training; 33% Validation; 33% Test	40×5 folds for each CVE model	40×5 folds for each CVE model	40×5 folds for each CVE model
NUMBER OF EXPLORED STRATEGIES[2]	1,000 induction strategies for the CVE on Training / Validation data 2,000 induction strategies for the IVE on synthetic data	1,000 ML strategies on Training / Validation data	1,000 ML strategies on Training / Validation data	1,000 ML strategies on Training / Validation data
NUMBER OF MODELS	3,000 CVE + selection of the top-CVE 2,000 IVE (for the reverse engineering of top-CVE) + selection of the top-IVE	1,000 CVE + selection of the top-CVE 1 top-IVE	1,000 CVE + selection of the top-CVE 1 top-IVE	1,000 CVE + selection of the top-CVE 1 top-IVE
TOP-IVE STRUCTURE				
NUMBER OF PREDICTORS (out of 8 Potential Predictors)	**8**	**8**	**8**	**8**
DECISION STRUCTURE	System with **86** unchained fuzzy rules, aggregated into **30** disjunctive rules	**172** trees; **76,196** binary rules	**337** chained trees; **10,719** binary rules	**2** hidden layer; **32** hidden nodes
MODEL INTELLIGIBILITY (& DECISION EXPLAINABILITY)	Only 6.7 predictors per rule on average Only a few rules are triggered at a time	Too many rules: 87 x number of learning points!	Tree #N corrects the error of the N-1 previous trees. Too many rules: 12 x number of learning points!	Unintelligible synthetic variables.
TOP-IVE REAL PERFORMANCE (External Test) — *Random*[3]				
Correlation — *0.253*	**0.970**	**0.967**	**0.984**	**0.949**
MAE — *16.5 (16.53%)*	3.6 (3.59%)	3.0 (3.04%)	2.2 (2.17%)	4.4 (4.37%)
RMSE — *21.2 (21.19%)*	**4.5 (4.55%)**	**4.5 (4.47%)**	**3.2 (3.18%)**	**5.6 (5.60%)**
Refusals — *N/A*	0.00%	N/A	N/A	N/A
MODEL ROBUSTNESS	#3	#2	#1	#4

1 Given the small number of reference cases of this dataset, the XTRACTIS Reverse-Engineering (CVE→IVE) is necessary to get a robust AND intelligible model.
2 All CVE and IVE models are optimized according to their validation RMSE. The XTRACTIS top-CVE and top-IVE are selected according to their validation RMSE while checking that it remains close to their training RMSE.
3 Baseline performances that models must exceed to perform better than chance (P-value = 0.001; 100,000 models generated by random permutation of the output values).

More Use Cases:
xtractis.ai/use-cases/