Centre for
Data Analytics

Insight

Explainable Machine Learning Models for Structured Data

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Overview

- **Structured Data**
  - Symbolic Sequences (e.g., DNA, malware)
  - Numeric Sequences (e.g., time series)

- **Explainable Learning Models**
  - Black-Box vs Linear Models with Rich Features

- **SEQL: Sequence Learning with All-Subsequences**
  - Framework for Sequence Classification & Regression

Structured Data: Sequences & Time Series

Many Applications:

- **DNA**

Value	Data points
290.507	AGGGCATCATGGAGCTGTCCAG
679.305	ATCACAATTTTGCCGAGAGCGA
1998.715	GTACACCCCGTTCGGCGGCCCA
447.803	CCTTTAGCCCATCGTTGGCCAA

- **Malware**

Byte sequence

Class	Data points
+1	C7 01 24 04 5F 0E EA DC 00 E9 D6 4A 00 0C 66 89
+1	74 13 BA EF 01 00 06 68 95 14 88 B7 00 0F 0E EA
-1	08 F9 C8 1A 80 C1 8B 48 40 00 89 51 10 B8 04 00
-1	B8 00 00 00 00 50 E8 D8 00 00 00 83 C4 04 53 FF

- **Sensors**

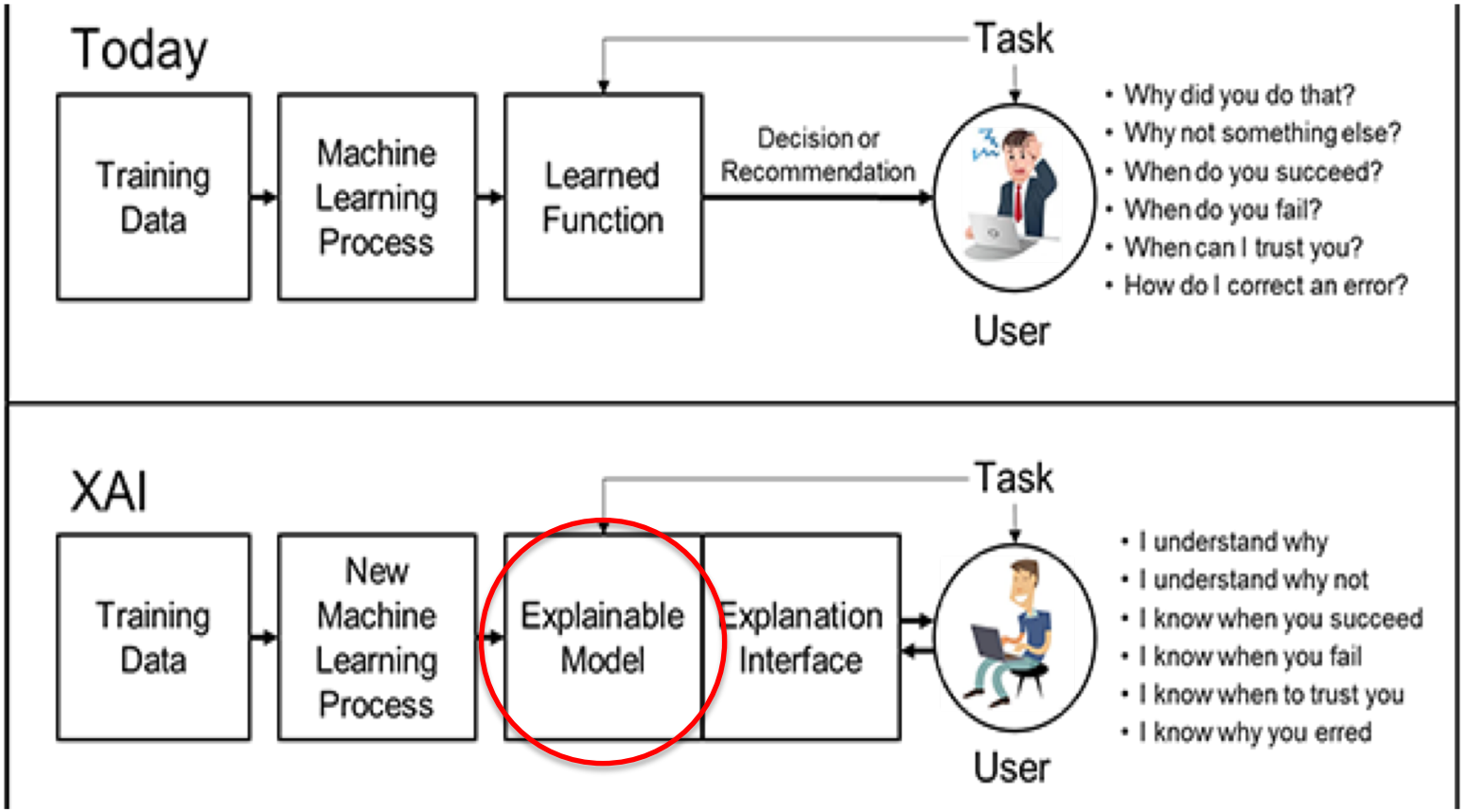
0	-0.26927	-0.26927	-0.26927	-0.26927	-0.26927
1	-0.46887	2.748	1.6263	-0.46887	-0.46887
0	2.2429	-0.39296	-0.39296	-0.39296	-0.39296
0	-0.45836	2.4229	-0.45836	2.5162	1.9876
0	-0.58609	-0.58609	-0.58609	-0.58609	-0.58609
0	1.8657	-0.44769	-0.44769	-0.44769	1.7914
0	1.3541	1.9638	-0.53962	-0.53962	-0.53962

Explainable Machine Learning Models

- **Accuracy & Efficiency:**
  - Many accurate algorithms: e.g., ensembles (Random Forest), Deep Neural Networks; but hard to interpret big, complex models
  - Large volumes of data, need efficient models

- **Interpretability:**
  - White box (linear models) vs black box (deep nets)
  - Interpretable AI is a big deal: Darpa Explainable AI (XAI; 2016), EU GDPR legislation (May 2018)

Darpa Explainable AI (XAI)



[**Source:** http://www.darpa.mil/program/explainable-artificial-intelligence]

SEQL: Sequence Learning with All-Subsequences

Key Idea: Linear Models with Rich Features are Accurate and Interpretable

- Linear models are **interpretable and well understood** (linear regression, logistic regression).
- Linear models with rich features are **accurate** (similar accuracy to ensembles, kernel-SVM, deep nets).
- **Efficiently optimize linear models:** We exploit the structure of a massive feature space (all-subsequences) to quickly select good features.

SEQL: Linear Models for Symbolic Sequences

Solution Approach

SEQL: all-subsequences are candidate features; focus on selecting good features quickly

Score	Sequence
290.5	AGTC**CACAA**GGCTAGGATAGCTA**TCCG**GATCGA
315.1	TATCCTGCAGTACAAG**TCCG**TAATT**CACAA**TCCA
805.6	AGTCCGC**TAGGCT**AGGATAGCTAGCCCGATCGA
799.7	AGCCAAGACCTGAAA**TAGGCT**CCTGAGATACAG
???	CGGGTCGTA**TCCG**CACTGAATATC**TAGGCT**TACG

Goal is to learn a mapping:

$$f : S \rightarrow \mathbb{R}$$

SEQL Model:

Weight	*k*-mer
796.6	TAGGCT
402,5	CACAA
-125.3	TCCG

Linear model (weighted sum of features):

$f(x) = \beta^t x$, with β the feature weights and x the feature vector

SEQL: Linear Models for Symbolic Sequences

Add features iteratively with greedy coordinate descent + branch-and-bound (bound the search for the best feature)

Algorithm 1 Coordinate Descent with Gauss Southwell Selection

1: Set $\beta^{(0)} = 0$
2: **while** termination condition not met **do**
3: Calculate objective function $L(\beta^{(t)})$
4: Find coordinate j_t with maximum gradient value
5: Find optimal step size η_{j_t}
6: Update $\beta^{(t)} = \beta^{(t-1)} - \eta_{j_t} \frac{\partial L}{\partial \beta_{j_t}}(\beta^{(t-1)}) e_{j_t}$
7: Add corresponding feature to feature set
8: **end while**

How do we find coordinate j_t efficiently?

Key Ideas

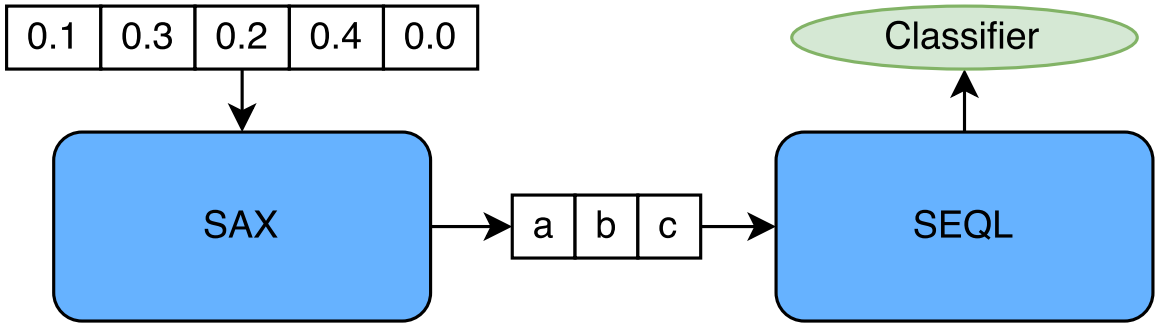
Bound gradient of k-mer using only information about its sub-k-mers.

Example

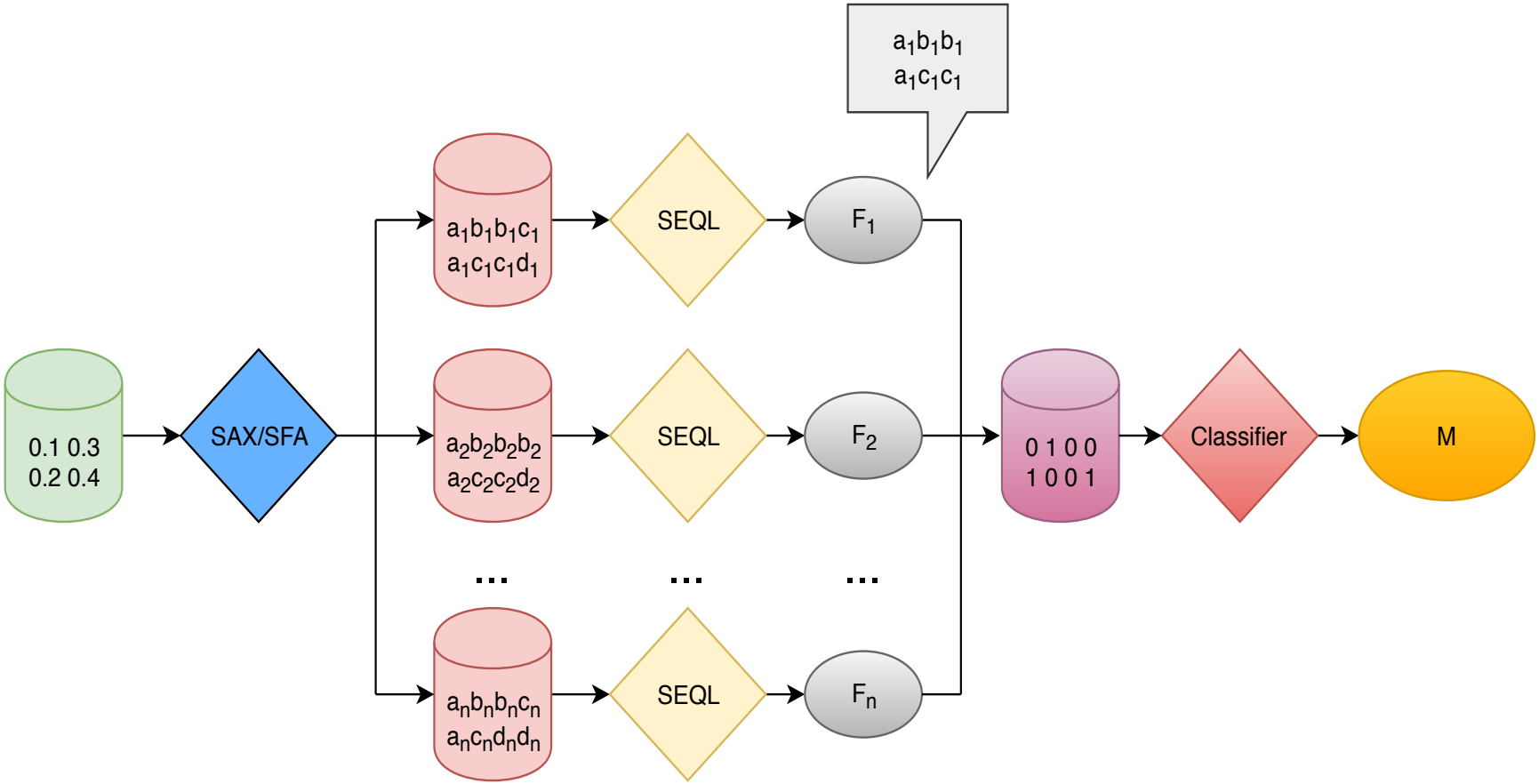
Given: $s_p = "ACT"$
Calculate bound: $\mu(s_p)$
$s_1 = "ACTC"$ -> $gradient(s_1) \leq \mu(s_p)$
$s_2 = "AACT"$ -> $gradient(s_2) \leq \mu(s_p)$
$s_3 = "TACTG"$ -> $gradient(s_3) \leq \mu(s_p)$

SEQL for Time Series Classification

Time Series → Discretisation (SAX, SFA) → Symbolic Sequence → Sequence Learner (SEQL)



SEQL for Time Series Classification



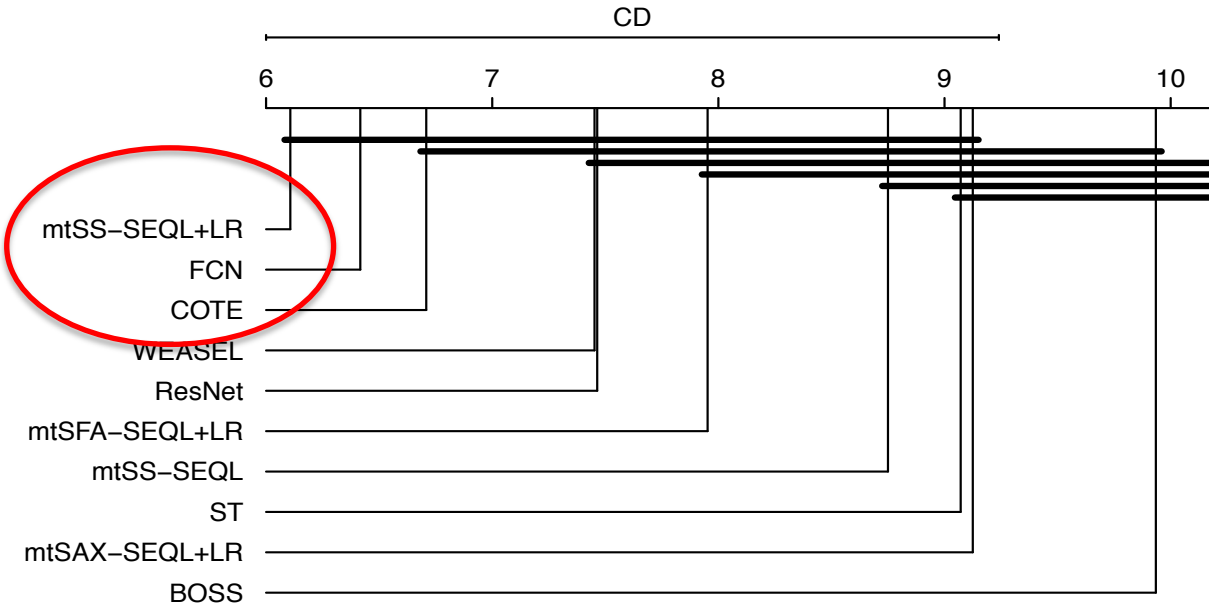
Evaluation on Time Series Classification

Ranking of learning algorithms by Accuracy

UCR Archive (85 TSC datasets: sensors, images, ECG)

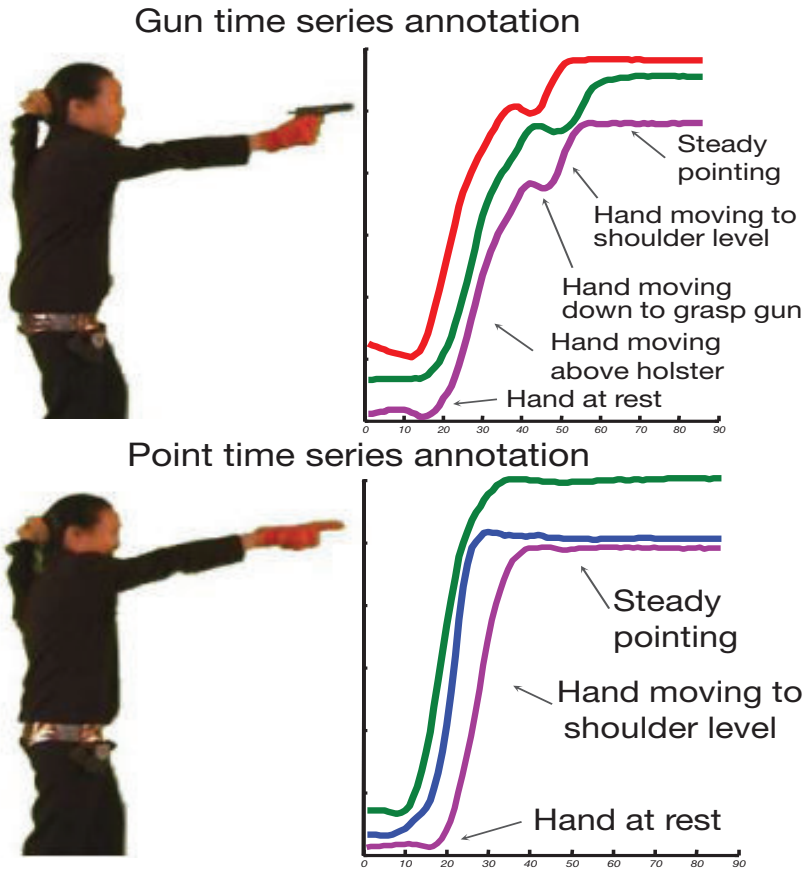
Top-3 models:

1. mtSS-SEQL+LR (our method, a linear model)
2. FCN (deep neural network)
3. COTE (ensemble of 35 classifiers)



Interpretability

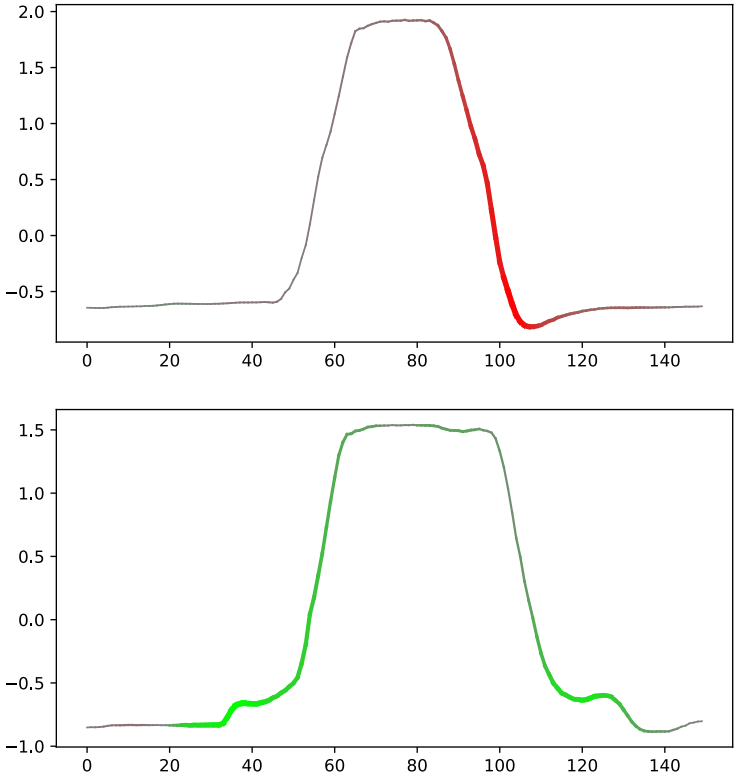
- GunPoint dataset tracking hand movement w/o Gun



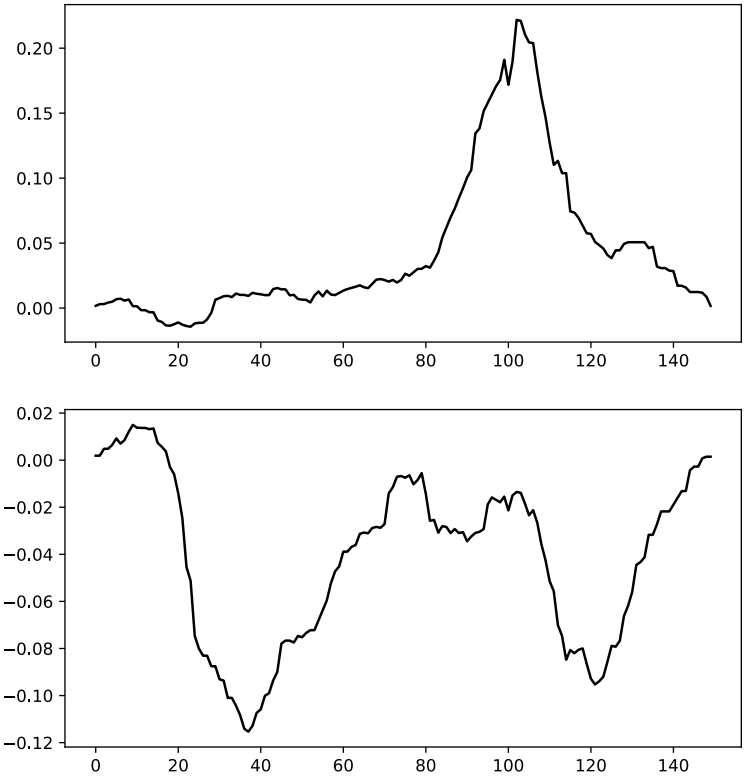
Interpretability

Coefficients	Subsequences
0.065 84	cbaab
0.062 47	db
0.062 23	ddddb
0.062 00	da
0.059 72	bbbbbbbbbbcdddd
−0.053 72	aaaaaabbbb
−0.054 39	bbbbaaaaaa

Point (top) and Gun (bottom)



Salient Region for Classification Decision



Github code for our work: https://github.com/heerme?tab=repositories

Recap SEQL

- Family of machine learning algorithms to train/predict (with) linear models for sequences
- Coordinate descent with Gauss-Southwell feature selection + Branch-and-bound for efficient feature search

- **Sequence Classificati**on (KDD08, KDD11): Logistic loss, l2-SVM loss
- **Sequence Regression** (ECMLPKDD17): Least-squares loss
- **Time Series Classification** (ICDE17): SEQL + SAX discretization

- Future Work:
  - Multi-dimensional Sequences

References

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