

Cyclic Boosting

A Pure-Python, Explainable, and Efficient ML Method

Felix Wick, April 2023



This is old stuff.



But it just works.



Cyclic Boosting ML Methods

family of off-the-shelf, general-purpose supervised machine learning methods for both regression and classification tasks (focus on structured data)

closest relatives: Generalized Additive Models (not a deep learning approach)

main difference: estimation of factors for each bin of the different features (instead of estimation of parameters like coefficients in linear regression or weights in neural networks)

→ individual explainability

scientific papers describing the methods: [Cyclic Boosting](#), [Demand Forecasting with Cyclic Boosting](#)



Cyclic Boosting Library

scikit-learn-like usage of library

open source: [github](#)

Python package: [pypi](#)

documentation: [readthedocs](#)



Cyclic Boosting | Different Modes/Scenarios



(conditional mean)

$$Y \in [0, \infty)$$

Poisson /
Negative Binomial
distribution
(link function *ln*)

example

demand forecasts
(mean)



(conditional mean)

$$Y \in (-\infty, \infty)$$

Gaussian
distribution
(link function *identity*)

example

profit predictions



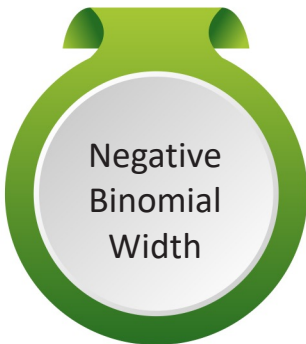
(probability)

$$Y \in [0, 1]$$

Bernoulli
distribution
(link function *logit*)

example

churn probability



(dispersion parameter)

$$Y \in [0, 1]$$

Negative Binomial
distribution
(link function *logit*)

example

demand forecasts as
full probability
distributions



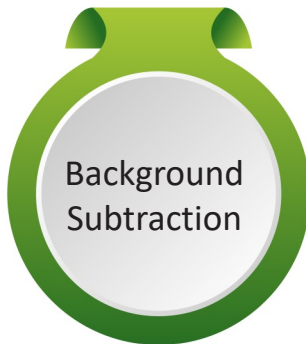
(elasticity parameter)

$$Y \in [0, \infty)$$

exponential
distribution
(link function *ln*)

example

individual price-
demand elasticities



(conditional mean)

$$Y \in (-\infty, \infty)$$

Gaussian
distribution
(link function *identity*)

example

individual causal
effects, e.g.,
customer targeting

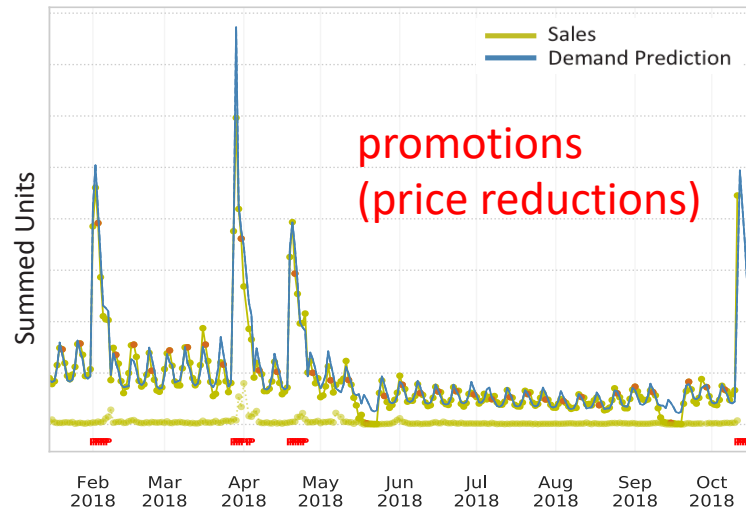


Example Use Case: Demand Forecasting

many individual time series to consider

typical retail grocery chain:

- products (items): ~20k
- locations (stores): ~500
- daily/hourly aggregated sales



advantages of machine learning over traditional univariate time series forecasting

combined learning on all time series of product-location combinations (rather than separately optimizing individual time series)
→ **reduces variance** by exploiting commonalities

natural consideration of many exogenous variables (prices, promotions, holidays, weather, ...)
→ **reduces bias**

to be noted:

- categorical features important (products and locations → high cardinality)
- mainly multiplicative effects
- demand (approximately) following Poisson (or rather negative binomial) distribution

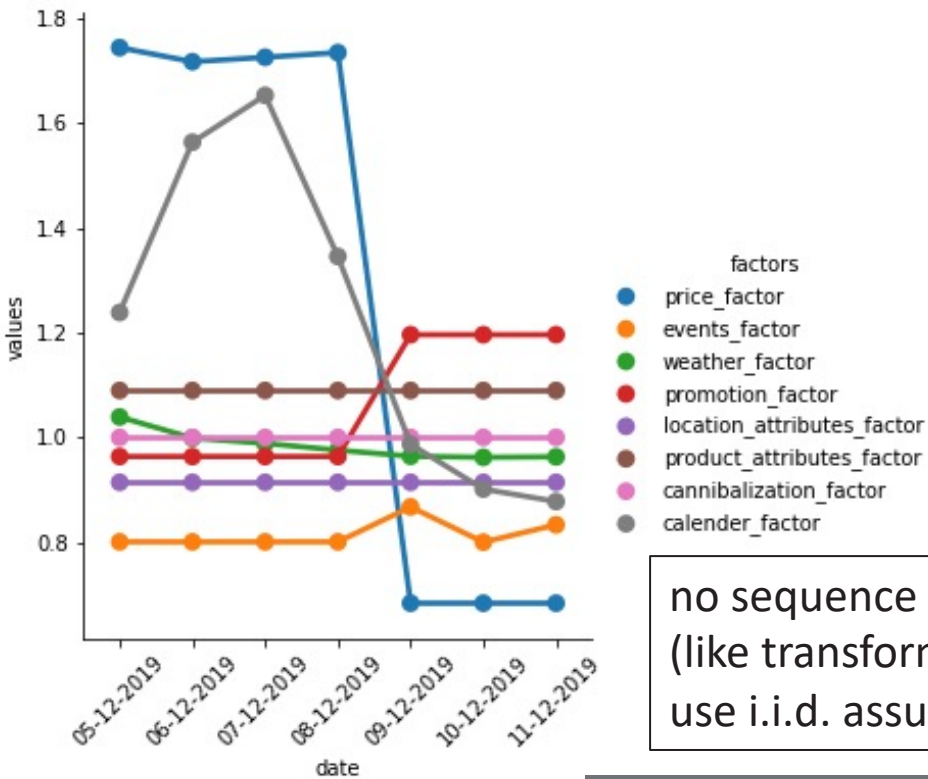


Cyclic Boosting - Prediction View | Individual Explainability

Cyclic Boosting in multiplicative regression mode

multiplicative model
variation proportional to level

individual item-store-day predictions



no sequence model
(like transformers),
use i.i.d. assumption

Cyclic Boosting allows for detailed explanation of each individual prediction by means of contributions (in form of factors) of each feature in the model.

prediction: look up learned factors of relevant bin for each feature

$$\hat{y}_i = \mu \cdot \prod_{j=1}^p f_j^k \quad \text{with} \quad k = \{x_{j,i} \in b_j^k\}$$

global target
average

product over factors
for all p features in
corresponding bins of
sample i

bin k of feature j

do not confuse explainability with causality though
→ need for causal assumptions (e.g., specific smoothing)



Cyclic Boosting Training

Coordinate Descent: Boosting-like Update of Factors

1. calculate global average μ , initialize all factors to 1
2. cyclically iterate through features and calculate factors for each feature bin (corresponding to minimization of quadratic loss)

for simplicity: show only non-aggregated mode

$$f_j^k = \sum_i y_i / \sum_i \hat{y}_{j,i}$$

bin k

numerator: target values

feature j

sum over all samples i in bin k of feature j

denominator: predictions excluding factor from current feature

$$\hat{y}_{j,i} = \mu \cdot \prod_{l \neq j} f_l^k$$

factors for corresponding feature bins of sample i

product over all features excluding j

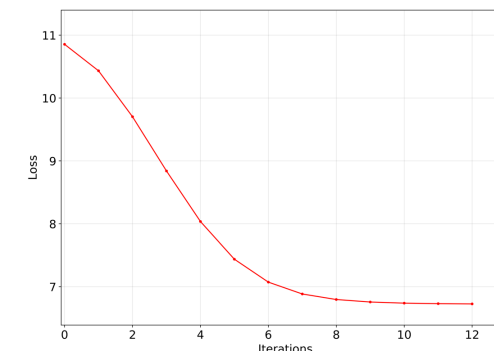
3. stop according to MAD or MSE criteria at end of iterations (full feature cycles) or when reaching given maximal number of iterations



Cyclic Boosting fitting procedure with three loops

```
while (stop criteria) iterations
...
    for (features) sequential
    ...
        for (samples) parallel
```

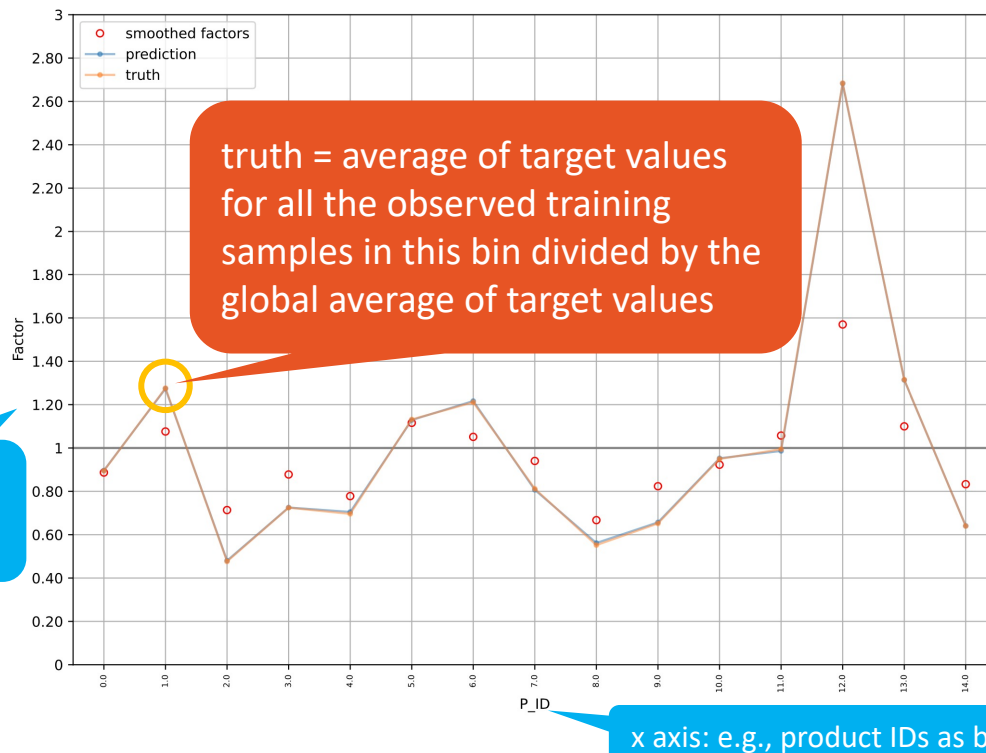
other modes work accordingly



Binning

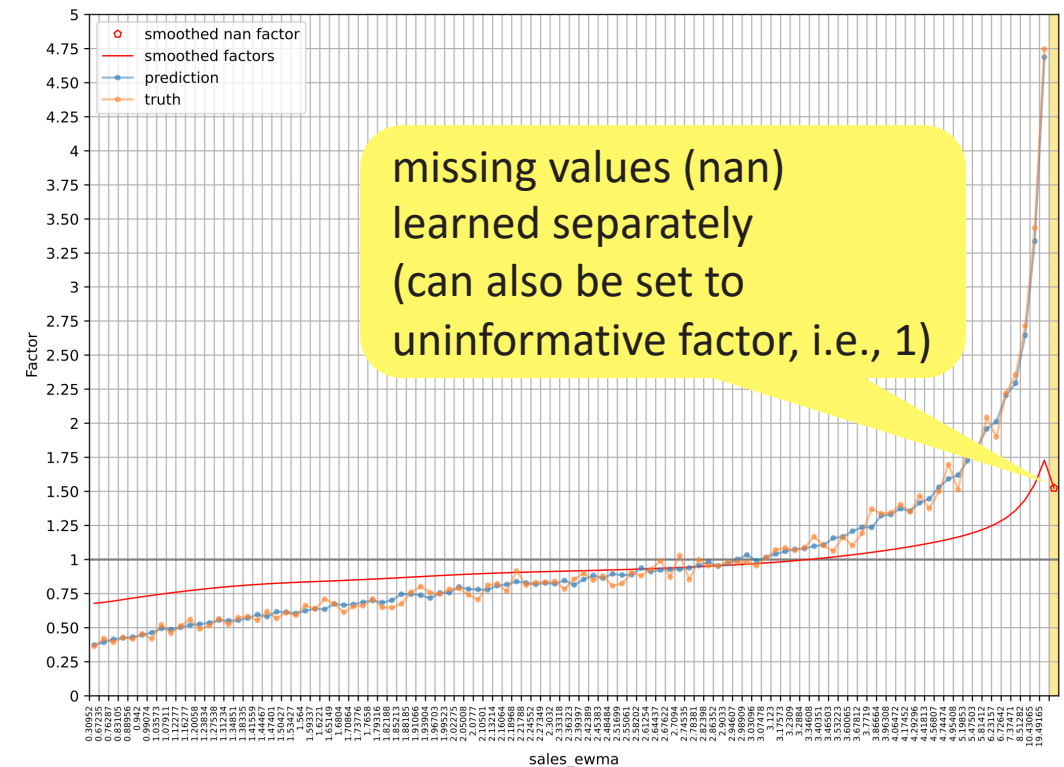
categorical features retain original categories (learning of specific factor for each of the bins)

→ supporting categorical features with high cardinality



continuous features discretized to:

- either having same bin width (equidistant binning)
- or containing approximately same number of observations (equistatistics binning) with different bin widths



local optimization in each bin: allows learning of rare effects with low bias



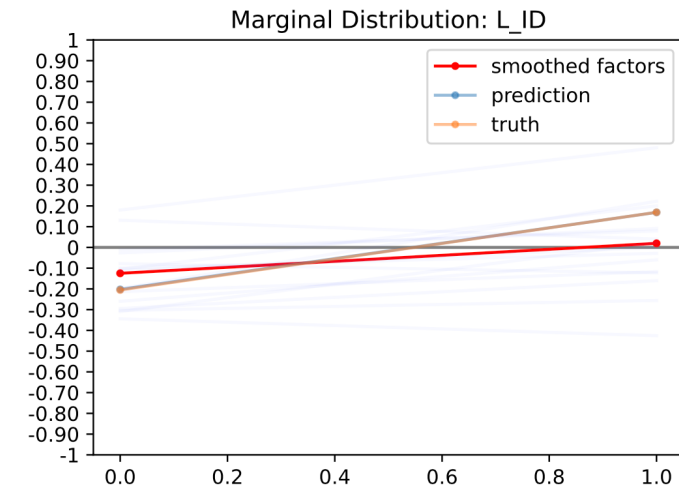
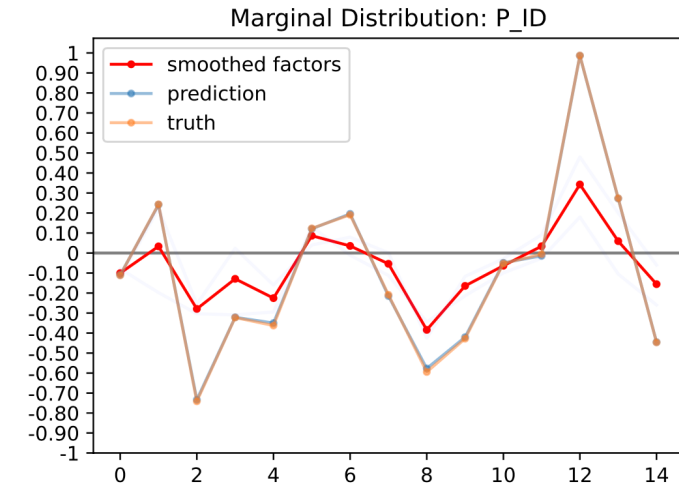
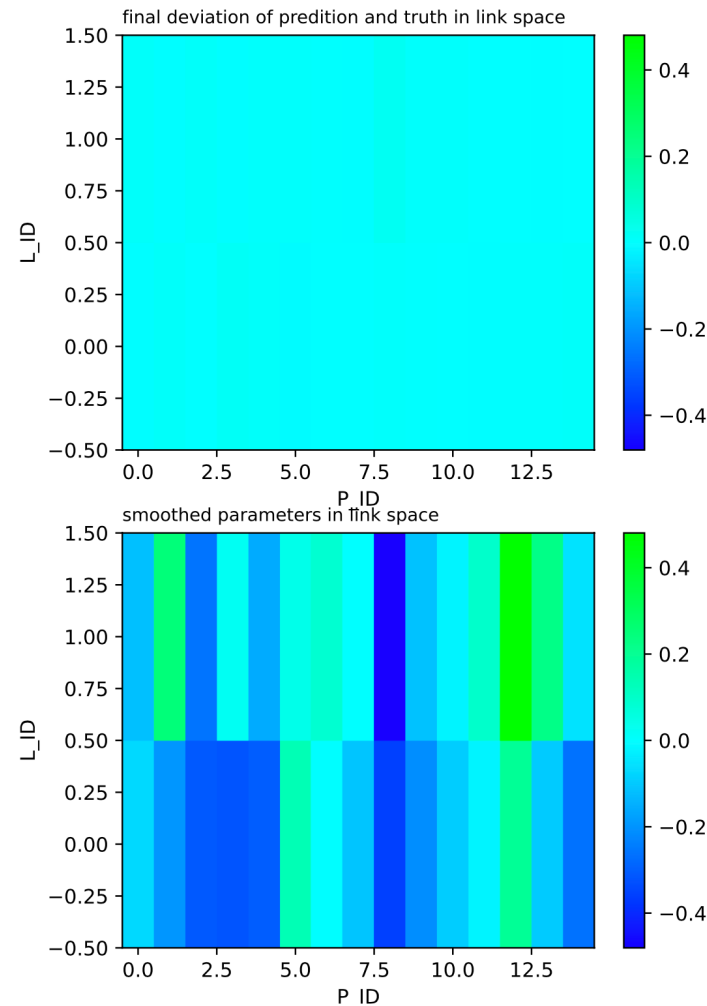
Interaction Terms

e.g., different holiday effects for different products

require even more local optimization (rare effects)

→ include binned interaction terms (e.g., 2D or 3D)

can (partly) enable hierarchical model structure (in combination with coordinate descent): interaction terms with product groups, products, locations



Smoothing

to avoid overfitting:
regularization (smoothing) across bins
→ **drastic reduction of variance** by
ignoring fluctuations

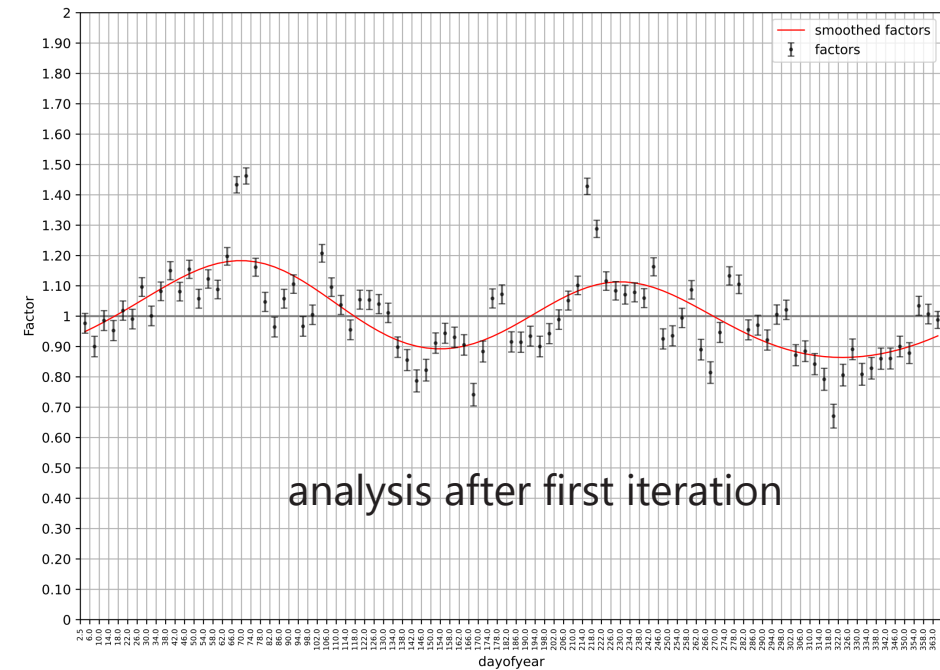
separate smoothings in each iteration

in general: orthogonal polynomials

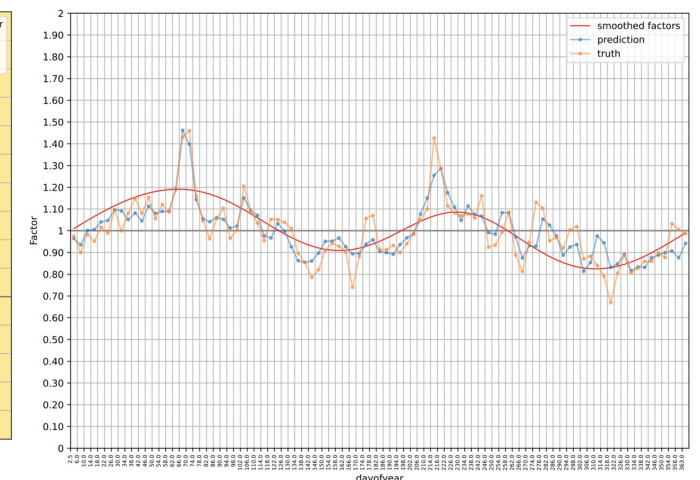
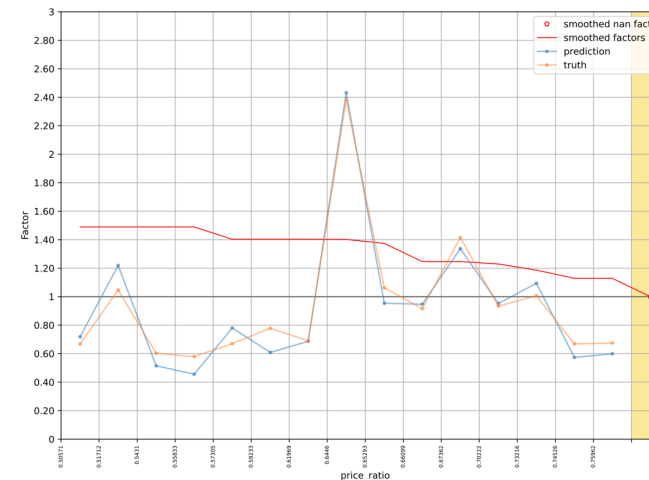
another way to include *prior knowledge* via

- monotonic requirements
- sinusoidal functions
- (piecewise) linear

use fitted functions (smoothed factors) instead of original factors



analysis after last iteration:



Analysis Plots

support EDA and modeling

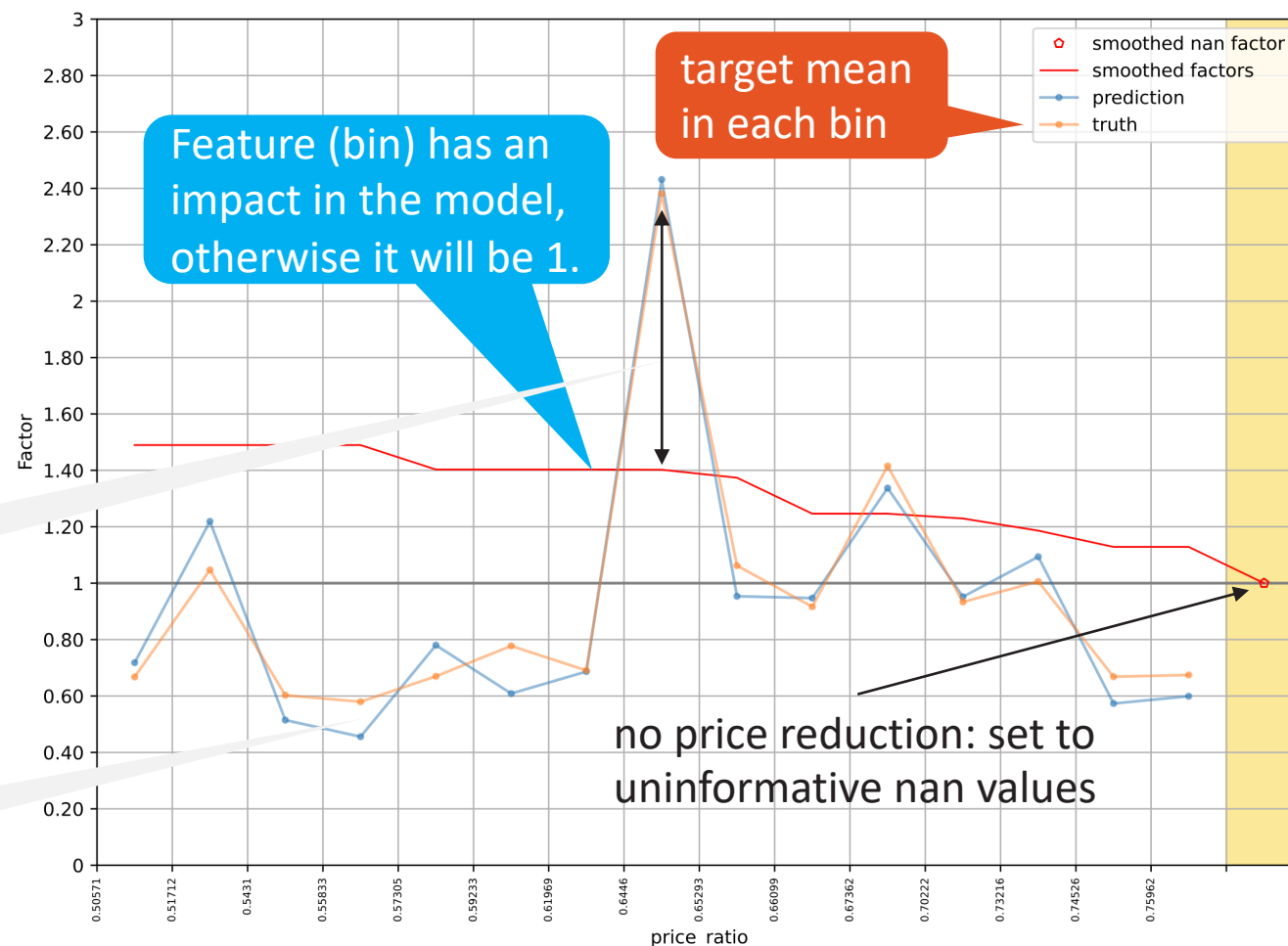
model transparency → ease of development

automatically generated

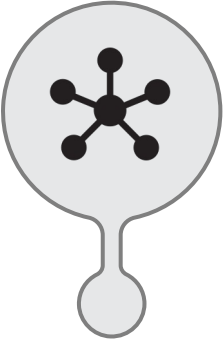
Deviations between smoothed factors and predictions come from correlations with other features.

Deviations of predictions from truths show potential model weaknesses (biases) in different bins.

analysis after last iteration:

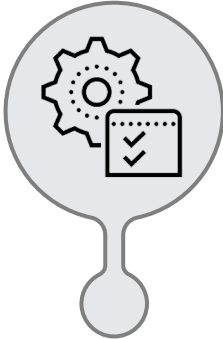


Cyclic Boosting | Characteristics



TOPOLOGY

Generalized
Additive Model



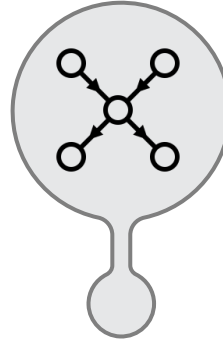
OPTIMIZATION

cyclic coordinate
descent



PREREQUISITE

binning of features



REGULARIZATION

Bayesian updates and
smoothing of factor
distributions

similarities to:

backfitting, forward-
stagewise modeling
(aka boosting)

LightGBM



Off-The-Shelf Method for Structured Data

- “simple” algorithm, but robust and fast
- few hyperparameters to be tuned
- not much data pre-processing needed
- easily configurable for different data types
- supporting missing values in input data
- assisting model development with individual analysis plots for features
- allowing building of complex models by means of interaction terms
- (multiplicative or additive) regression (location parameter)
- classification



Other Modes: Width Prediction (Scale)

important business application: automated replenishment

full, individual PDF predictions (e.g., probability distributions for each product-location-day combination)

by means of separate ML models for mean and variance (actually, indirect prediction of variance via dispersion parameter), assuming negative binomial distribution of target (e.g., demand) in maximum likelihood estimation

1. Forecast Probabilities



We understand internal & external factors. By forecasting the probability density, we know the risks of e.g. lost sales vs. waste.

2. Optimize Decisions



3. Automate Orders



Knowing these risks we calculate the order, which minimizes these risks and balances them according to strategy set by the retailer.



using factors in exponential terms

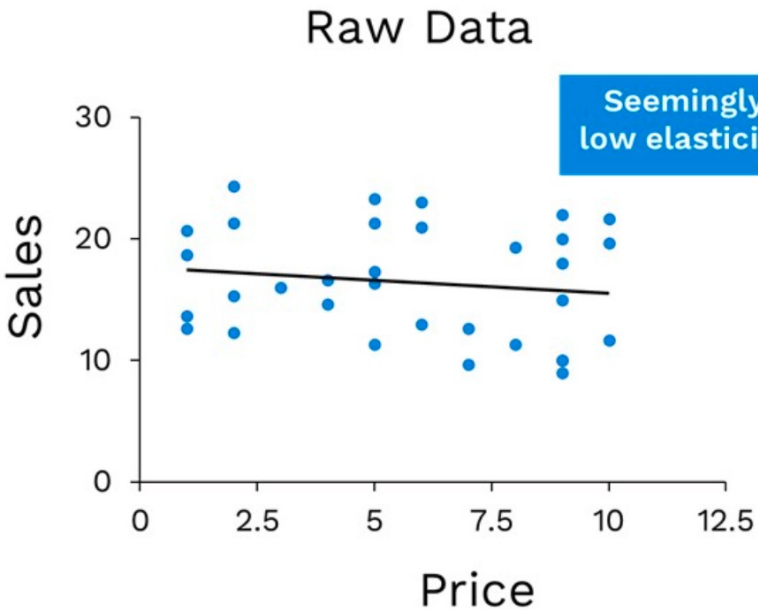
using negative sample weights

Other Modes: Elasticity Prediction (Shape), Background Subtraction

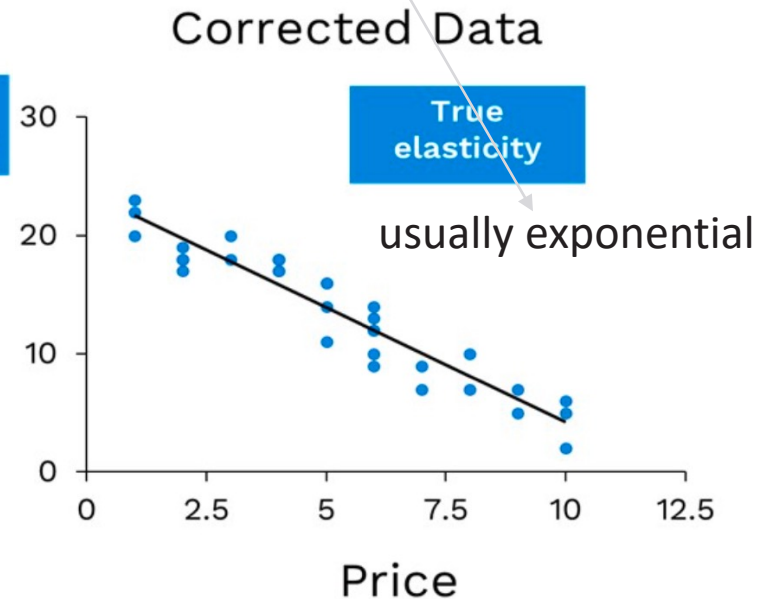
other business application: demand shaping by causal inference (mainly beyond ML/CB), examples:

- dynamic pricing: influence demand of different products by price setting
- customer targeting: influence individual customer demand by couponing (subtract unaffected customers)

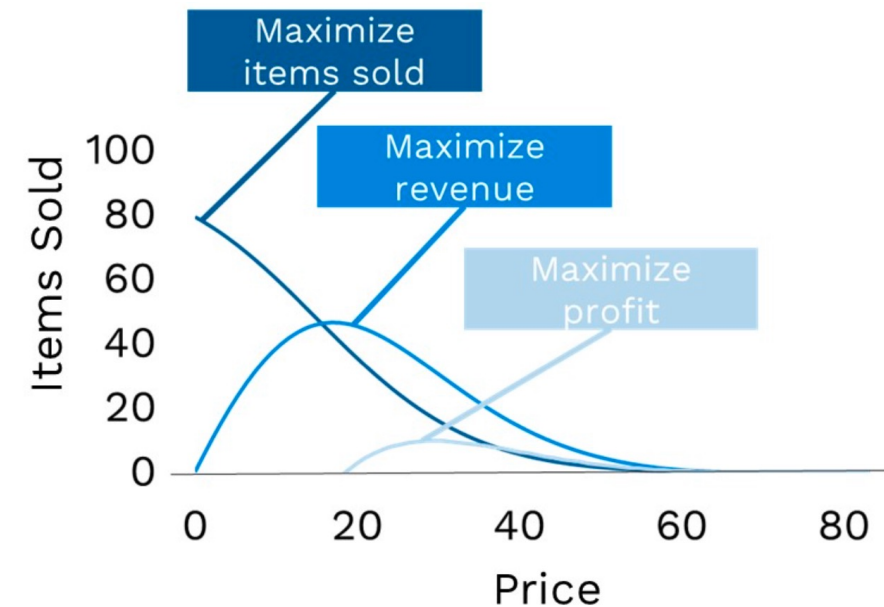
confounded effect:



after de-confounding:



use for pricing policies:



Now Try It Yourself ...

hackathon at Blue Yonder booth

task: retail demand forecasting

You can also try to beat Cyclic Boosting with other methods like Gradient Boosting or a transformer.





Fulfill your potential™