

# 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



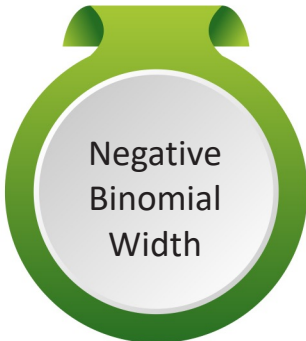
(probability)

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

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

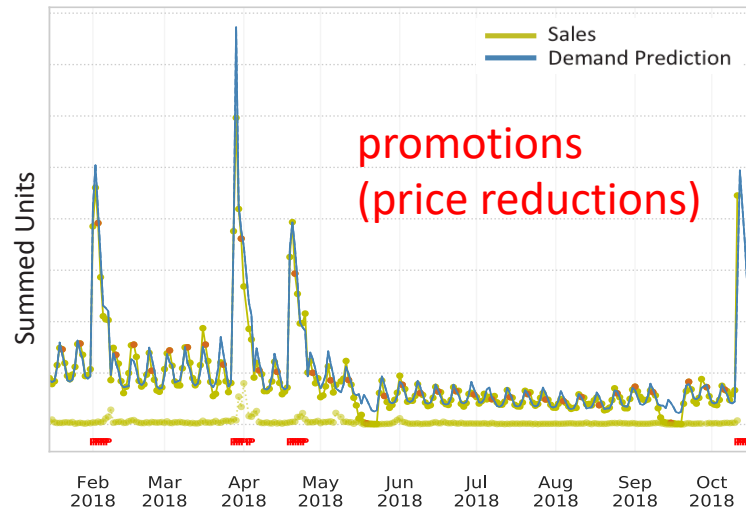


# Example Use Case: Demand Forecasting

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:

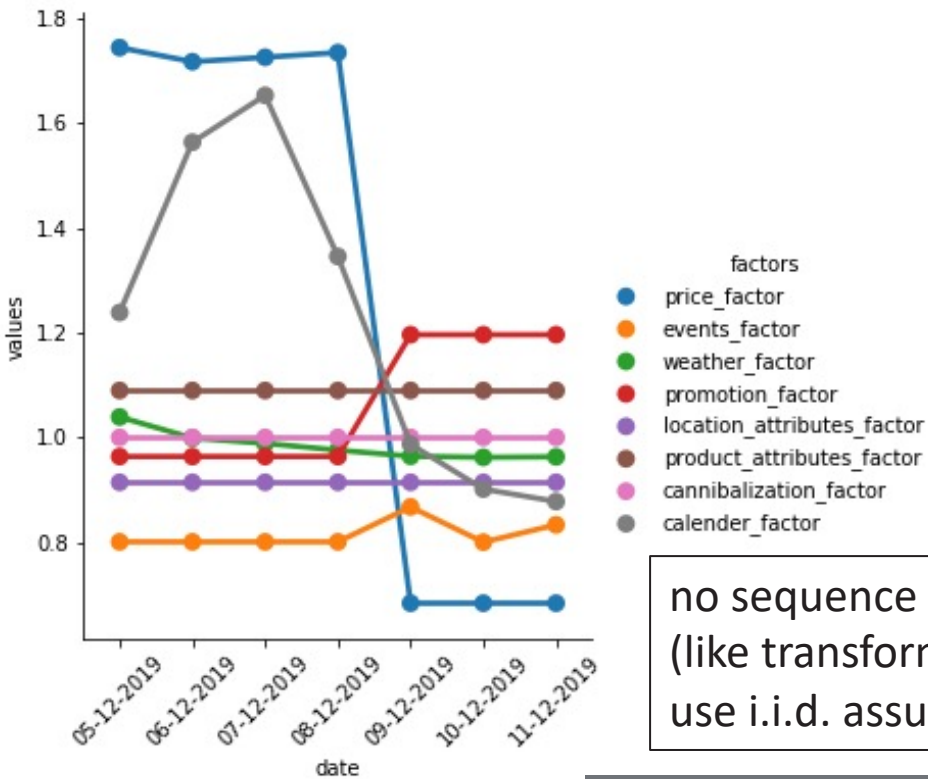
- categorical features important (products and locations → high cardinality)
- mainly multiplicative effects
- demand (approximately) following Poisson (or rather negative binomial) distribution



# Cyclic Boosting - Prediction View | Individual Explainability

Cyclic Boosting in multiplicative regression mode

## 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

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

global  
average

factor for feature  
j in bin k

multiplicative model  
variation proportional to level

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





# Cyclic Boosting Training

## Coordinate Descent with Boosting-like Update of Factors

1. calculate global average  $\mu$ , initialize all factors to 1
2. cyclically iterate through features and calculate for each feature bin partial and corresponding aggregated factors (with  $t$  and  $\tau$  referring to iterations of full feature cycles,  $\tau = t$  or  $\tau = t - 1$ )

$$g_{j,t}^k = \frac{\sum_{x_{j,i} \in b_j^k} y_i}{\sum_{x_{j,i} \in b_j^k} \hat{y}_{i,\tau}}$$

numerator: target values  
 denominator: estimation  
 bins  
 features

where  $f_{j,t}^k = \prod_{s=1}^t g_{j,s}^k$

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)
...
    for (features)
...
        for (samples)
  
```

iterations

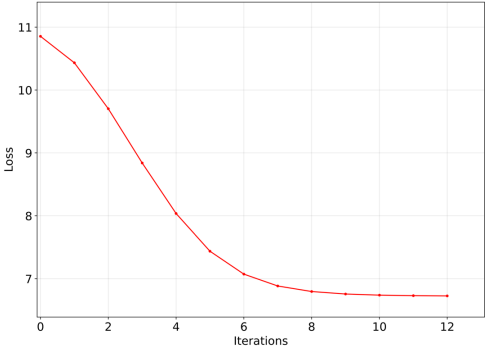
sequential

parallel

other modes work accordingly

$$\hat{y}_{i,\tau} = \mu \cdot \prod_{j=1}^p f_{j,\tau}^k$$

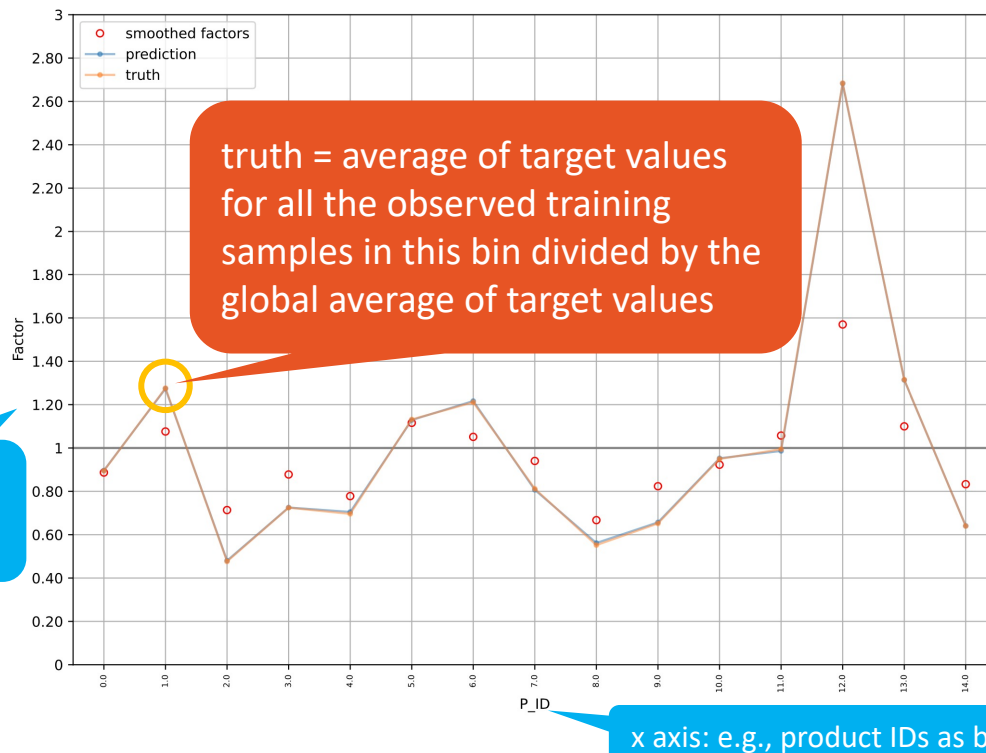
global average  
 product of all factors



# Binning

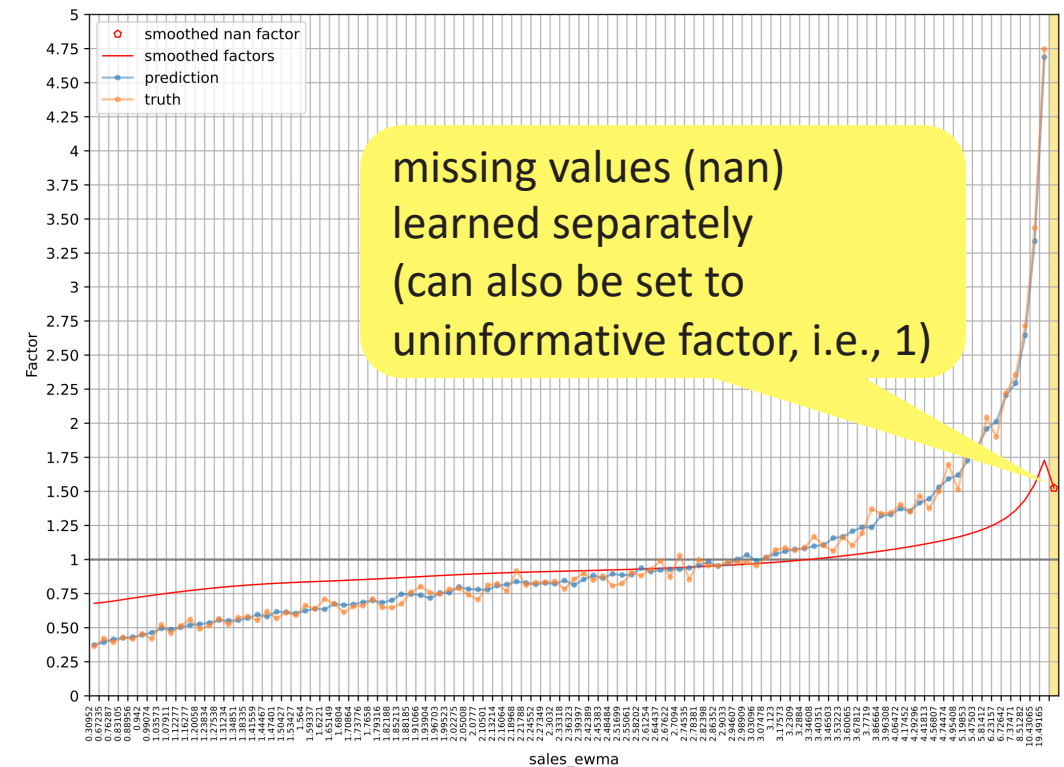
categorical features retain original categories (learning of specific factor for each of the bins)

→ 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



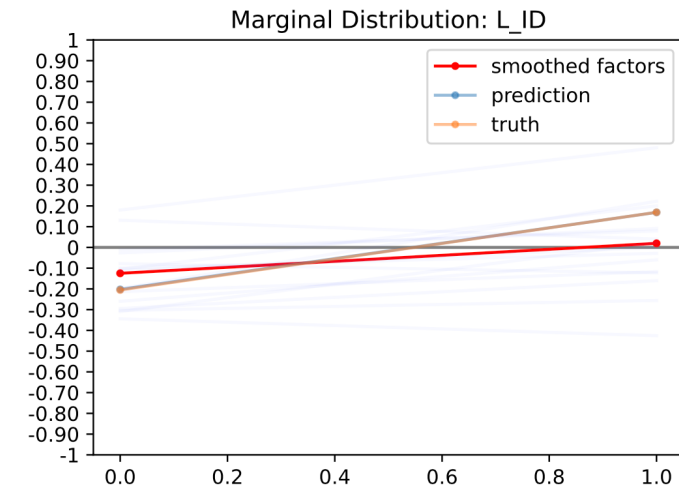
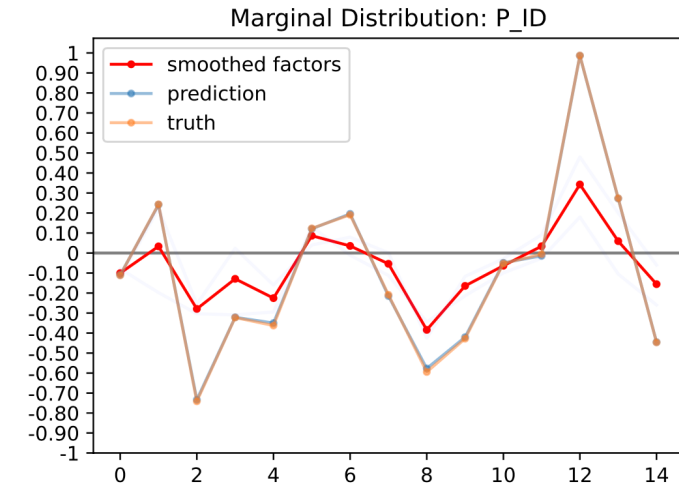
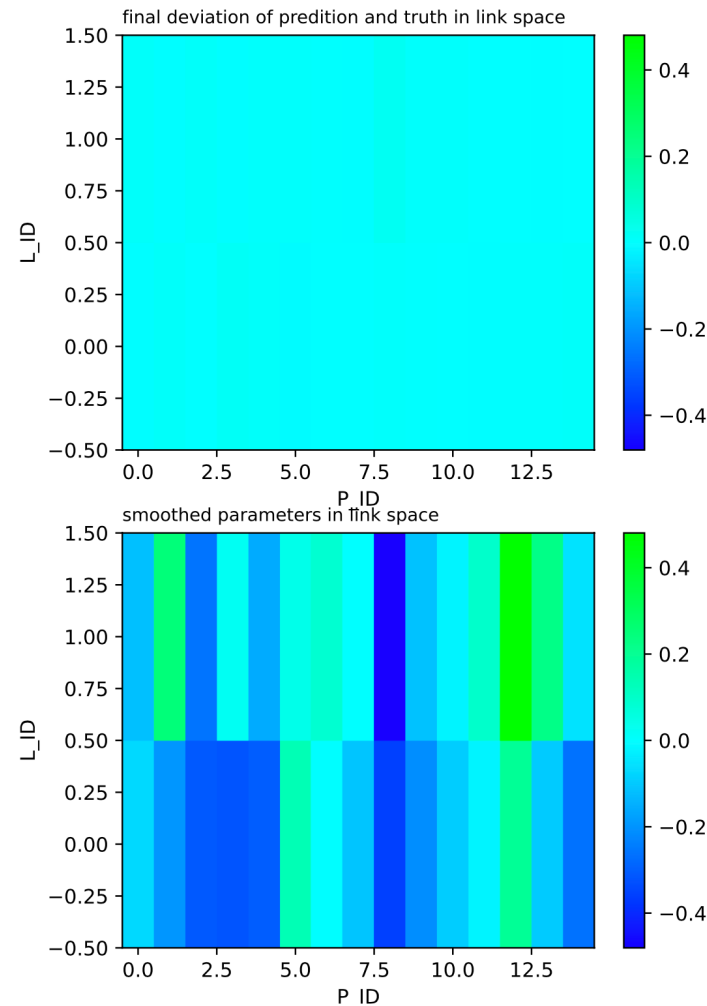
# Interaction Terms

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

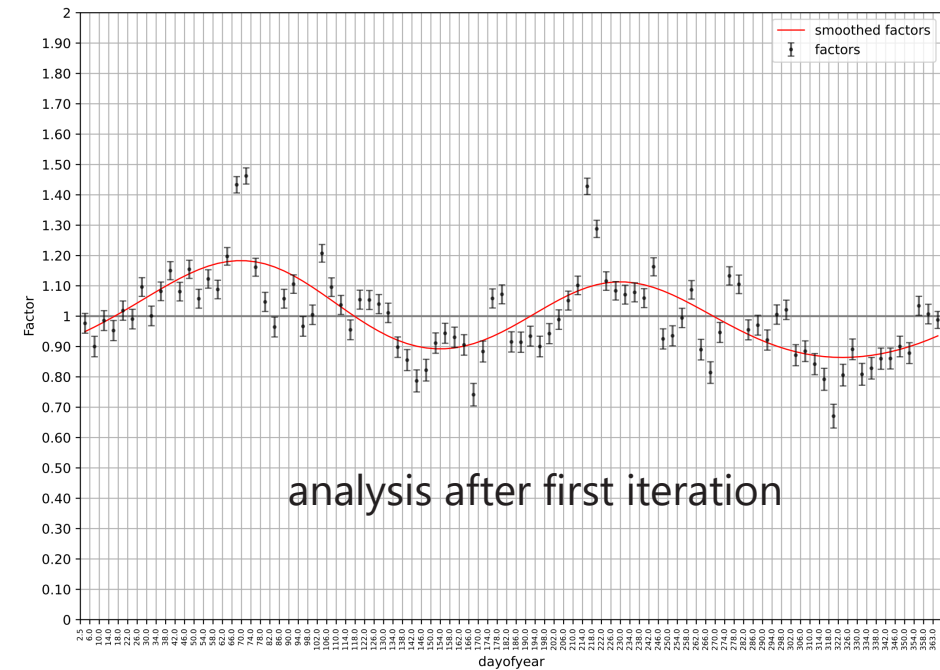
separate smoothings in each iteration

in general: orthogonal polynomials

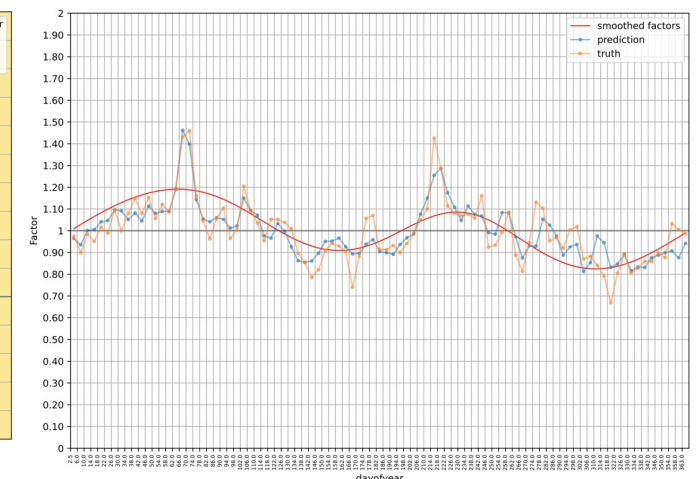
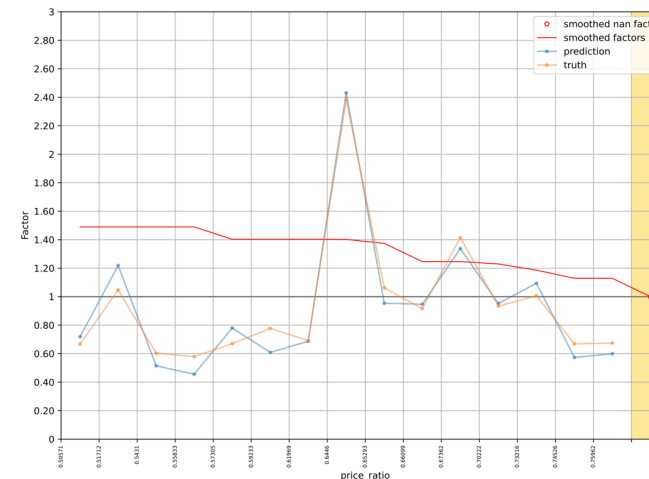
another way to include *prior knowledge* via

- 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

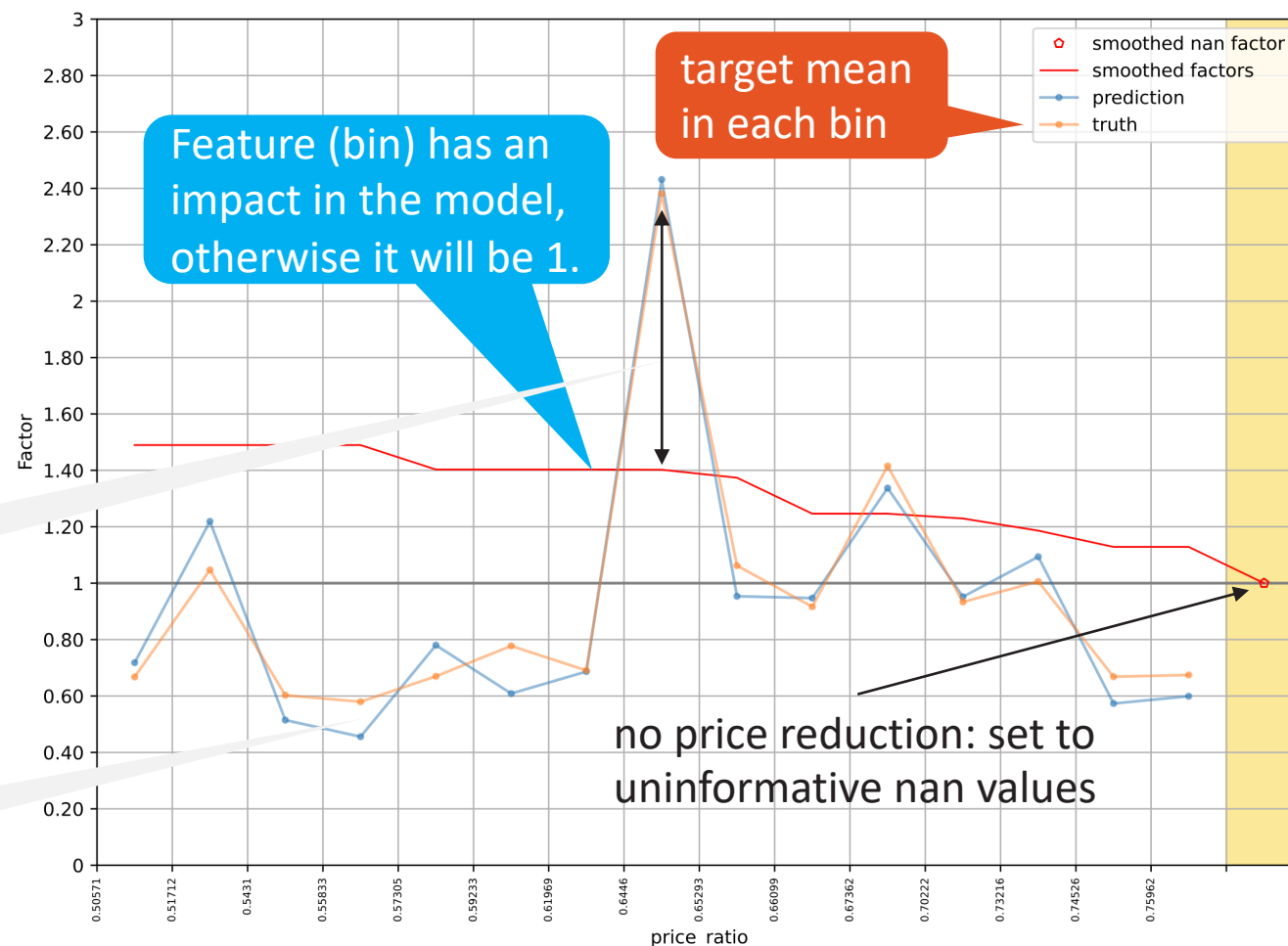
model transparency → ease of development

automatically generated

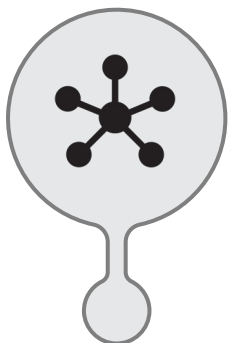
Deviations between smoothed factors and predictions come from correlations with other features.

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

analysis after last iteration:

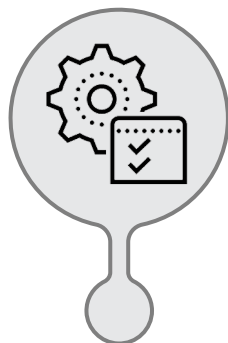


# Cyclic Boosting | Characteristics



## TOPOLOGY

Generalized  
Additive Model



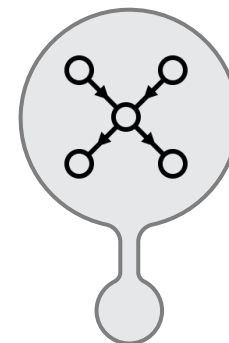
## OPTIMIZATION

cyclic coordinate  
descent with boosting-like  
update of factors



## 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

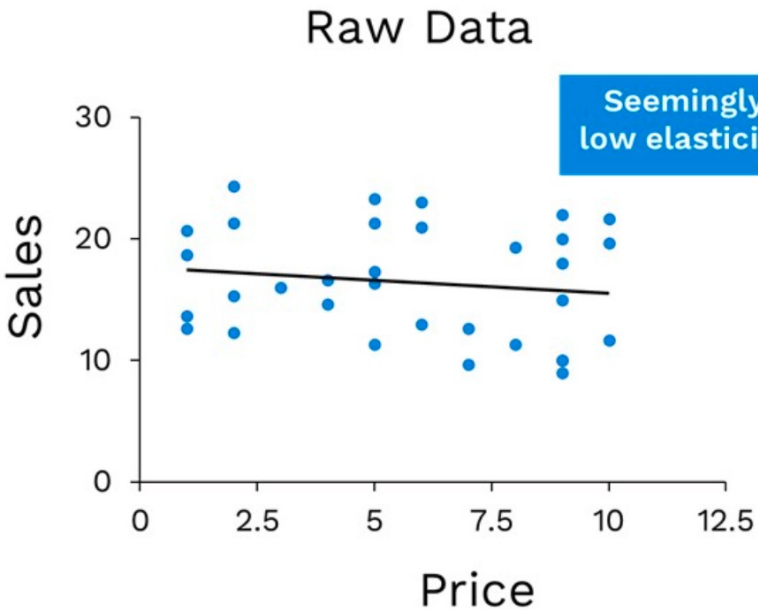
using negative sample weights

# Other Modes: Elasticity Prediction (Shape), Background Subtraction

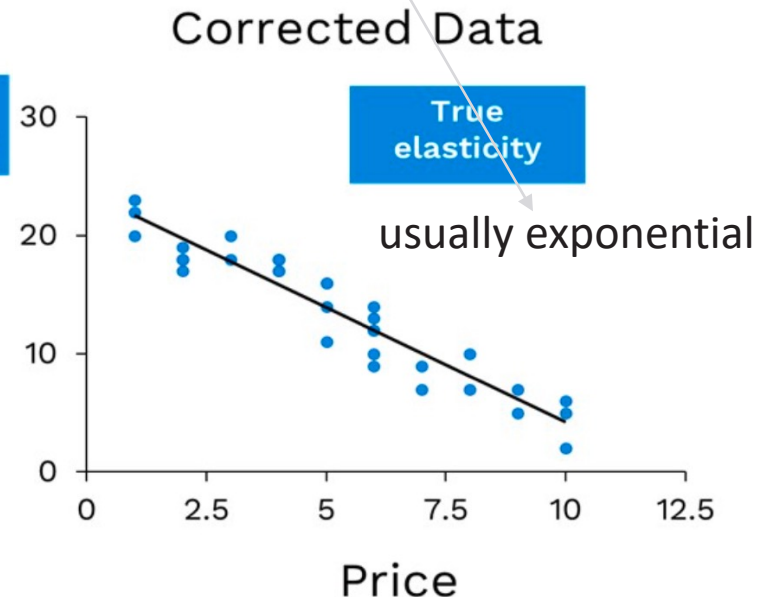
other business application: demand shaping by causal inference (mainly beyond ML/CB), examples:

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

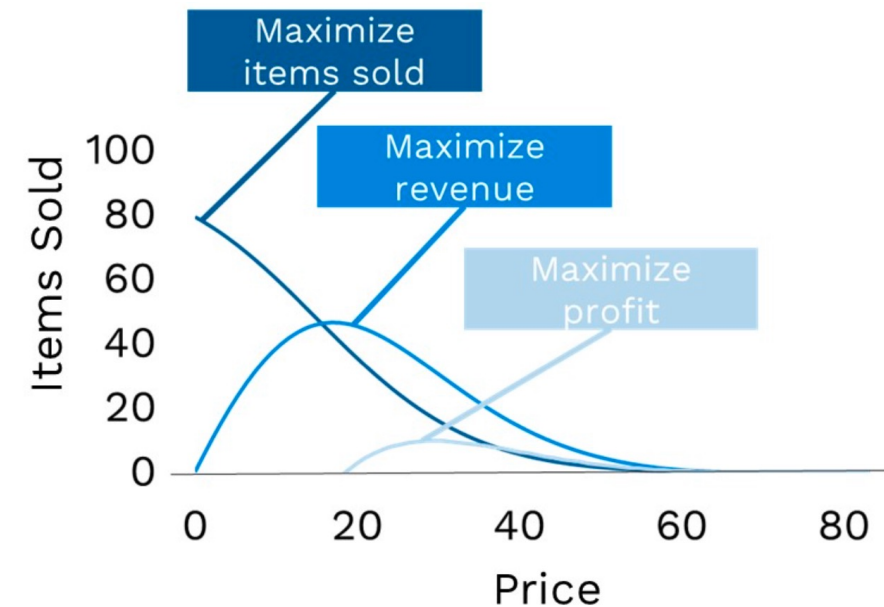
confounded effect:



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™