From Predictive to Prescriptive Analytics

Dimitris Bertsimas

Joint work with Nathan Kallus





Philosophy/Motivation

- Operations Research/Management Science typically starts with models and aims to make optimal decisions. Data is often an afterthought.
- Machine Learning/Statistics typically starts with data and aims to make predictions. Decisions are typically not considered.
- Models, in my opinion, exist in our imagination.
- Yet, we typically teach models to our students.

Opportunity

- Availability of data (often big data) in electronic form.
- Can we develop a theory that unifies OR/MS and ML/S that goes:

From data to predictions to prescriptions?

What are the implications in Education? Should we change our courses?

Contributions

- A theory that unifies OR/MS and ML/S that goes
 From data to predictive to prescriptive analytics.
- Asymptotic optimality, as the data increases the decisions are optimal.
- Computational Tractability
- Coefficient of Prescriptiveness P that measures how much auxiliary data improves a baseline, generalizing R² for predictions.
- Real world example that shows that this theory makes a material improvement in a Global Fortune 100 multimedia media company.

A Real World Problem

A Global Fortune 100 multimedia company.

1 billion units of entertainment media shipped per year

 Sells 1/2 million different titles on CD/DVD/Bluray at over 50,000 retailers worldwide



Key Issues

- Limited shelf space at retail locations
- Huge array of potential titles
- Highly uncertain demand for new releases
- Which titles to order and in what quantities?
- Maximize number media sold



Data

- 4 years of sales data across a network of 50,000 retailers
- Data harvested from public online sources







How to leverage all this data?

The general problem

- Data y^1, \ldots, y^N on quantities of interest Y E.g. demands at locations/of products,
- Data x^1, \ldots, x^N on associated covariates X E.g. recent sales figures, search engine attention
- Decision $z \in \mathcal{Z}$ to minimize $\mathit{uncertain}$ costs c(z;Y) after observing X=x

Outline

- From Predictive to Prescriptive Analytics
 - A gap in decision making
 - Our approach
 - Asymptotic optimality
 - Coefficient of Prescriptiveness
 - Real world problem

Standard Data-Driven Optimization

- Data y^1, \ldots, y^N on quantities of interest Y
- Decision $z \in \mathcal{Z}$ to minimize *uncertain* costs c(z;Y)
- Problem of interest is

$$\min_{z \in \mathcal{Z}} \mathbb{E}\left[c(z; Y)\right]$$

- But we only have data
- Distributions only exist in our imagination

Standard Data-Driven Optimization

Problem of interest is

$$\min_{z \in \mathcal{Z}} \mathbb{E}\left[c(z; Y)\right]$$

Standard data-driven solution is sample average approximation

$$\hat{z}_N^{\text{SAA}} \in \arg\min_{z \in \mathcal{Z}} \frac{1}{N} \sum_{i=1}^N c(z; y^i)$$

- Other approaches: Stochastic Approximation (Robins 1951),
 Robust SAA (Bertsimas, Gupta, Kallus 2014)
- General theorem: solutions from these approaches converge to the full-info problem (cf. Shapiro et al. 2009)
- In our problem data-driven approaches like SAA account for uncertainty but not for auxiliary data

Standard Supervised Learning in ML

- Data y^1, \ldots, y^N on quantities of interest Y
- Data x^1, \ldots, x^N on associated covariates X
- Obtain a prediction $\hat{m}_N(x)$ for the future value of Y after observing X=x so that the squared difference between our best prediction and the true value is small.
- For example, a random forest!

Standard Supervised Learning in ML

Problem of interest is

$$\mathbb{E}\left[Y\middle|X=x\right]$$

- How to use for decision-making?
- Fit a ML predictive model $\hat{m}_N(x) \approx \mathbb{E}\left[Y \middle| X = x\right]$ (e.g. a random forest) and solve a deterministic problem

$$\hat{z}_N^{\text{point-pred}}(x) \in \arg\min_{z \in \mathcal{Z}} c(z; \hat{m}_N(x))$$

 In our problem, this point-prediction-driven decision accounts for auxiliary data but not for uncertainty

The predictive prescription problem

Problem of interest:

$$z^*(x) \in \arg\min_{z \in \mathcal{Z}} \mathbb{E}\left[c(z;Y) \middle| X = x\right]$$

Task:

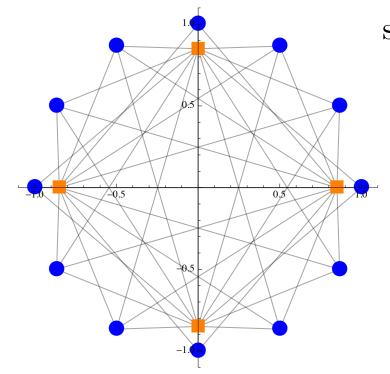
use data $S_N = \{(x^1, y^1), \dots, (x^N, y^N)\}$ to construct a data-driven predictive prescription

$$\hat{z}_N(x): \mathcal{X} \to \mathcal{Z}$$

Shipment planning example

- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week

$$c(z;y) = p_1 \sum_{i=1}^{d_z} z_i + \min \left(p_2 \sum_{i=1}^{d_z} t_i + \sum_{i=1}^{d_z} \sum_{j=1}^{d_y} c_{ij} s_{ij} \right)$$



s.t.
$$t_i \geq 0$$

$$s_{ij} \ge 0$$
 $\forall i, j$

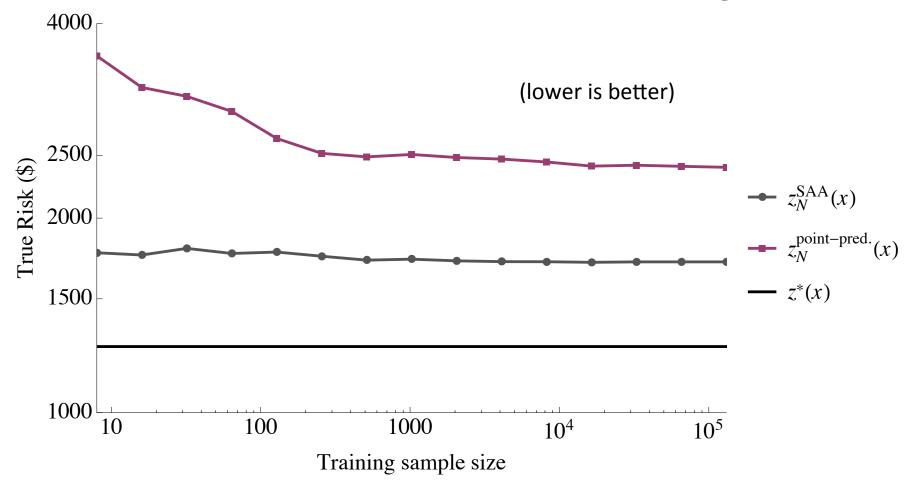
 $\forall i$

$$\sum_{i=1}^{d_z} s_{ij} \ge y_j$$
 $\forall j$

$$\sum_{j=1}^{d_y} s_{ij} \le z_i + t_i \qquad \forall i$$

Shipment planning example

- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week X: Sales, weather forecasts, volume of Google searches



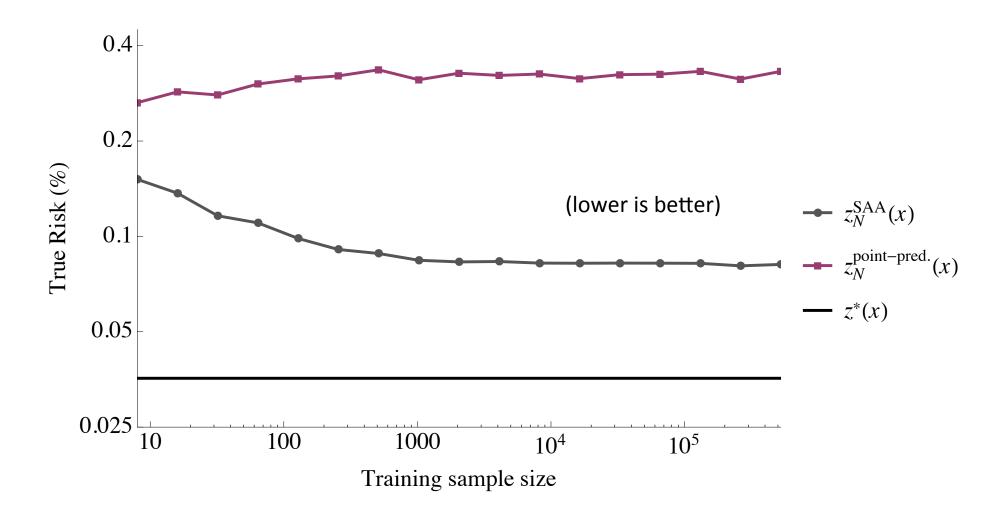
Portfolio example

- Mean-CVaR_{15%} portfolio allocation with 12 securities
- Observe market factors X correlated with future returns

$$c((z,\beta);y) = \beta + \frac{1}{\epsilon} \max\left\{-z^T y - \beta, 0\right\} - \lambda z^T y$$
$$\mathcal{Z} = \{\beta \in \mathbb{R}, z \ge 0, \sum_{i=1}^{d_z} z_i = 1\}$$

Portfolio example

- Mean-CVaR_{15%} portfolio allocation with 12 securities
- Observe market factors X correlated with future returns



Outline

- From Predictive to Prescriptive Analytics
 - A gap in decision making
 - Our approach
 - Asymptotic optimality
 - Coefficient of Prescriptiveness
 - Real world problem

Our approach

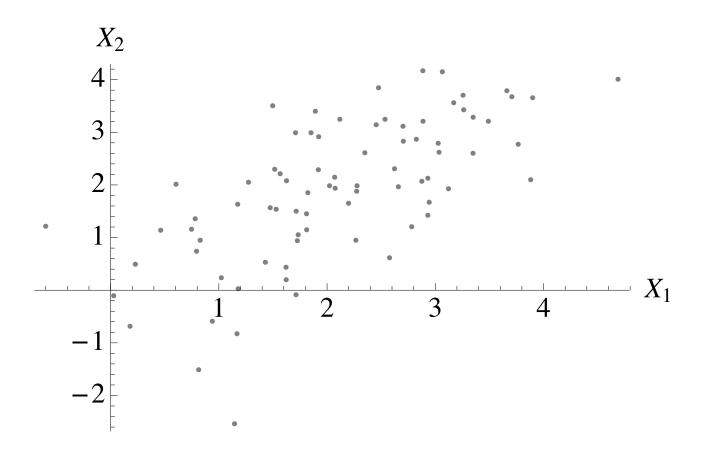
Construct predictive prescriptions of the form

$$\hat{z}_N(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N w_N^i(x) c(z; y^i)$$

Thm: if c(z;y) is convex, $\mathcal Z$ convex, then we can compute $\hat z_N(x)$ in polynomial time.

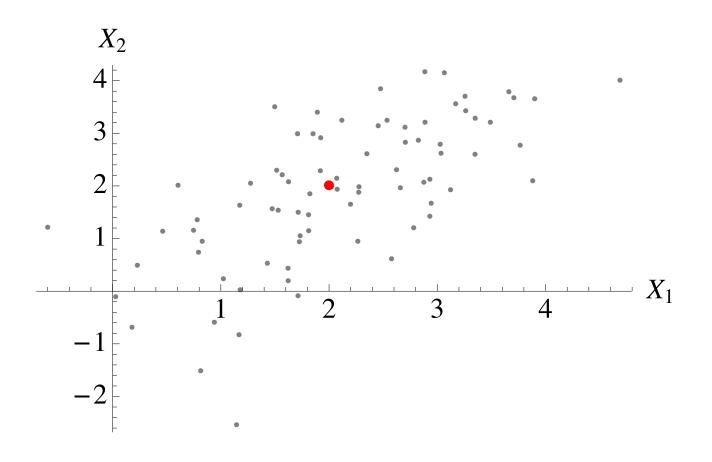
*k*NN

$$\hat{z}_N^{k\text{NN}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{x^i \text{ is } k\text{NN of } x} c(z; y^i)$$



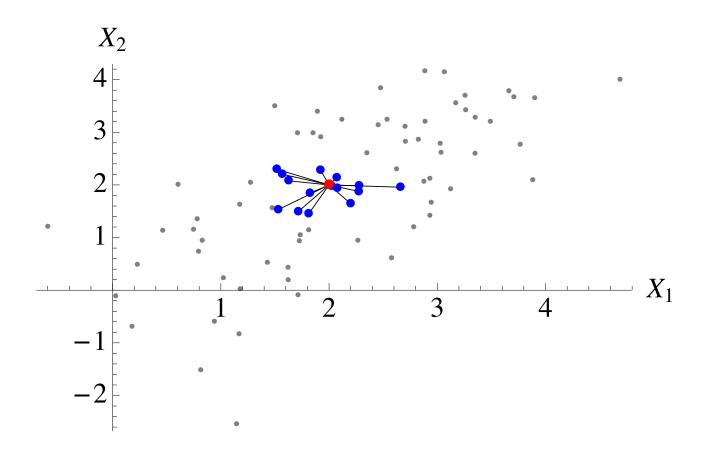
kNN

$$\hat{z}_N^{k\text{NN}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{x^i \text{ is } k\text{NN of } x} c(z; y^i)$$

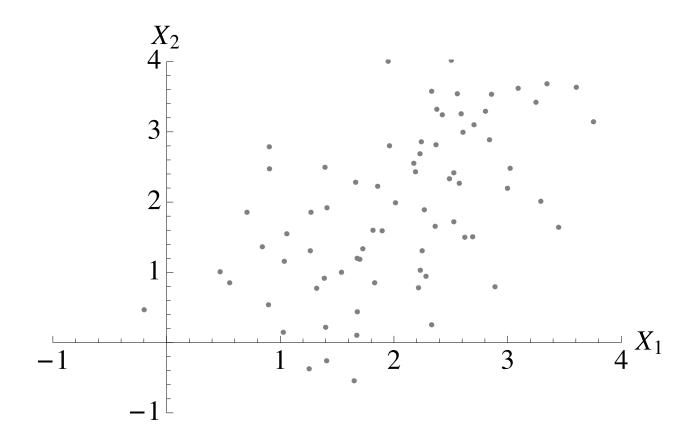


kNN

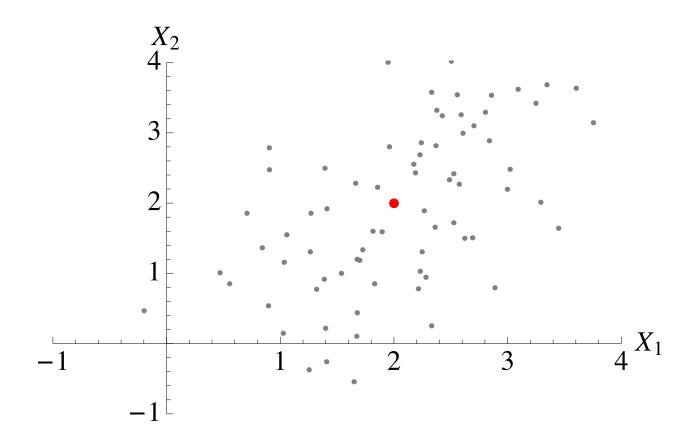
$$\hat{z}_N^{k\text{NN}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{x^i \text{ is } k\text{NN of } x} c(z; y^i)$$



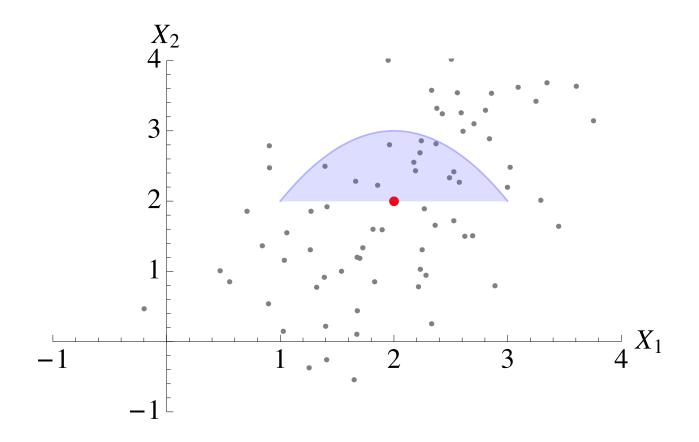
$$\hat{z}_N^{\mathrm{KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_N) c(z; y^i)$$



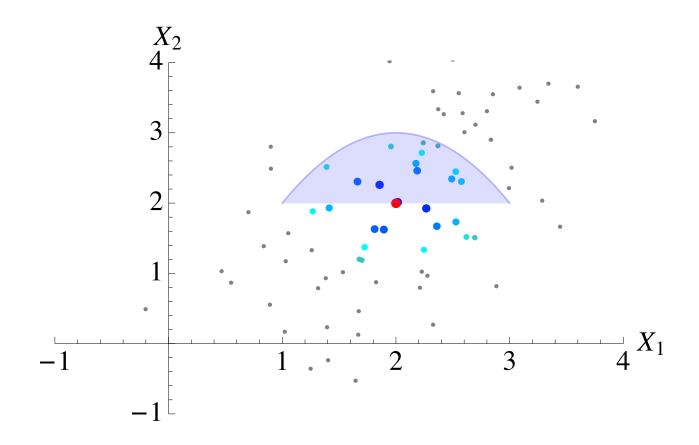
$$\hat{z}_N^{\mathrm{KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_N) c(z; y^i)$$



$$\hat{z}_N^{\mathrm{KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_N) c(z; y^i)$$

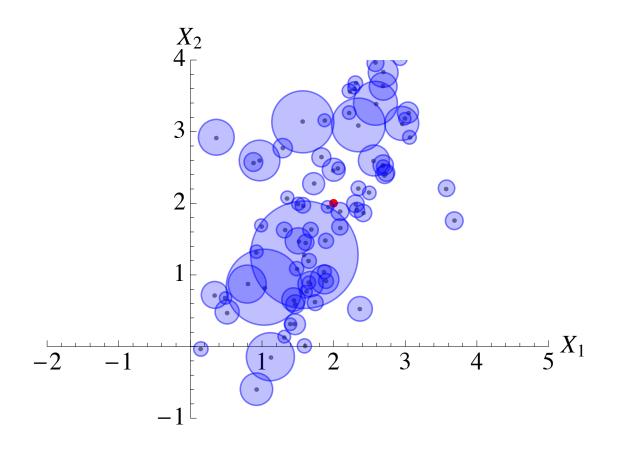


$$\hat{z}_N^{\mathrm{KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_N) c(z; y^i)$$



Recursive Parzen windows

$$\hat{z}_N^{\text{Rec-KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_{i})c(z; y^i)$$



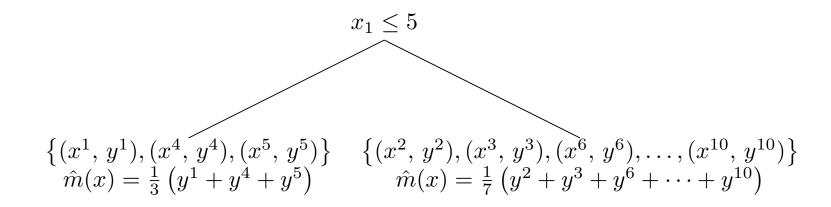
Local linear regression

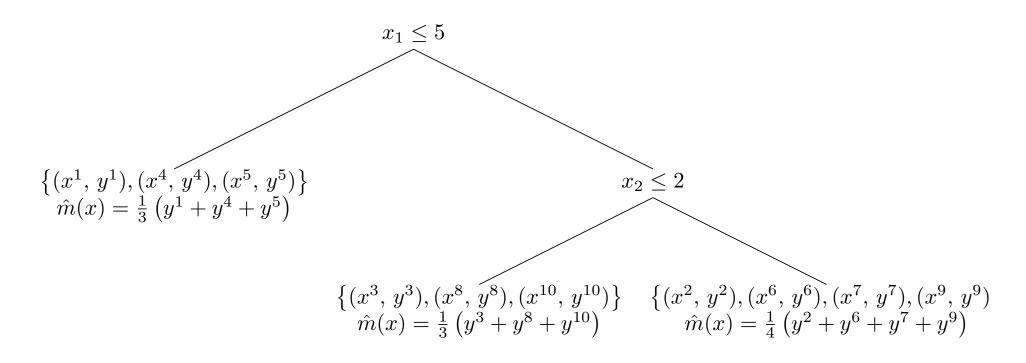
$$\hat{z}_{N}^{\text{LOESS}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^{N} k_{i}(x) \left(1 - \sum_{j=1}^{n} k_{j}(x)(x^{j} - x)^{T} \Xi(x)^{-1}(x^{i} - x) \right) c(z; y^{i})$$

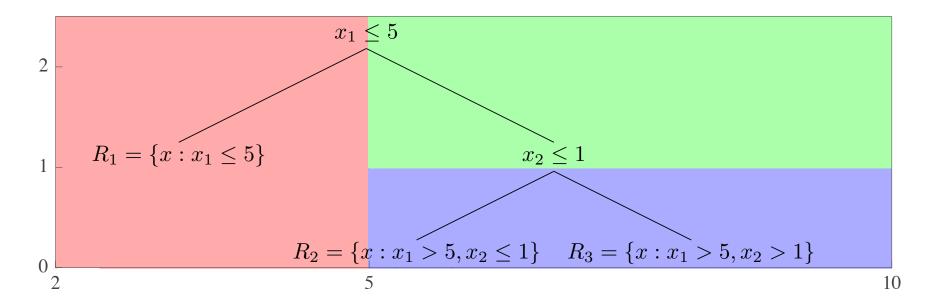
$$\Xi(x) = \sum_{i=1}^{n} k_i(x)(x^i - x)(x^i - x)^T \quad k_i(x) = \left(1 - \left(\left|\left|x^i - x\right|\right| / h_N\right)^3\right)^3 \mathbb{I}\left[\left|\left|x^i - x\right|\right| \le h_N\right]$$

$$\left\{ (x^1, y^1), (x^2, y^2), (x^2, y^2), (x^3, y^3), (x^4, y^4), (x^5, y^5), (x^6, y^6), (x^7, y^7), (x^8, y^8), (x^9, y^9), (x^{10}, y^{10}) \right\}$$

$$\hat{m}(x) = \frac{1}{10} \left(y^1 + y^2 + y^3 + y^4 + y^5 + y^6 + y^7 + y^8 + y^9 + y^{10} \right)$$







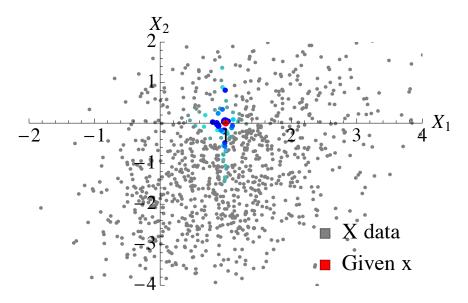
Implied binning rule $R(x) = (j \text{ s.t. } x \in R_j)$

$$\hat{z}_{N}^{\text{CART}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{\mathcal{R}(x^{i}) = \mathcal{R}(x)} c(z; y^{i})$$

Random Forest

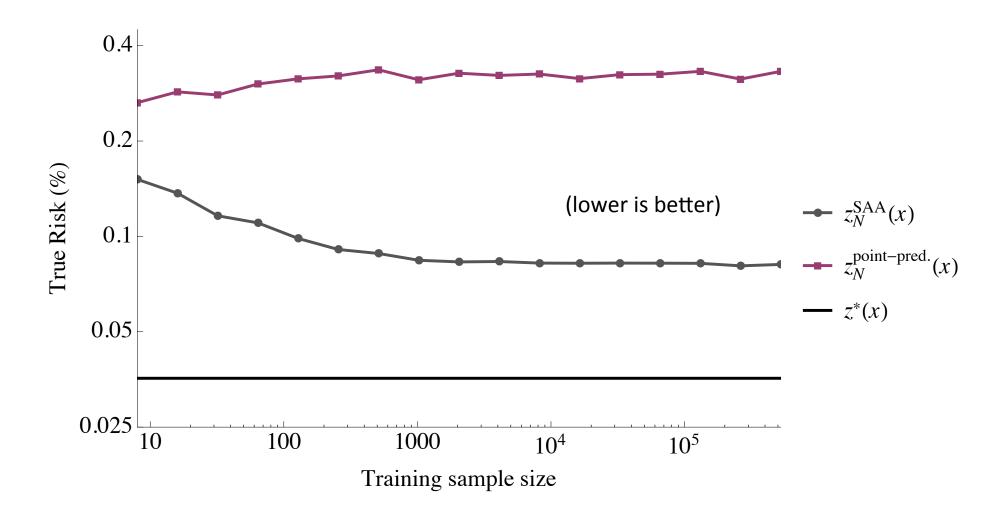
- Train T trees on bootstrapped samples and randomly selected feature subsets
- Get T binning rules $R^t(x) = (j \text{ s.t. } x \in R_j^t)$

$$\hat{z}_{N}^{\text{RF}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{t=1}^{T} \frac{1}{|\{j : R^{t}(x^{j}) = R^{t}(x)\}|} \sum_{R^{t}(x^{i}) = R^{t}(x)} c(z; y^{i})$$



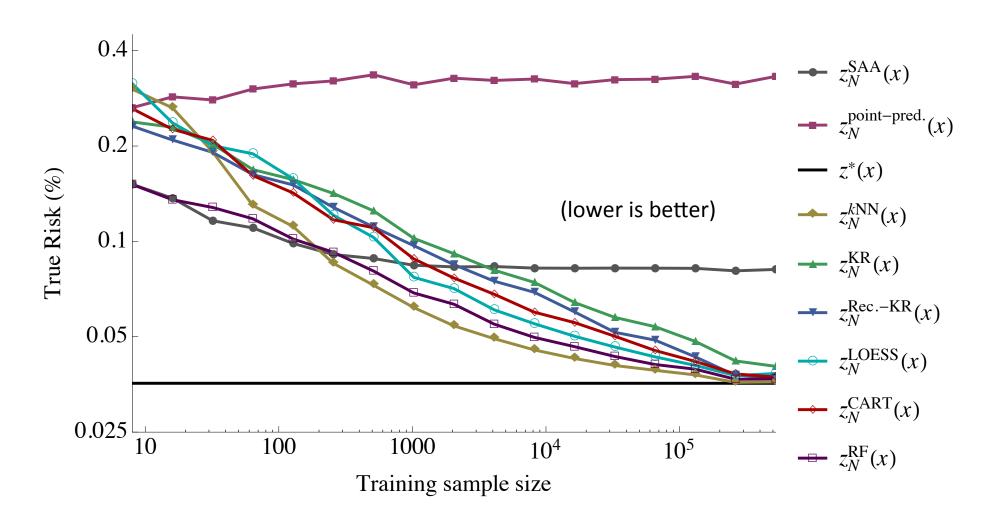
Portfolio example

- Mean-CVaR_{15%} portfolio allocation with 12 securities
- Observe market factors X correlated with future returns

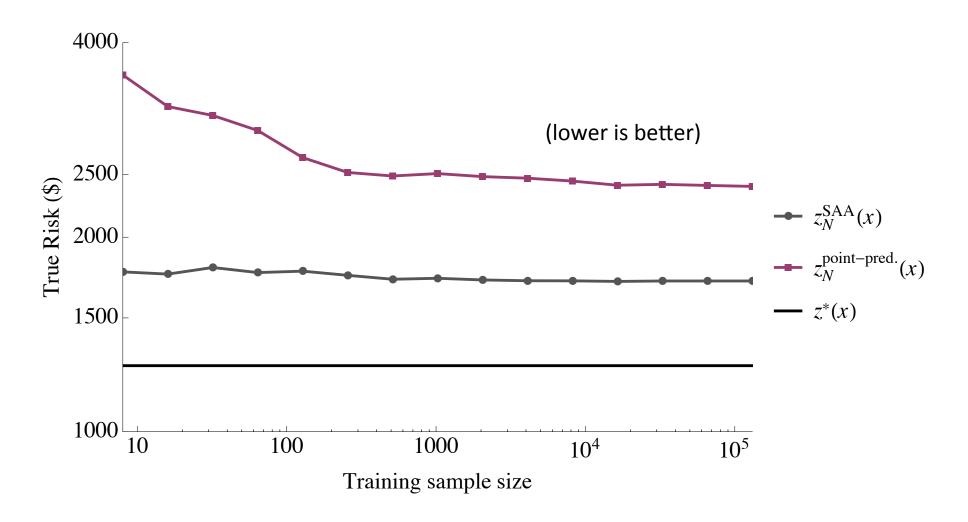


Portfolio example

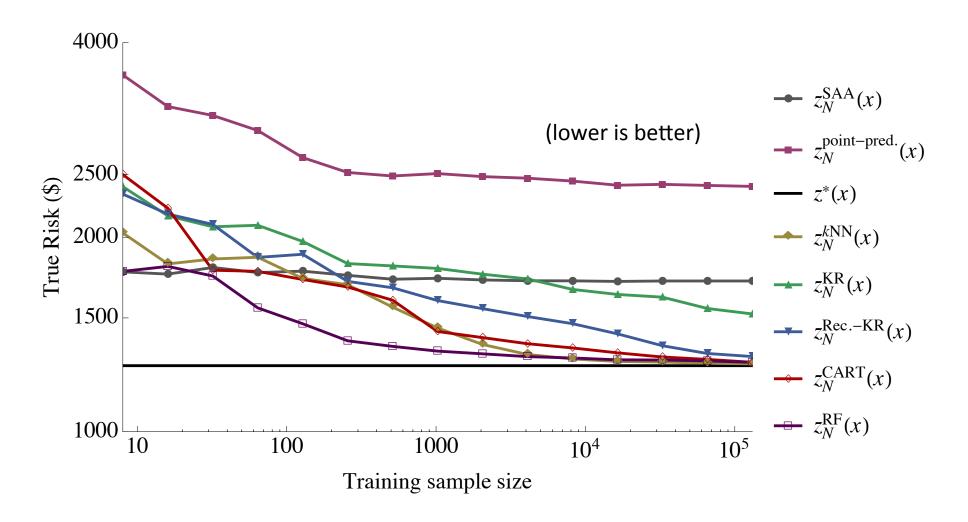
- Mean-CVaR_{15%} portfolio allocation with 12 securities
- Observe market factors X correlated with future returns



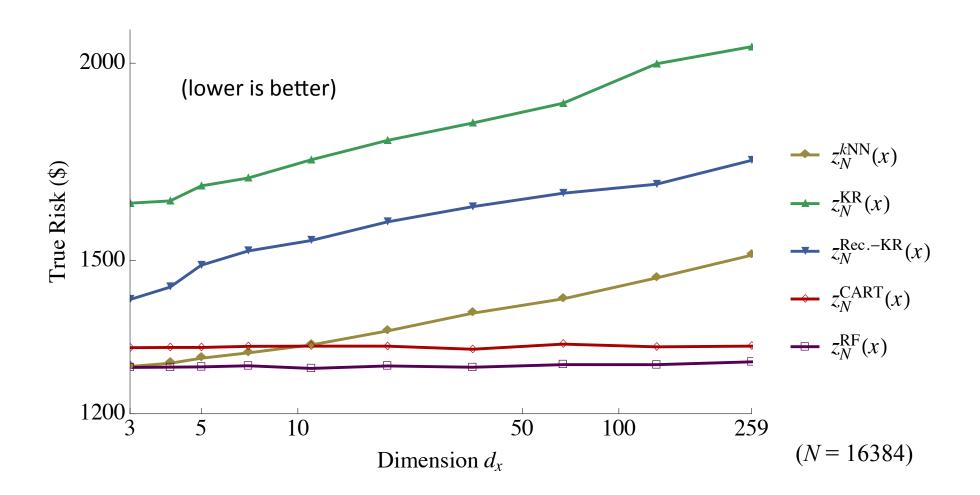
- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week



- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week



- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week



Outline

- From Predictive to Prescriptive Analytics
 - A gap in decision making
 - Our approach
 - Asymptotic optimality
 - Coefficient of Prescriptiveness
 - Real world problem

Asymptotic Optimality

Want

Def: predictive prescription $\hat{z}_N(x)$ is *asymptotically optimal* if, with probability 1, for almost everywhere x, as $N \to \infty$ $\lim_{N \to \infty} \mathbb{E}\left[c(\hat{z}_N(x);Y)\big|X=x\right] = \min_{z \in \mathcal{Z}} \mathbb{E}\left[c(z;Y)\big|X=x\right]$ $L\left(\{\hat{z}_N(x):N \in \mathbb{N}\}\right) \subset \arg\min_{z \in \mathcal{Z}} \mathbb{E}\left[c(z;Y)\big|X=x\right]$

Need

Assumption 1: The full-info problem is well defined, i.e., $\mathbb{E}\left[|c(z;Y)|\right] < \infty$

Assumption 2: c(z;y) is equicontinuous in z.

Assumption 3: \mathcal{Z} is closed and bounded, and c(z;y) is convex.

Data collection as a mixing process

Instead of IID consider a data collection process

$$(x_1, y_1), (x_2, y_2), \dots$$

that is a stationary mixing process

• i.e., as the lag ℓ gets bigger,

$$(x_1,\,y_1),\ldots,(x_t,\,y_t)$$
 and $(x_{t+\ell},\,y_{t+\ell}),(x_{t+\ell+1},\,y_{t+\ell+1}),\ldots$

are more and more independent.

- Encompasses ARMA, GARCH, Markov processes.
- Can represent more realistic data collection from interdependent weekly demands, stock returns, volume of Google searches on a topic, ...

Asymptotic Optimality: *k*NN

$$\hat{z}_N^{k\text{NN}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{x^i \text{ is } k\text{NN of } x} c(z; y^i)$$

Thm: Suppose Assumptions 1, 2, & 3 hold, data collection is

IID, and $k = \min \{ \lceil CN^{\delta} \rceil, N - 1 \}$ with $0 < \delta < 1$.

Then $\hat{z}_N^{k\mathrm{NN}}(x)$ is asymptotically optimal.

Asymptotic Optimality: Parzen Windows

$$\hat{z}_N^{\mathrm{KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_N) c(z; y^i)$$

Thm: Suppose Assumptions 1, 2, & 3 hold, data collection is mixing, costs satisfy $\mathbb{E}\left[|c(z;Y)|\left(\log|c(z;Y)|\right)_+\right]<\infty$, K is one of given kernels, and $h_N=CN^{-\delta}$, $0<\delta<1/d_x$. Then $\hat{z}_N^{\mathrm{KR}}(x)$ is asymptotically optimal.

Asymptotic Optimality: Recursive Parzen Windows

$$\hat{z}_N^{\text{Rec-KR}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^N K((x^i - x)/h_{\textcolor{red}{\boldsymbol{i}}}) c(z; y^i)$$

Thm: Suppose Assumptions 1, 2, & 3 hold, data collection is mixing, K is one of given kernels,

and
$$h_i = Ci^{-\delta}$$
, $0 < \delta < 1/(2d_x)$.

Then $\hat{z}_N^{\mathrm{Rec-KR}}(x)$ is asymptotically optimal.

Asymptotic Optimality: LOESS

$$\hat{z}_{N}^{\text{LOESS}}(x) \in \arg\min_{z \in \mathcal{Z}} \sum_{i=1}^{N} k_{i}(x) \left(1 - \sum_{j=1}^{n} k_{j}(x) (x^{j} - x)^{T} \Xi(x)^{-1} (x^{i} - x) \right) c(z; y^{i})$$

$$\Xi(x) = \sum_{i=1}^{n} k_i(x)(x^i - x)(x^i - x)^T \quad k_i(x) = \left(1 - \left(\left|\left|x^i - x\right|\right| / h_N\right)^3\right)^3 \mathbb{I}\left[\left|\left|x^i - x\right|\right| \le h_N\right]$$

Thm: Suppose Assumptions 1, 2, & 3 hold, data collection is mixing, μ_X abs. continuous, costs bounded $|c(z;y)| \leq g(z)$, and $h_N = CN^{-\delta}$, $0 < \delta < 1/d_x$.

Then $\hat{z}_N^{\mathrm{LOESS}}(x)$ is asymptotically optimal.

Outline

- From Predictive to Prescriptive Analytics
 - A gap in decision making
 - Our approach
 - Asymptotic optimality
 - Coefficient of Prescriptiveness
 - Real world problem

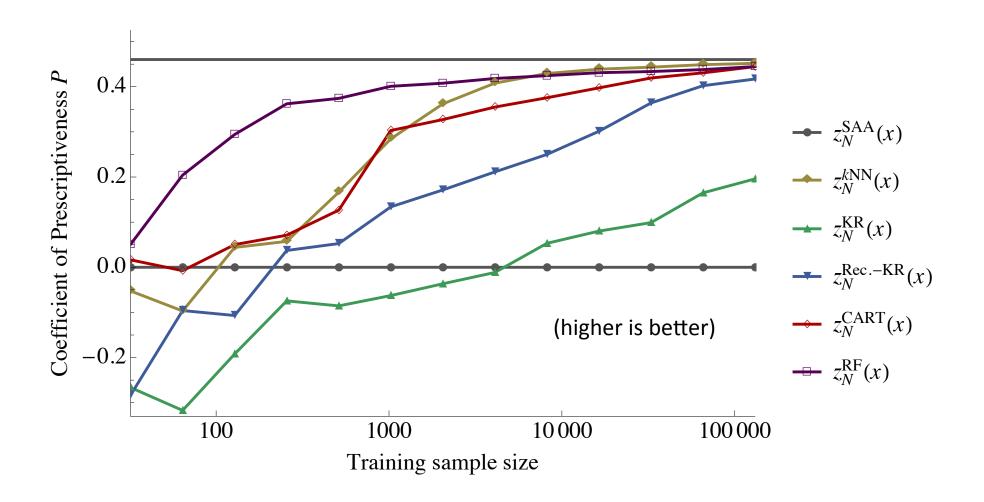
Value of a Prescription

Coefficient of Prescriptiveness

$$P = \frac{\min_{z \in \mathcal{Z}} \sum_{i=1}^{N} c(z; y^{i}) - \sum_{i=1}^{N} c(\hat{z}_{N}(x^{i}); y^{i})}{\min_{z \in \mathcal{Z}} \sum_{i=1}^{N} c(z; y^{i}) - \sum_{i=1}^{N} \min_{z \in \mathcal{Z}} c(z; y^{i})} \stackrel{\leq 1}{\to [0, 1]}$$

- Measures the prescriptive value of X
 and of the of the prescription trained
- Contrast with R².

- Stock 4 warehouses to fulfill demand in 12 locations
- Observe predictive features X about demand in a week



Outline

- From Predictive to Prescriptive Analytics
 - A gap in decision making
 - Our approach
 - Asymptotic optimality
 - Coefficient of Prescriptiveness
 - Real world problem

Back to our media distribution application

- Recall: want to maximize number of items sold.
- Focus on video media, Europe
- r index locations, t index periods, j index products.
- Y_j demand for j, z_{trj} order, x_{tr} auxiliary data.

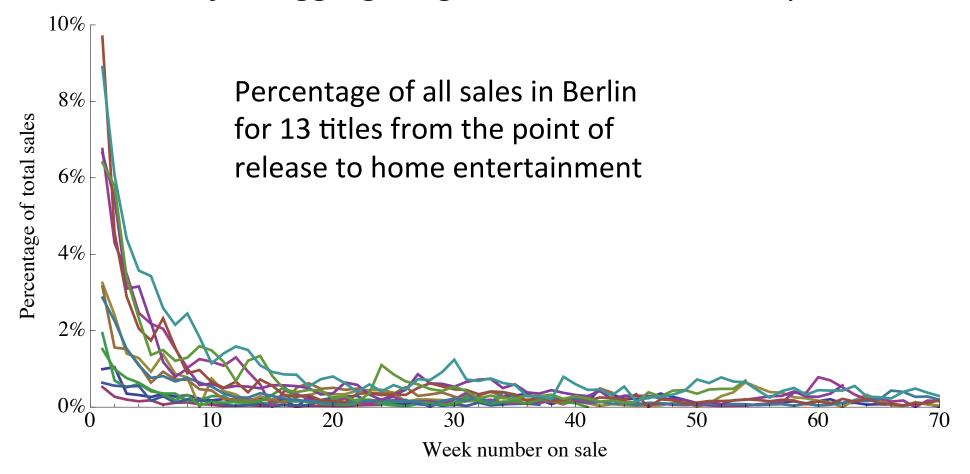
$$\max \mathbb{E}\left[\sum_{j=1}^{d} \min\left\{Y_j, z_{trj}\right\} \middle| X = x_{tr}\right]$$

s.t.
$$\sum_{j=1}^{d} z_{trj} \le K_r$$
$$z_{trj} \ge 0$$

$$\forall j=1,\ldots,d$$

Internal Company Data

- Sales by item/location, 2010 to present
- ~50GB after aggregating transaction records by week



Dealing with Censored Data

Observe sales, not demand (quantity of interest Y)

$$U = \min\{Y, V\}$$

Adjust weights for right-censored data

$$\tilde{w}_{N,(i)}(x) = \begin{cases} \left(\frac{w_{N,(i)}(x)}{\sum_{\ell=i}^{N} w_{N,(\ell)}(x)}\right) \prod_{k \le i-1 : u^{(k)} < v^{(k)}} \left(\frac{\sum_{\ell=k+1}^{N} w_{N,(\ell)}(x)}{\sum_{\ell=k}^{N} w_{N,(\ell)}(x)}\right) & \text{if } u^{(i)} < v^{(i)}, \\ 0 & \text{otherwise.} \end{cases}$$

Thm: Under same assumptions as before and if in addition (a) Y and V conditionally independent given X, (b) Y and V share no atoms, and (c) upper support of V greater than that of Y given X = x, then $\hat{z}_N(x)$ is **asymptotically optimal**.

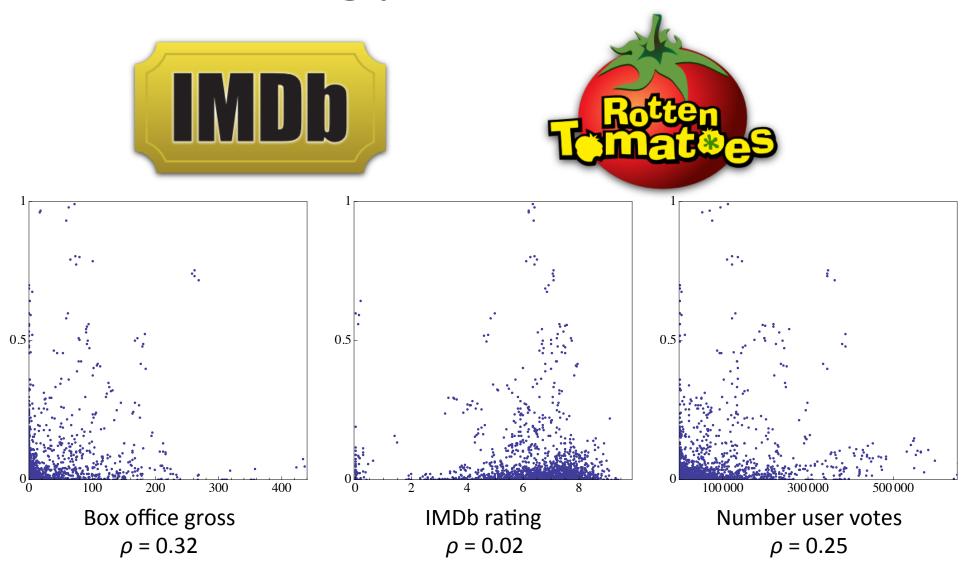
Internal Company Data

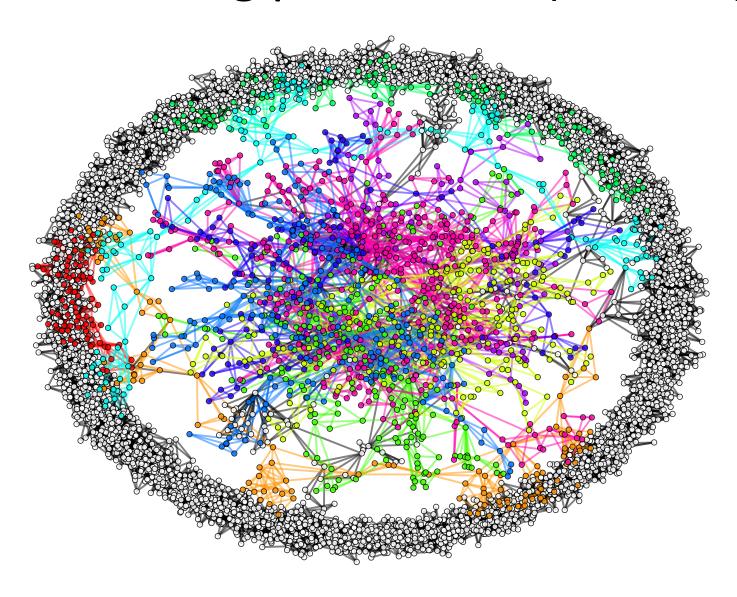
- Sales by item/location, 2010 to present
- ~50GB after aggregating transaction records by week
- Location info:
 - Address
 - Google Geocoding API
- Item info:
 - Medium (DVD/BLU)
 - Obfuscated title
 - Disambiguation

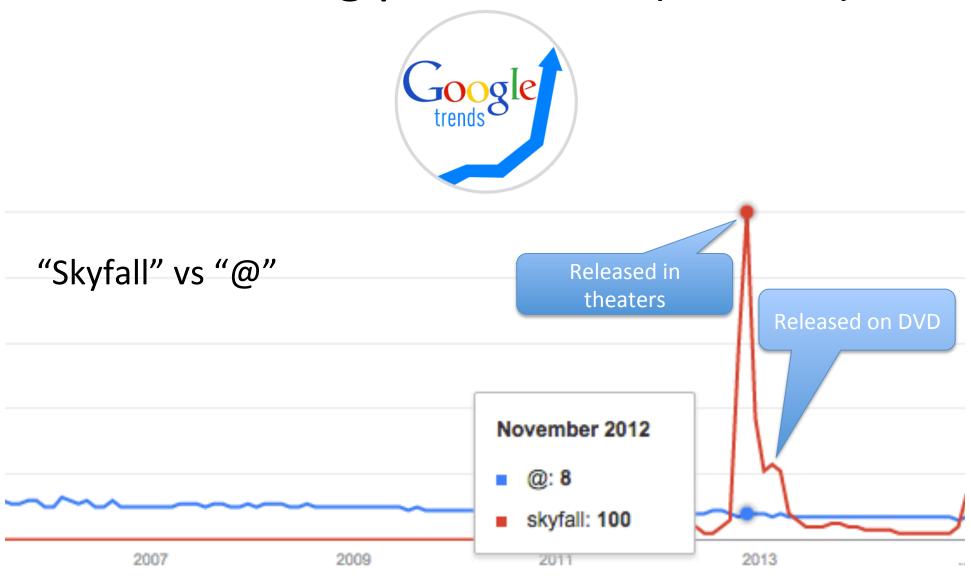


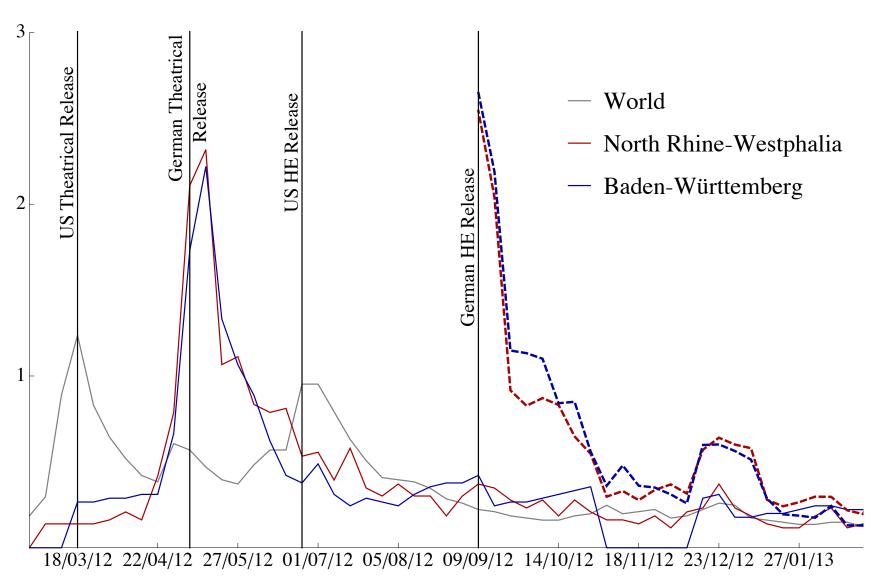


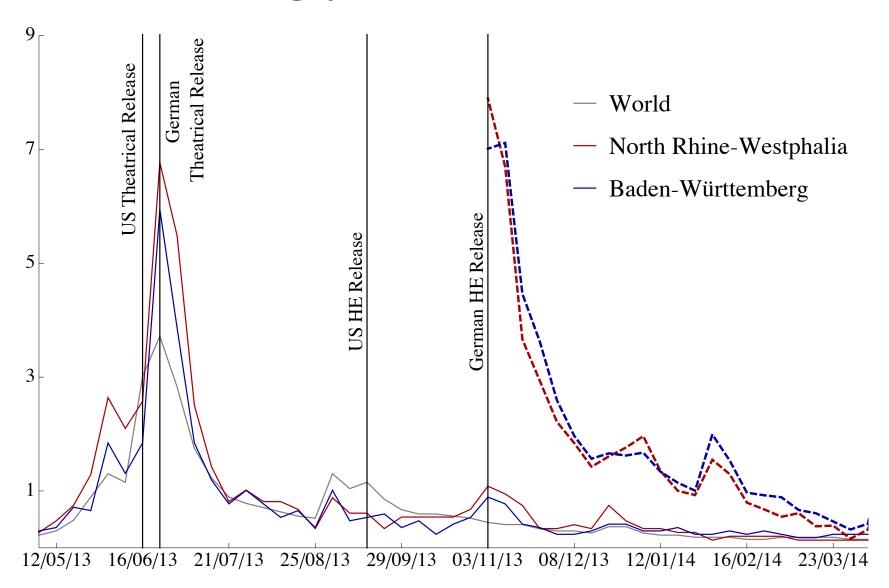
- Movie/series
- Actors (find actor communities; Blondel et al 2008)
- Plot summary (cosine similarities, hierarchically clustered)
- Box office gross, US
- Oscar wins and nominations and other awards
- Professional (meta-)ratings, user ratings
- Num of user ratings
- Genre (can be multiple)
- MPAA rating

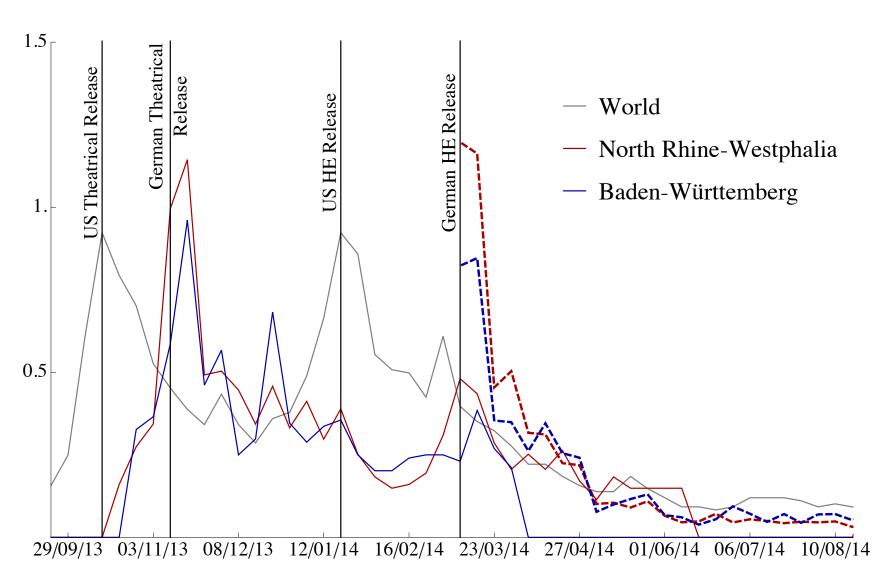








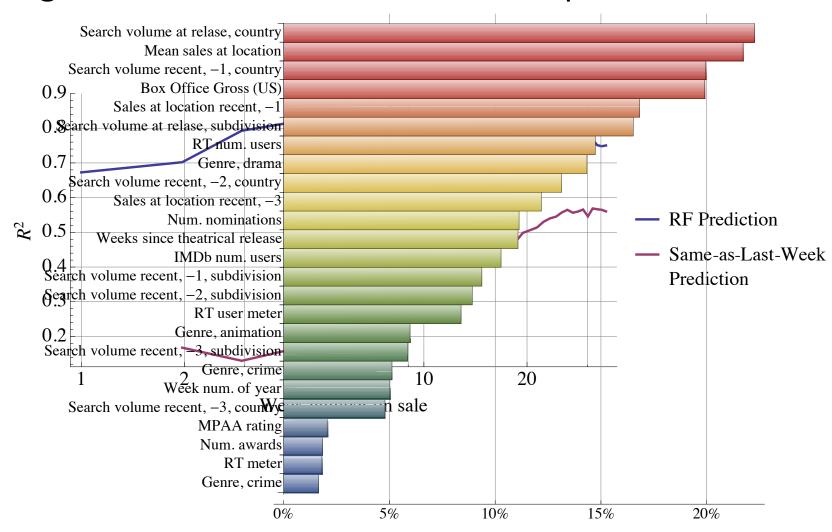




Predicting Demand

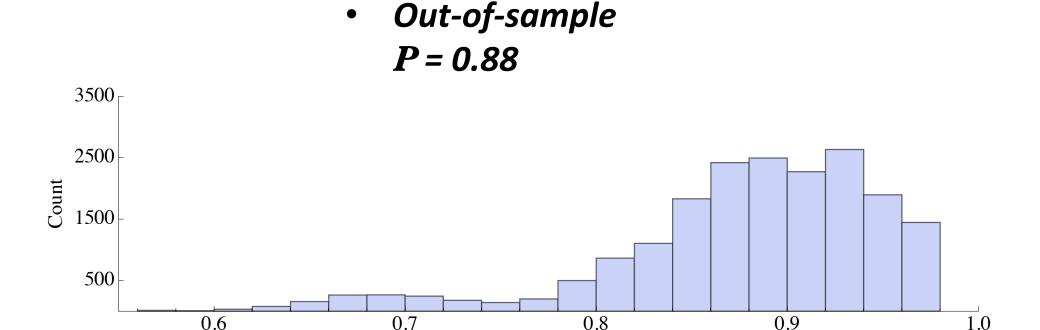
 Random forest regressor

• *New* titles: out-of-sample $R^2 = 0.67$



Prescribing Order Quantities

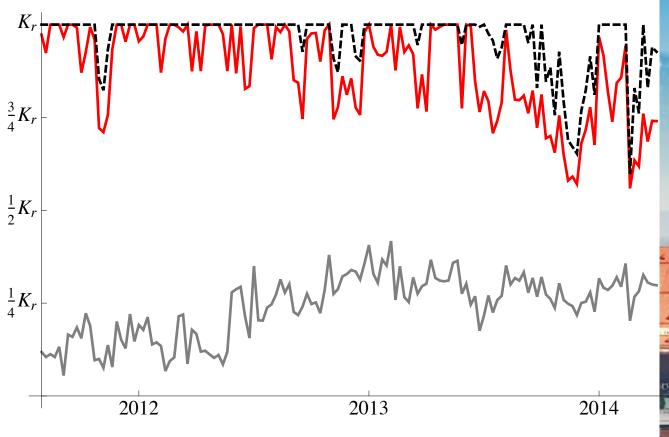
 Construct a predictive prescription based on our random forest...



Coefficient of Prescriptiveness P

Munich

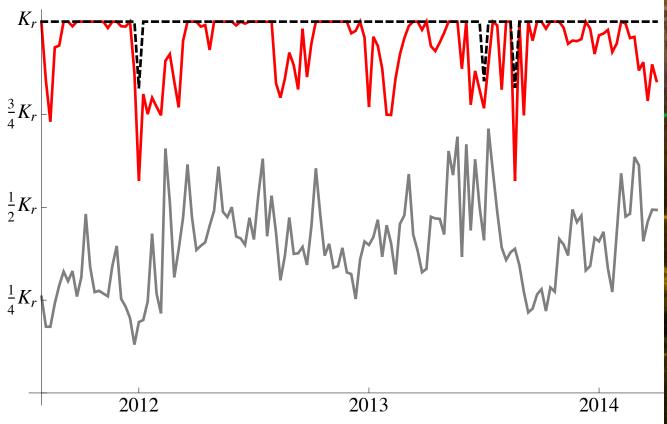
$$P = 0.89$$

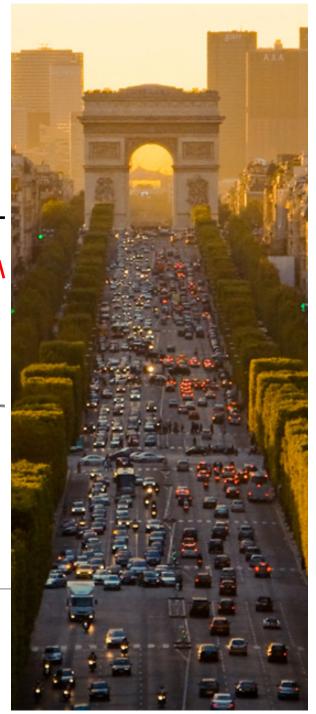




Paris

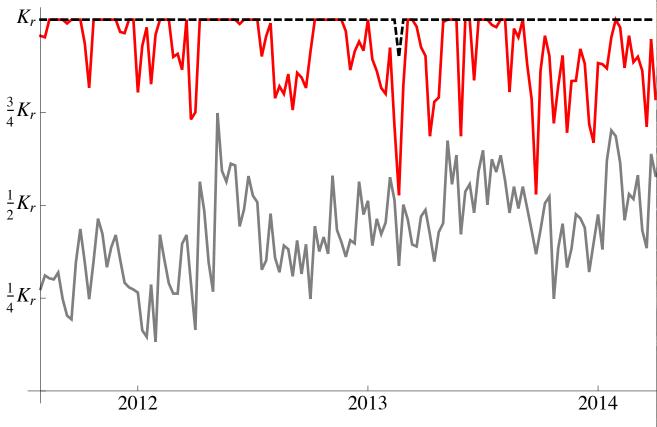
$$P = 0.90$$





Waterloo

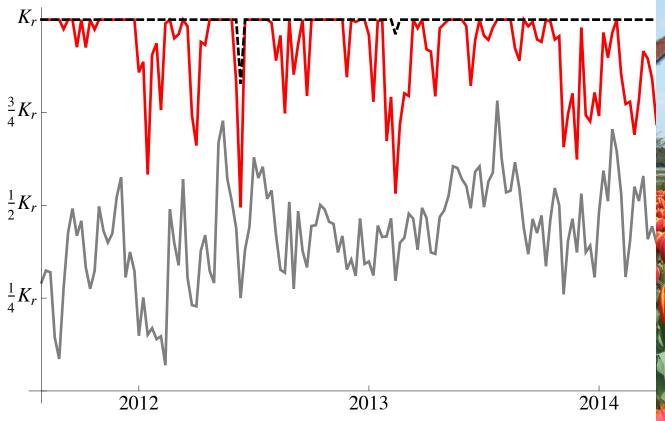
$$P = 0.85$$





The Hague

$$P = 0.86$$





Conclusions

A new framework

- Unifies ML and OR/MS
- General purpose

Theory

- Computational tractability
- Asymptotic optimality

Performance metric

Coefficient of prescriptiveness

Practice

Material Improvement for A Global Fortune 100 company.

Education

- A new class at the Master level that starts with Data: Analytics Edge
- A new class at the PhD level that aspires to go
 From Data to predictions to prescriptions.