

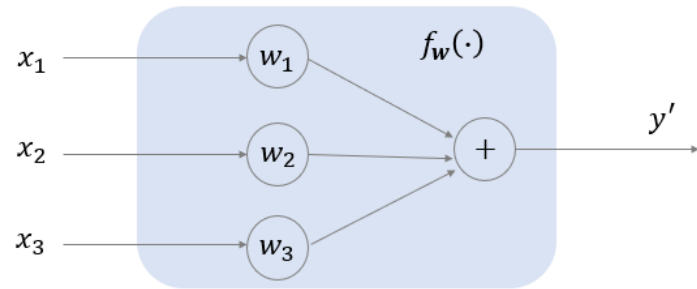
CS 4501/6501 Interpretable Machine Learning

Interpretable Generalized Additive Models

Hanjie Chen, Yangfeng Ji
Department of Computer Science
University of Virginia
{hc9mx, yangfeng}@virginia.edu

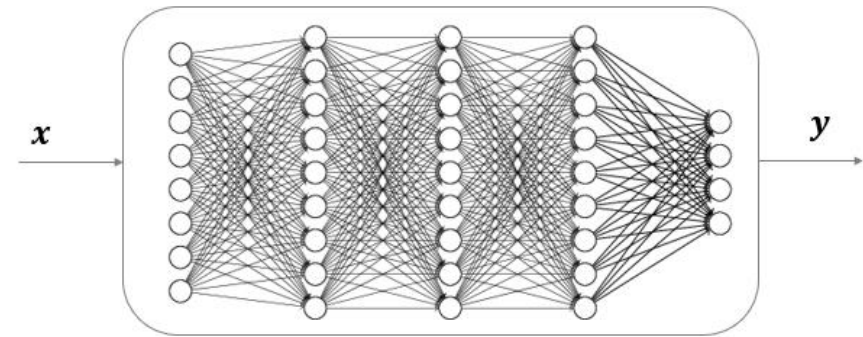
Interpretability

Bad performance
Good interpretability



- Three parameters (w_1, w_2, w_3)
- $y' = w_1x_1 + w_2x_2 + w_3x_3$
- Contributions:
 - $x_1: w_1x_1$
 - $x_2: w_2x_2$
 - $x_3: w_3x_3$

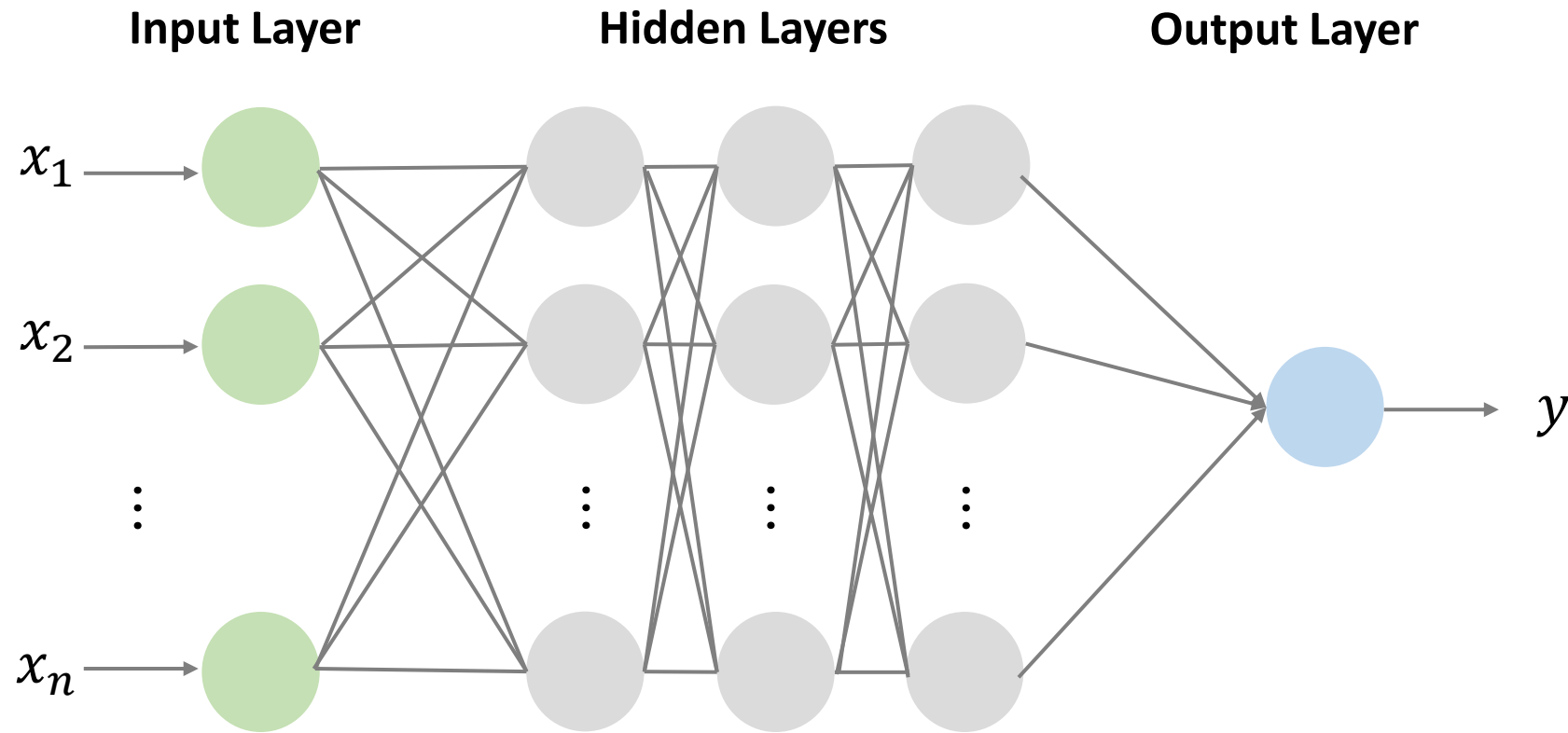
Good performance
Bad interpretability



- Millions of parameters
- $y' = f_w(x)$ (complex transformations)
- Model decision-making and feature attributions are unclear

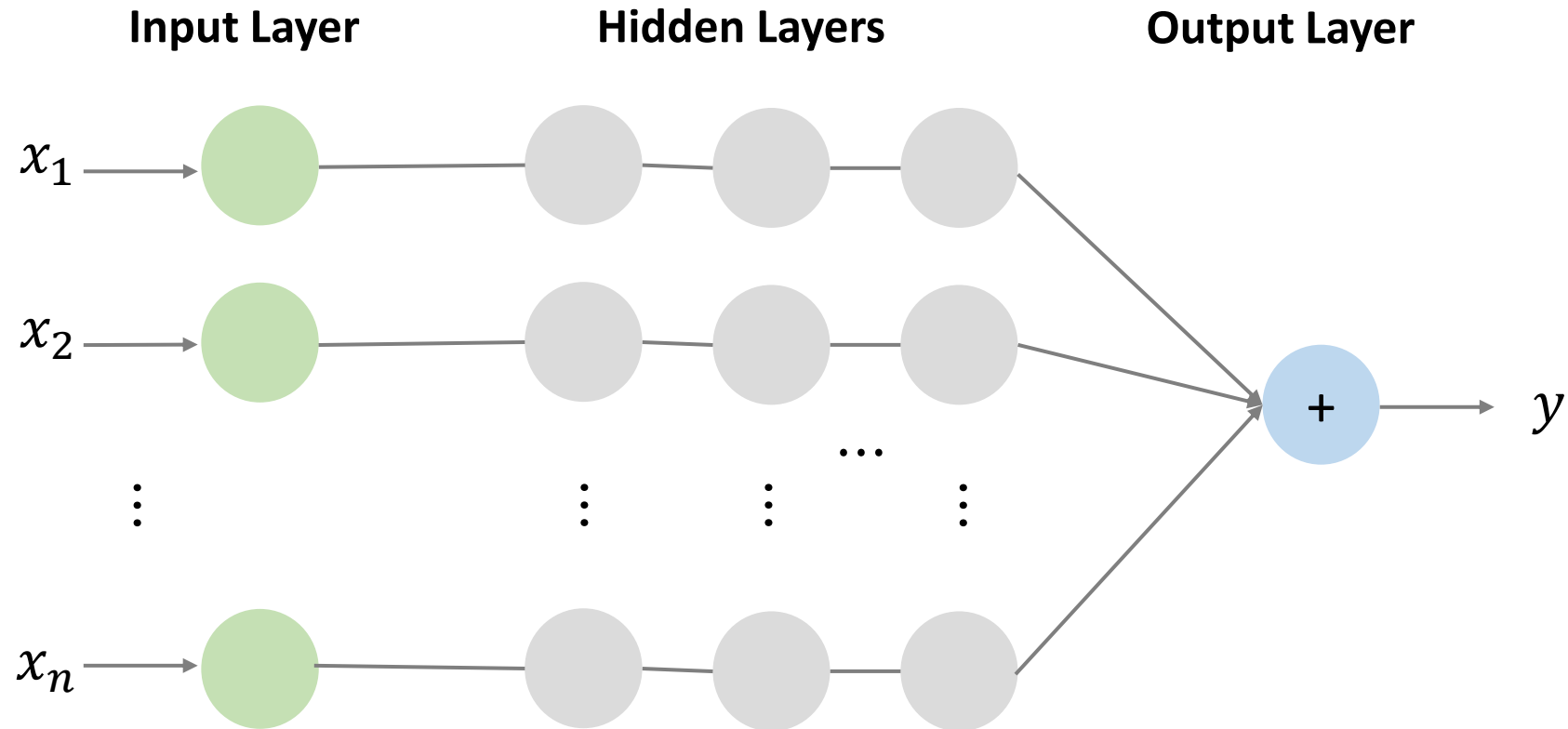
Trade-off

The information of input features is mixed



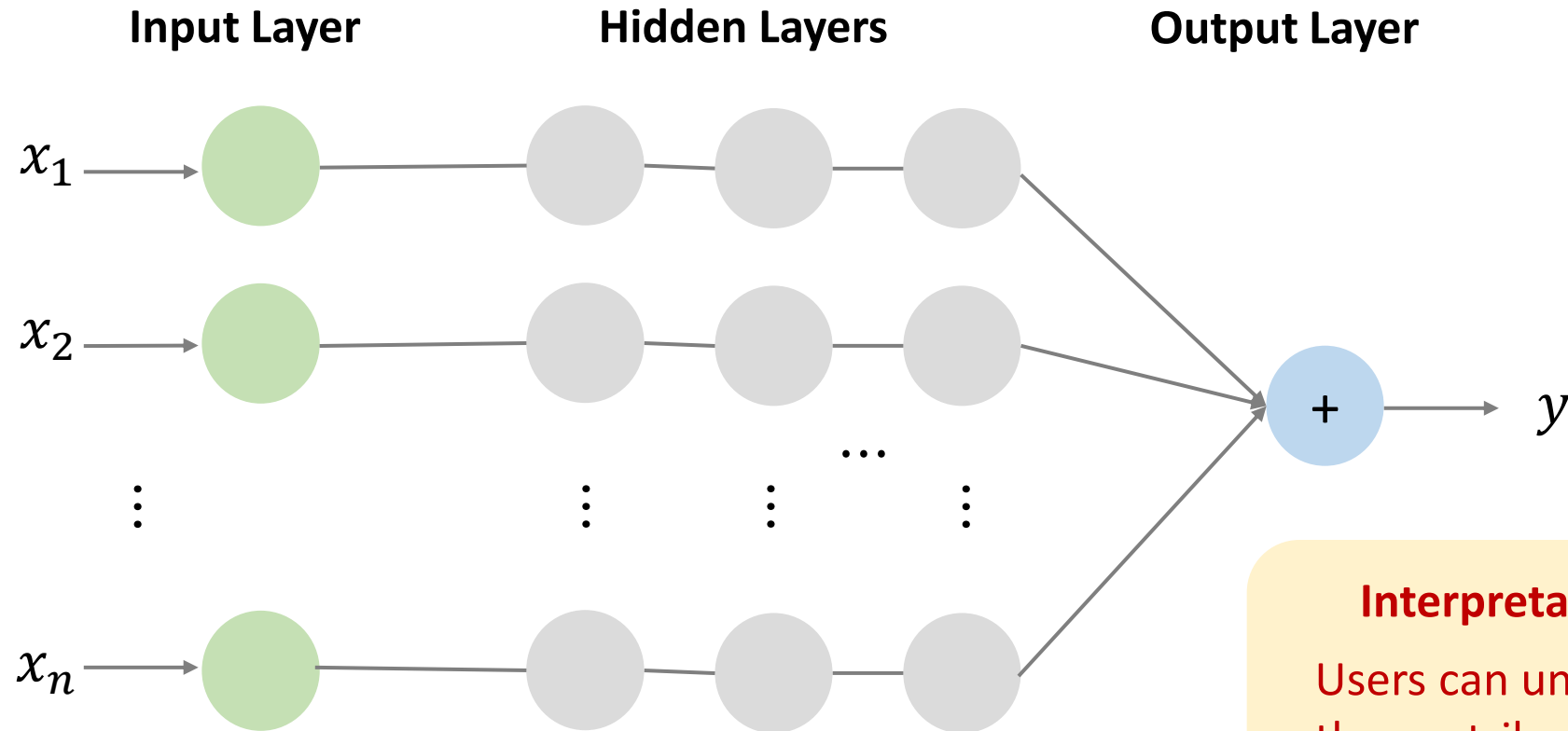
Trade-off

Keep the information of individual features “locally”



Trade-off

Keep the information of individual features “locally”



Interpretability
Users can understand the contributions of individual features

Trade-off

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

- Permit complex relationships between individual features (x_i) and the target ($g(y)$)
- Exclude complex interactions between features

GAM

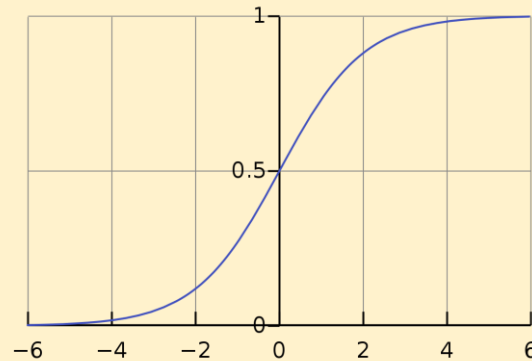
Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

- $g(\cdot)$: link function
 - Identity: $g(y) = y \longrightarrow$ Regression
 - Logistic function: $g(y)$ represents the probability on a class \longrightarrow Classification

$$\frac{L}{1 + e^{-k(x-x_0)}}$$

$$(L = 1, k = 1, x_0 = 0)$$

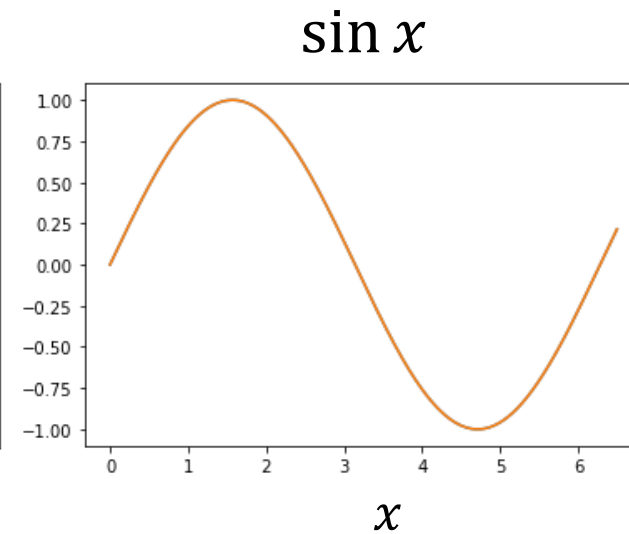
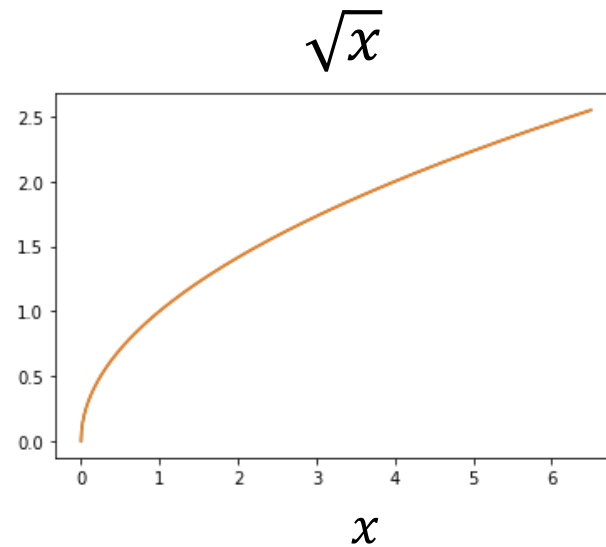
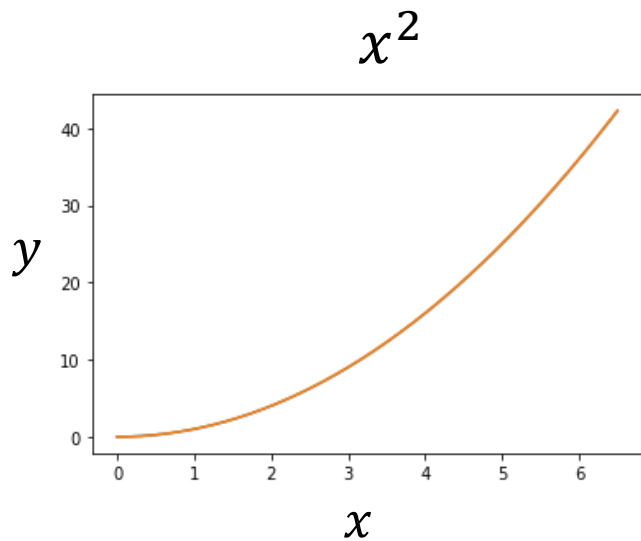


GAM

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

- $f_i(\cdot)$: shape function
 - Splines

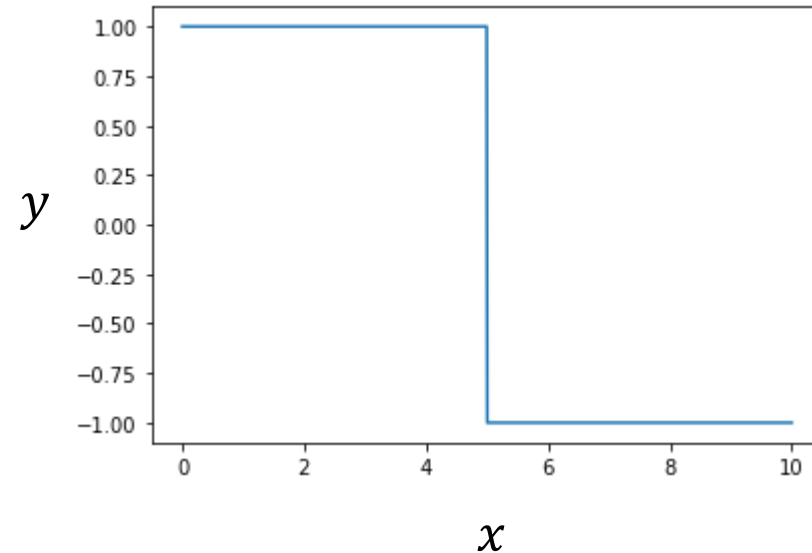
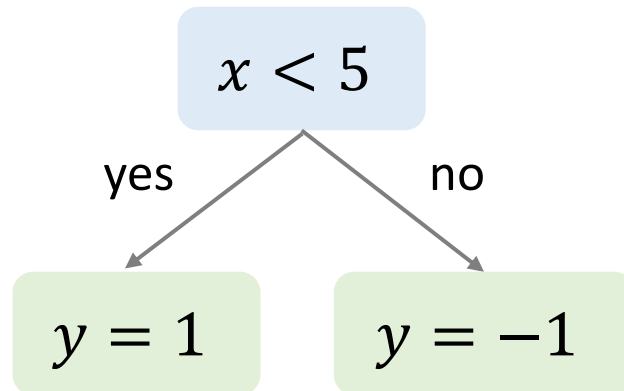


GAM

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \dots + f_n(x_n)$$

- $f_i(\cdot)$: shape function
 - Binary Trees

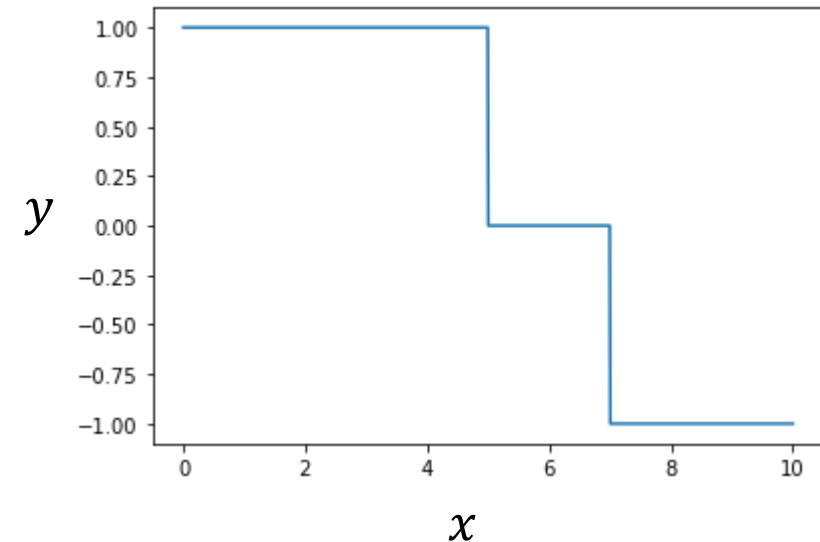
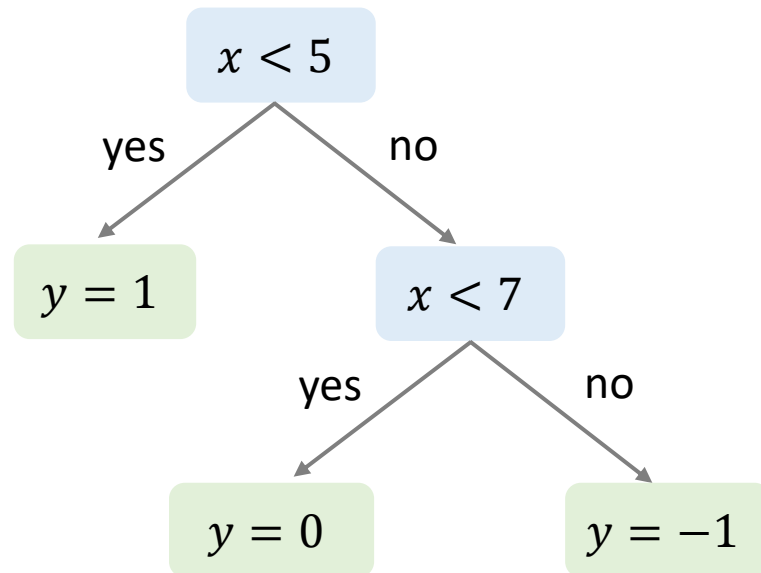


GAM

Generalized additive models (GAMs)

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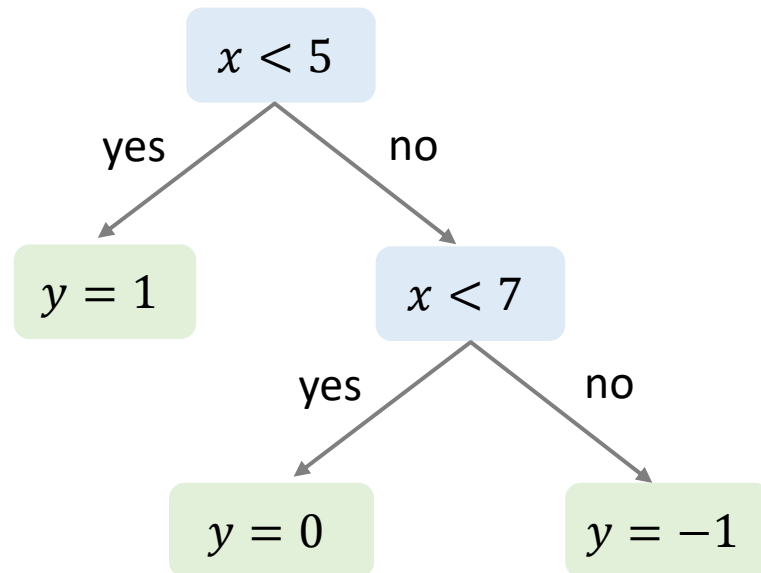


GAM

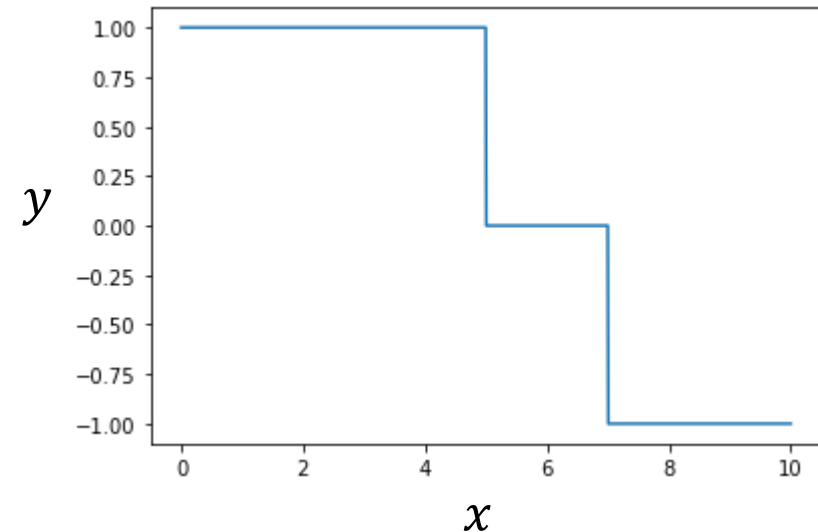
Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \dots + f_n(x_n)$$

- $f_i(\cdot)$: shape function
 - Binary Trees



For interpretability, we control tree complexity (nodes, leaves, depth)

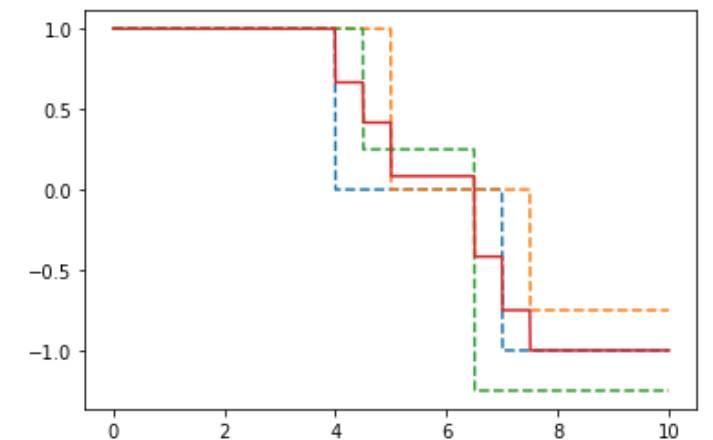
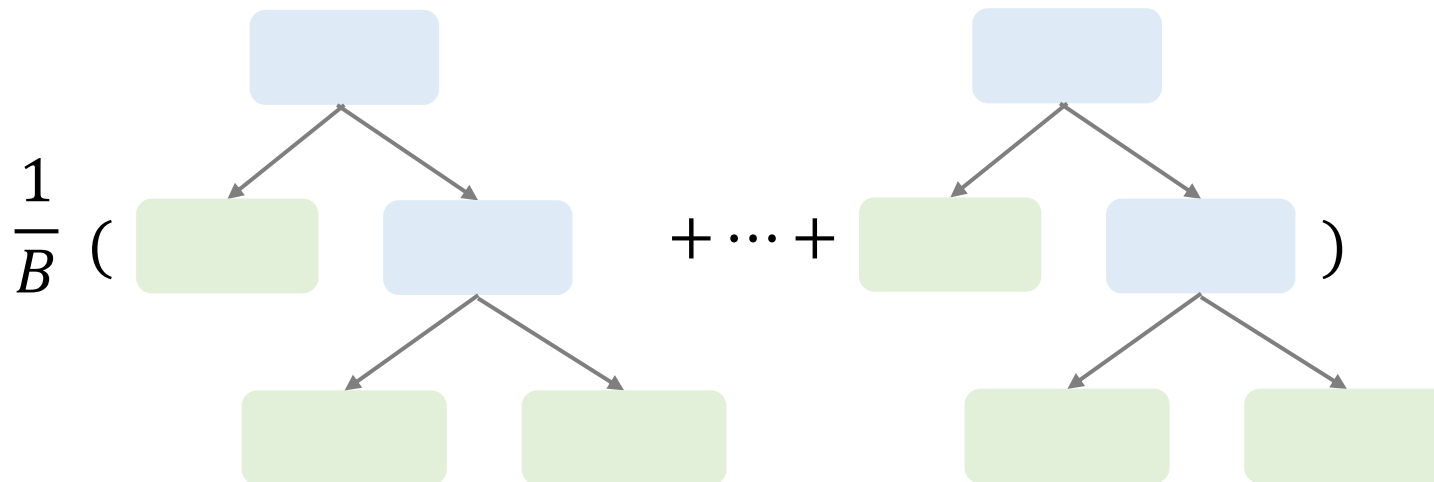


GAM

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \dots + f_n(x_n)$$

- $f_i(\cdot)$: shape function
 - Bagged Trees (reduce the variance)



GAM

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \dots + f_n(x_n)$$

- Training
 - Shape functions for individual features
 - Learning methods

Learning GAM

- Gradient Boosting
 - Learning tree or tree ensemble shape functions

Algorithm Gradient Boosting for GAM

1. $f_j \leftarrow 0, j = 1, \dots, n$ Initialize all shape functions as zero
 2. **for** $m = 1, \dots, M$ **do** Loop over M iterations
 3. **for** $j = 1, \dots, n$ **do** Loop over all features
 4. $\mathcal{R} \leftarrow \left\{ x_{ij}, y_i - \sum_{k=1}^N f_k \right\}_{i=1}^N$ Calculate residuals
 5. Learning shape function $S: x_j \rightarrow y$ using \mathcal{R} as training data Learn the one-dimensional function to predict the residuals
 6. $f_j \leftarrow f_j + S$ Update the shape function
-

Learning GAM

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Learn the one-dimensional function to predict the residuals

6. $f_j \leftarrow f_j + S$ Update the shape function

Learning GAM

- Gradient Boosting

Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$

i	x_1	x_2	\dots	x_j	\dots	x_n	y
1	x_{11}	x_{12}	\dots	x_{1j}	\dots	x_{1n}	y_1
x_2 2	x_{21}	x_{22}	\dots	x_{2j}	\dots	x_{2n}	y_2
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
N	x_{N1}	x_{N2}	\dots	x_{Nj}	\dots	x_{Nn}	y_N

Learning GAM

- Gradient Boosting

Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$

i	x_1	x_2	\dots	x_j	\dots	x_n	y
1	x_{11}	x_{12}	\dots	x_{1j}	\dots	x_{1n}	y_1
2	x_{21}	x_{22}	\dots	x_{2j}	\dots	x_{2n}	y_2
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
N	x_{N1}	x_{N2}	\dots	x_{Nj}	\dots	x_{Nn}	y_N

Learning GAM

- Gradient Boosting

Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$

i	x_1	x_2	\dots	x_j	\dots	x_n	y
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\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
N	x_{N1}	x_{N2}	\dots	x_{Nj}	\dots	x_{Nn}	y_N

Learning GAM

- Gradient Boosting

Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$

i	x_1	x_2	\dots	x_j	\dots	x_n	y
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\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
N	x_{N1}	x_{N2}	\dots	x_{Nj}	\dots	x_{Nn}	y_N

f_j

Residuals

$$\begin{aligned} \rightarrow y_1 - \sum_k f_k \\ \rightarrow y_2 - \sum_k f_k \\ \vdots \\ \rightarrow y_N - \sum_k f_k \end{aligned}$$

(errors made by the current model)

Learning GAM

- Gradient Boosting

Update f_j based on $\left\{ \underbrace{(x_{ij}, y_i - \sum_k f_k)}_{\substack{x \\ y}} \right\}_{i=1}^N$

- Learn a shape function S that fits: $x \rightarrow y$
- Update $f_j \leftarrow f_j + S$

Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
3	8
9	7

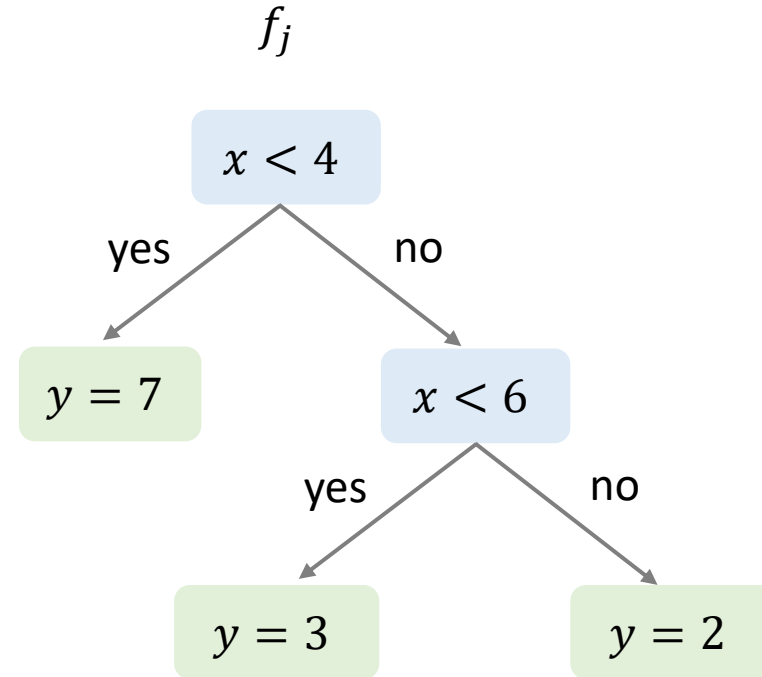
Residuals

$$8 - 7 = 1$$

$$5 - 3 = 2$$

$$8 - 7 = 1$$

$$7 - 2 = 5$$



Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
3	8
9	7

Residuals

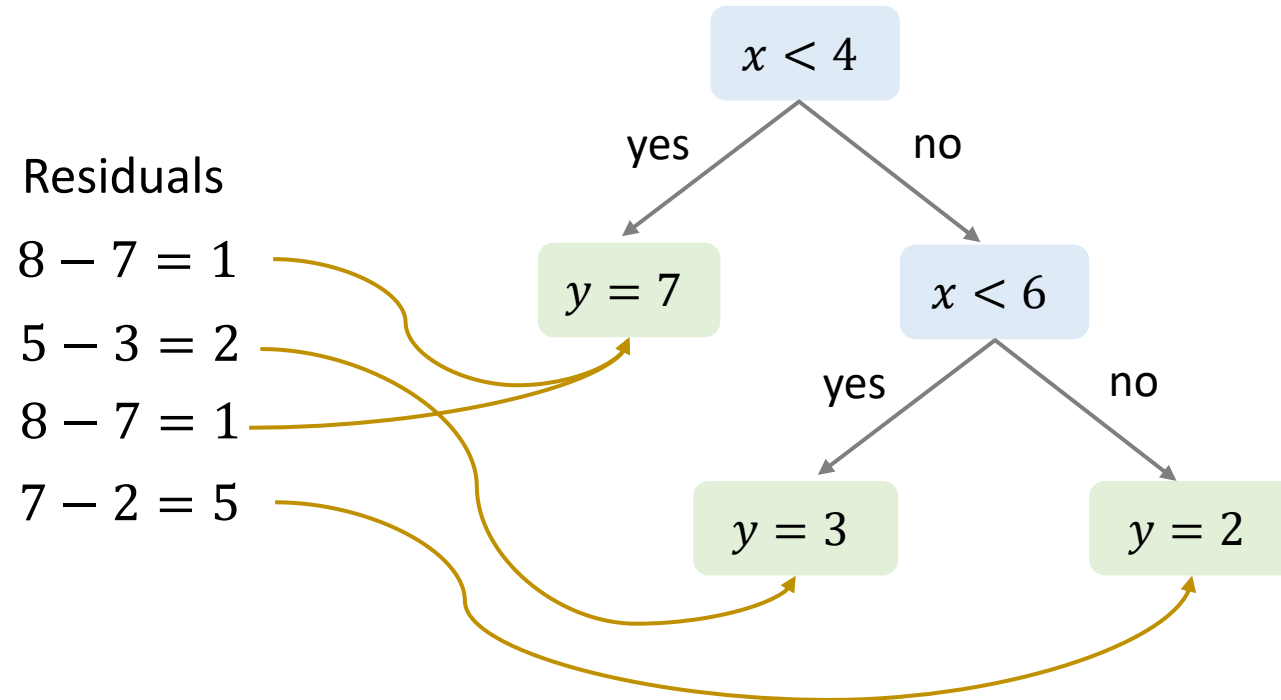
$$8 - 7 = 1$$

$$5 - 3 = 2$$

$$8 - 7 = 1$$

$$7 - 2 = 5$$

f_j



Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
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9	7

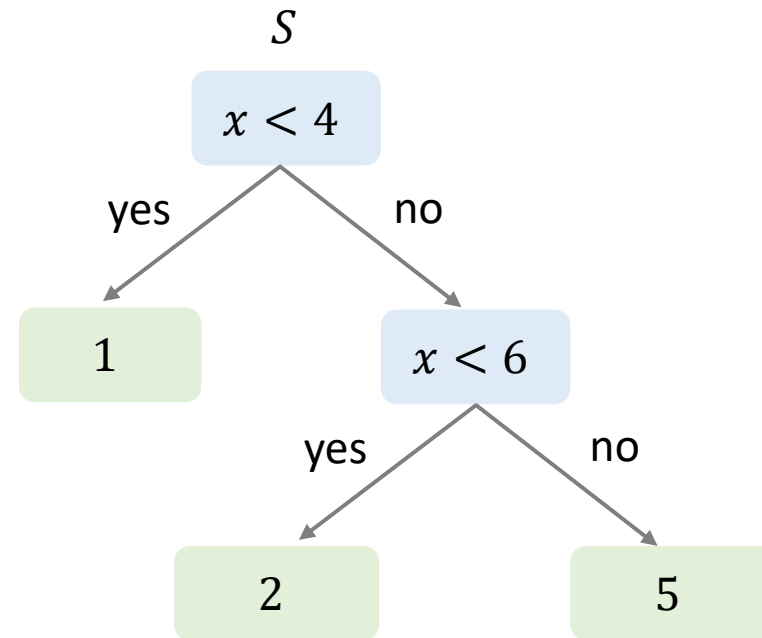
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Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
3	8
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Residuals

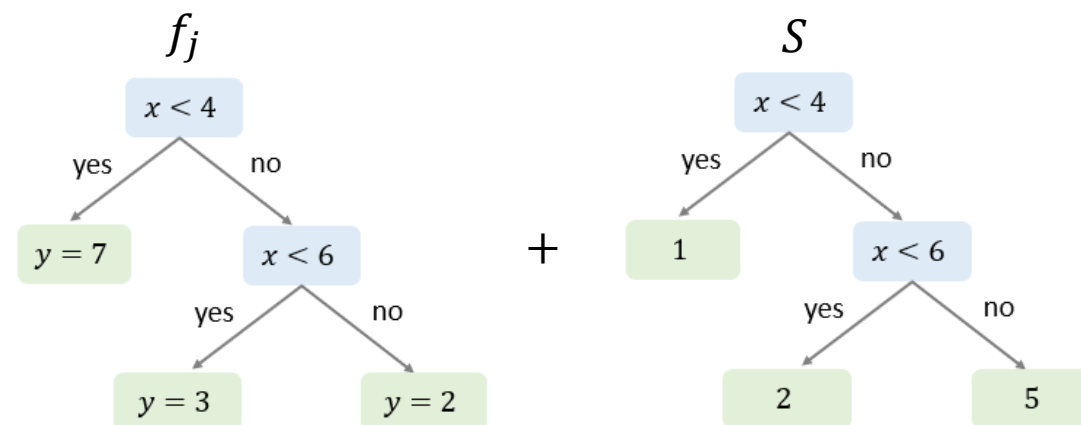
$$8 - (7 + 1) = 0$$

$$5 - (3 + 2) = 0$$

$$8 - (7 + 1) = 0$$

$$7 - (2 + 5) = 0$$

Update $f_j \leftarrow f_j + S$



Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
3	8
9	7

Residuals

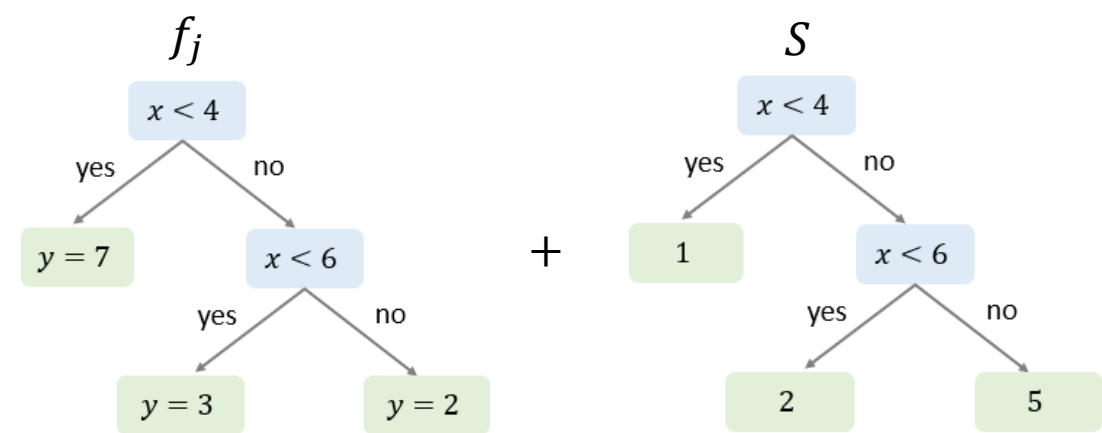
$$8 - (7 + 1) = 0$$

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$$8 - (7 + 1) = 0$$

$$7 - (2 + 5) = 0$$

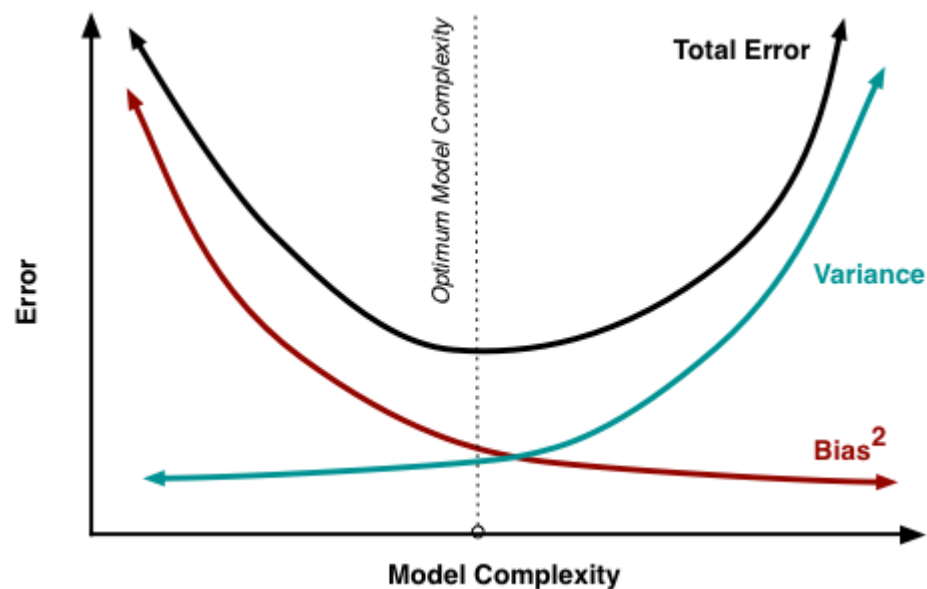
Update $f_j \leftarrow f_j + S$



Do we learn a perfect model?

Learning GAM

The model fits training data too well



We have low bias, but probably have high variance

Source: <http://scott.fortmann-roe.com/docs/BiasVariance.html>

Learning GAM

- Gradient Boosting

Example

x	y
1	8
5	5
3	8
9	7

Residuals

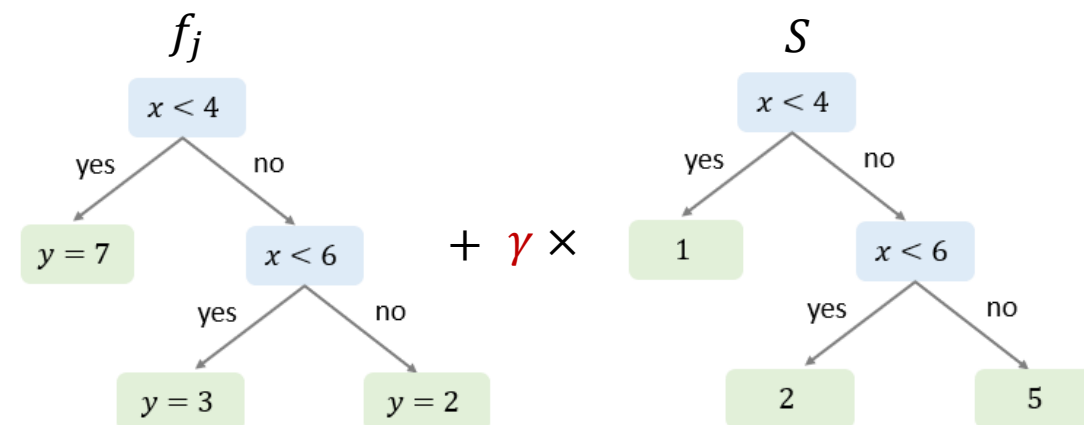
$$8 - (7 + 0.1 \times 1) = 0.9$$

$$5 - (3 + 0.1 \times 2) = 1.8$$

$$8 - (7 + 0.1 \times 1) = 0.9$$

$$7 - (2 + 0.1 \times 5) = 4.5$$

$$\text{Update } f_j \leftarrow f_j + \gamma \times S$$



Add a learning rate to scale the contribution of the new tree

Learning GAM

- Gradient Boosting
 - Learning tree or tree ensemble shape functions

Algorithm Gradient Boosting for GAM

1. $f_j \leftarrow 0, j = 1, \dots, n$ Initialize all shape functions as zero

2. **for** $m = 1, \dots, M$ **do** Loop over M iterations

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4. $\mathcal{R} \leftarrow \left\{ x_{ij}, y_i - \sum_{k=1}^n f_k \right\}_{i=1}^N$ Calculate residuals

5. Learning shape function $S: x_j \rightarrow y$ using \mathcal{R} as training data

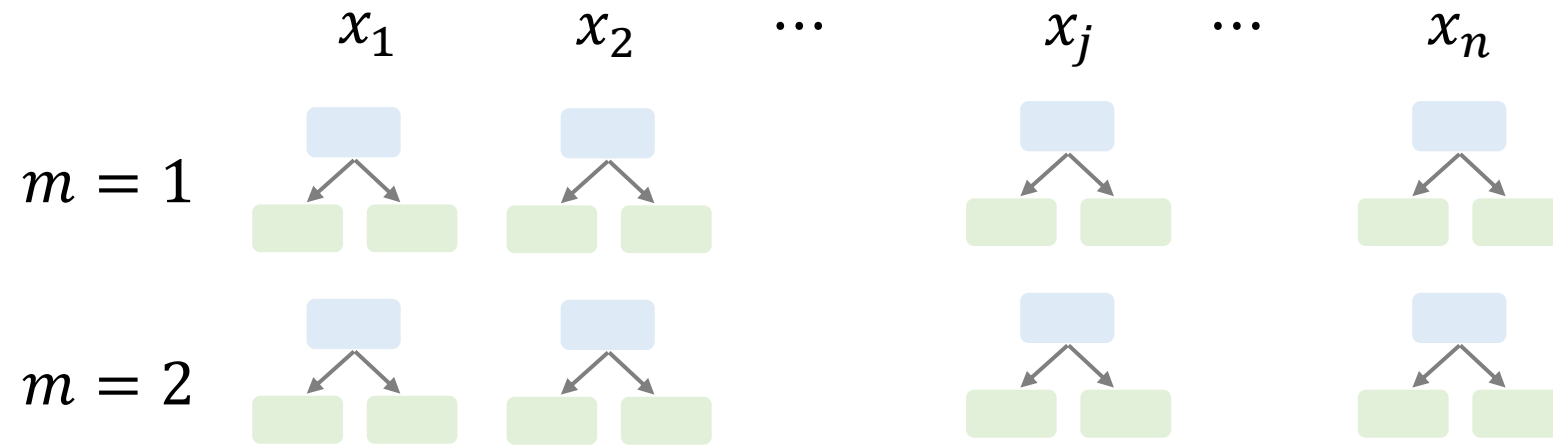
Learn the one-dimensional function to predict the residuals

6. $f_j \leftarrow f_j + S$ Update the shape function

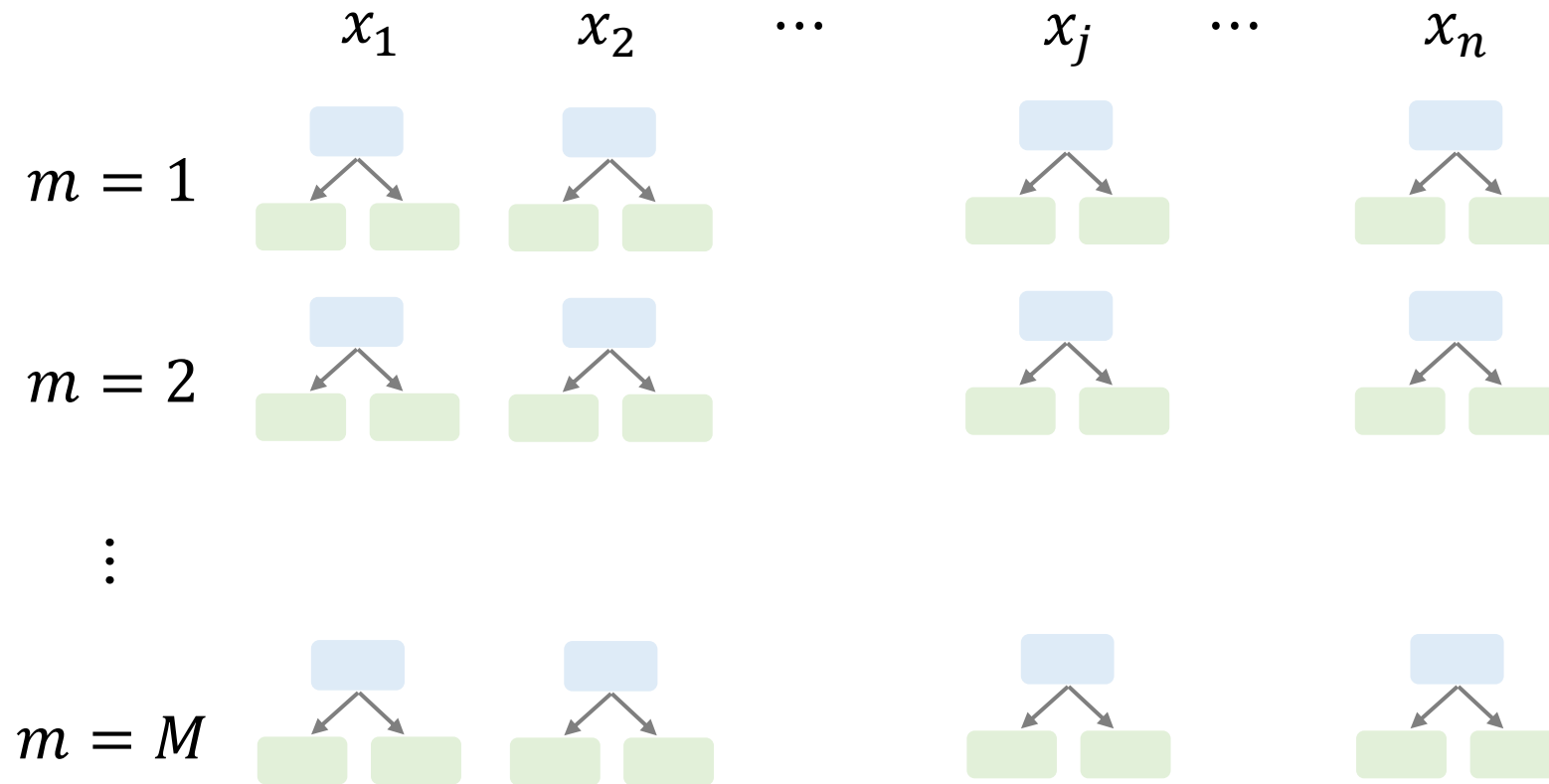
Learning GAM



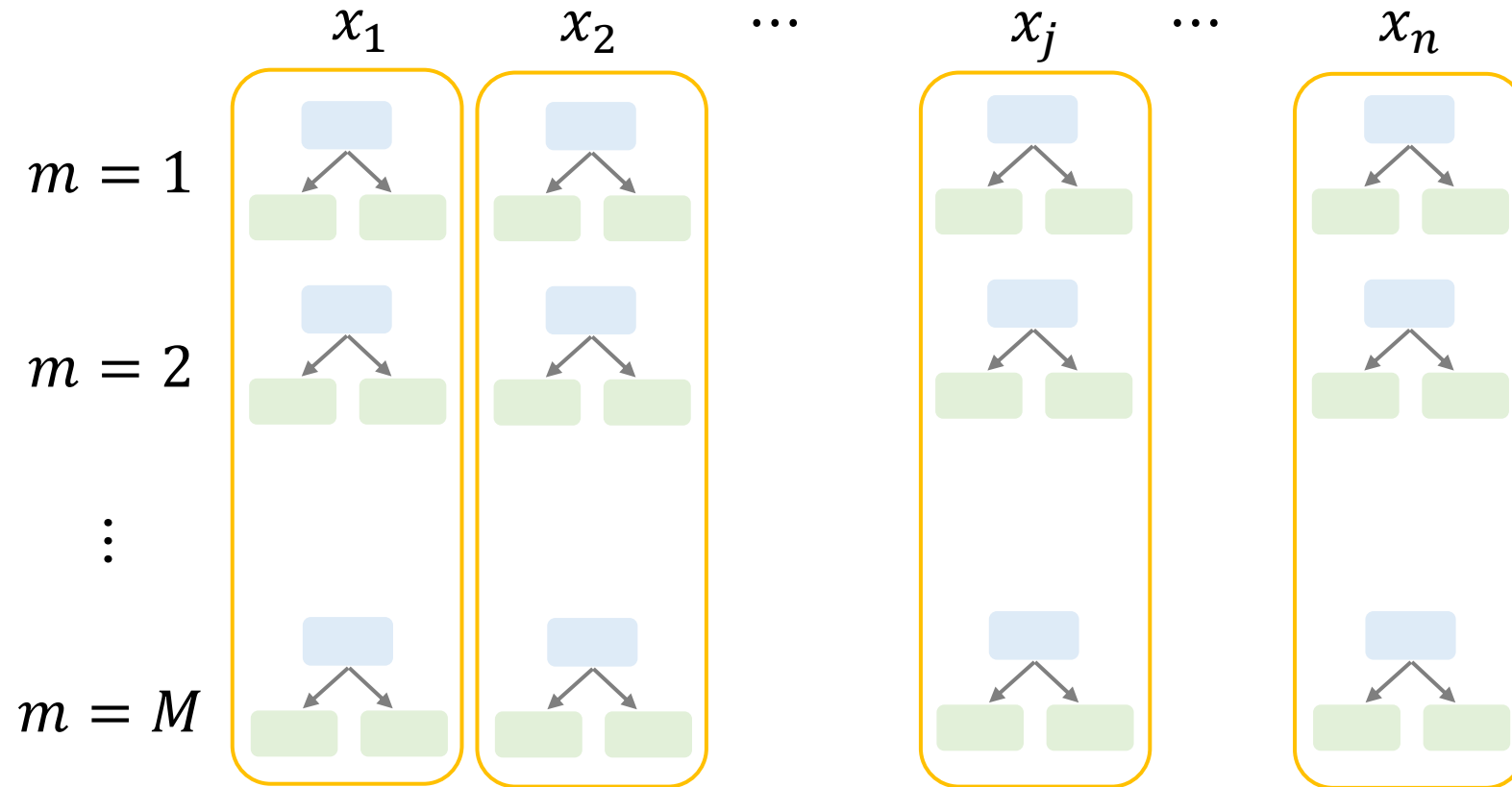
Learning GAM



Learning GAM



Learning GAM



Question?

Learning GAM

- Backfitting
 - Learning tree or tree ensemble shape functions

Algorithm Backfitting for GAM

1. $f_j \leftarrow 0, j = 1, \dots, n$ Initialize all shape functions as zero
2. Learn f_1 using the training set $\{(x_{i1}, y_i)\}_{i=1}^N$
3. **for** $j = 2, \dots, n$ **do** Loop over rest features
4. $\mathcal{R} \leftarrow \left\{ x_{ij}, y_i - \sum_{k=1}^{j-1} f_k \right\}_{i=1}^N$ Calculate residuals
5. Learning shape function $S: x_j \rightarrow y$ using \mathcal{R} as training data Learn the one-dimensional function to predict the residuals
6. $f_j \leftarrow S$ Update the shape function
7. Retrain f_1 based on the residuals of other $n - 1$ shape functions

Learning GAM

- Least Squares
 - Learning spline shape functions
 - Reducing to fitting a linear model

$$g(y) = \beta_1 x_1^2 + \beta_2 \sqrt{x_2} + \cdots + \beta_n \sin x_n$$

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}$$

$$\underline{\mathbf{X}}_i = [x_{i1}^2, \sqrt{x_{i2}}, \cdots, \sin x_{in}]$$

*i*th example

$$\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_n]^T$$

Objective

$$\min \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2$$

Learning GAM

- Least Squares
 - Learning spline shape functions
 - Reducing to fitting a linear model

$$g(y) = \beta_1 x_1^2 + \beta_2 \sqrt{x_2} + \cdots + \beta_n \sin x_n$$

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*i*th example

$$\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_n]^T$$

Objective

$$\min \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2$$

Simple, but not flexible

Summary

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

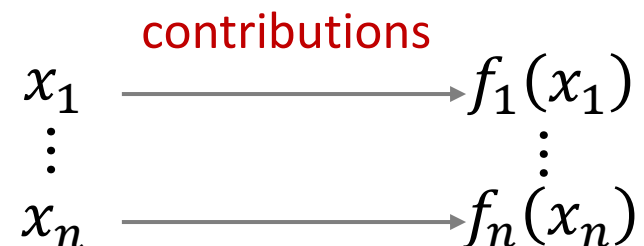
- Training
 - Shape functions for individual features: splines, trees, ensembles of trees
 - Learning methods: Least Squares, Gradient Boosting, Backfitting

Summary

Generalized additive models (GAMs)

$$g(y) = f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n)$$

- Training
 - Shape functions for individual features: splines, trees, ensembles of trees
 - Learning methods: Least Squares, Gradient Boosting, Backfitting
- Interpretability



Application

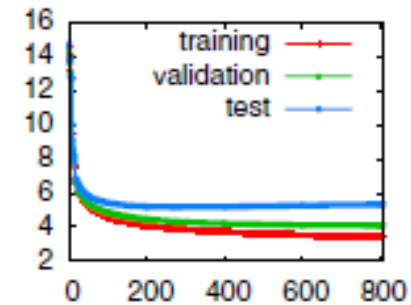
- Dataset: “Concrete” (Blast Furnace Slag, Fly Ash, Superplasticizer...)
- Task: predicting the compressive strength of concrete
- Models:

Shape Function	Least Squares	Gradient Boosting	Backfitting
Splines	P-LS/P-IRLS	BST-SP	BF-SP
Single Tree	N/A	BST-TR _x	BF-TR
Bagged Trees	N/A	BST-bagTR _x	BF-bagTR
Boosted Trees	N/A	BST-TR _x	BF-bstTR _x
Boosted Bagged Trees	N/A	BST-bagTR _x	BF-bbTR _x

Lou, Yin, Rich Caruana, and Johannes Gehrke. "Intelligible models for classification and regression." *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2012.

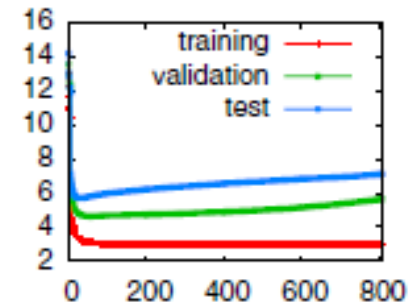
Empirical Results

- GAMs perform better than linear or logistic regression (without feature shaping)
- Tree-based shaping methods are more accurate than spline-based methods
- Bagged-trees with 2-4 leaves as shape functions in combination with gradient boosting as learning method perform better
- Controlling the complexity of trees can avoid overfitting



(a) BST-bagTR2

(2 leaves)



(b) BST-bagTR16

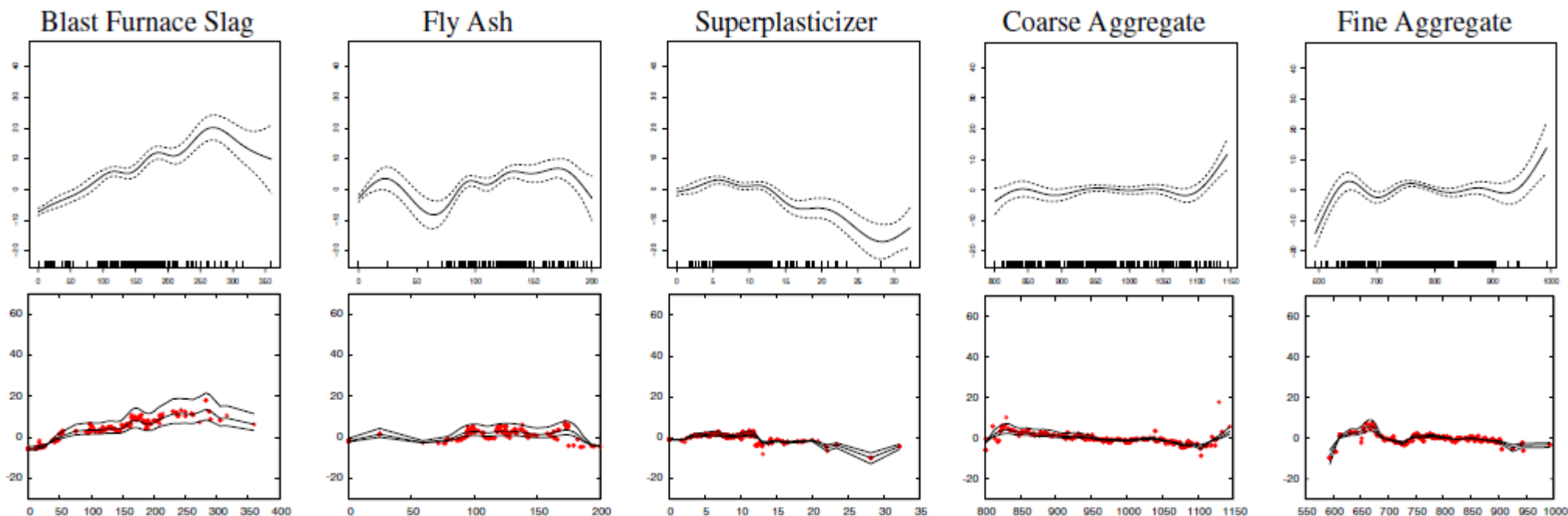
(16 leaves)

Lou, Yin, Rich Caruana, and Johannes Gehrke. "Intelligible models for classification and regression." *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2012.

Interpretation

Shapes of features for the “Concrete” dataset (versus the compressive strength of concrete)

(Splines)



(Bagged trees)

Lou, Yin, Rich Caruana, and Johannes Gehrke. "Intelligible models for classification and regression." *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2012.

Question?

GA²M

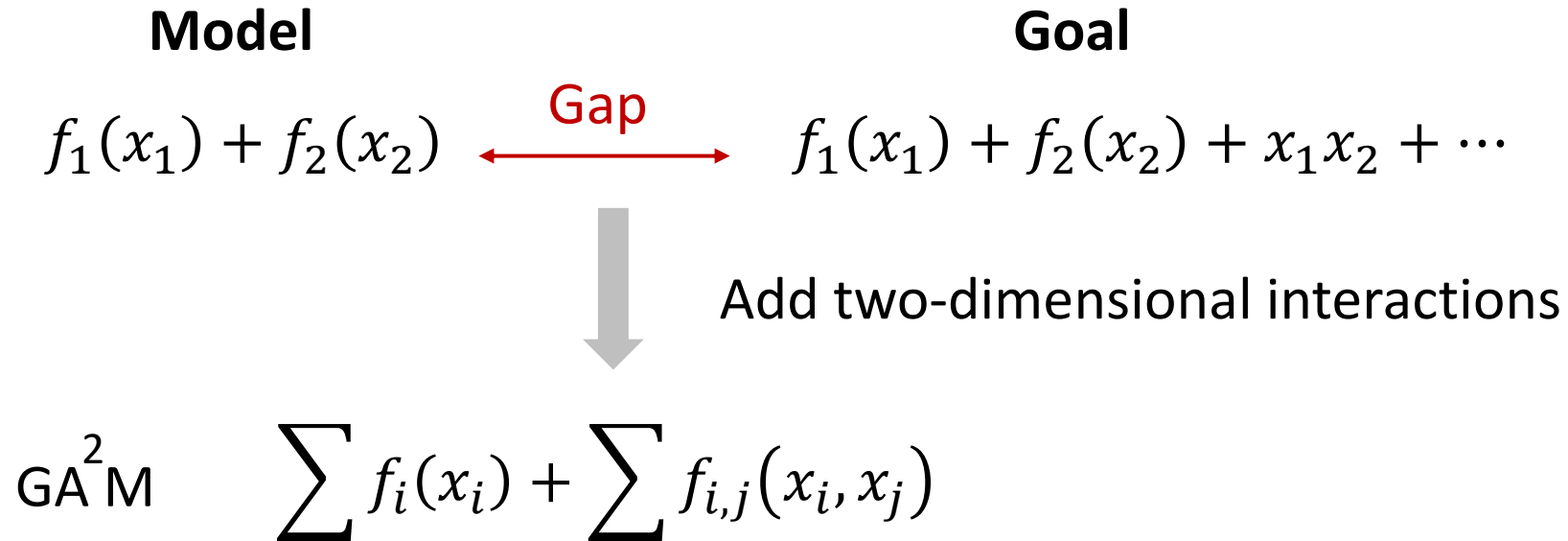
Limitation: GAMs do not consider feature dependency

Model	Goal
$f_1(x_1) + f_2(x_2)$	$f_1(x_1) + f_2(x_2) + x_1x_2 + \dots$

← Gap →

GA²M

Limitation: GAMs do not consider feature dependency



Definitions

- Dataset $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$
- $\mathbf{x}_i = [x_{i1}, \dots, x_{in}]$ with n features
- y_i is the response
- $\mathbf{x} = (x_1, \dots, x_n)$ denote the features in the dataset
- $U_1 = \{\{i\} | 1 \leq i \leq n\}, U_2 = \{\{i, j\} | 1 \leq i < j \leq n\}, U = U_1 \cup U_2$, i.e., U contains all indices for all features and pairs of features
- For any $u \in U$, let H_u denote the Hilbert space of $f_u(x_u)$
- $H = \sum_{u \in U} H_u, H_1 = \sum_{u \in U_1} H_u, H_2 = \sum_{u \in U_2} H_u$

GA²M

GA²M

$$F(\mathbf{x}) = \sum_{u \in U} f_u(x_u)$$

Objective

$$\min_{F \in \mathcal{H}} E[L(y, F(\mathbf{x}))]$$

L : non-negative convex loss function

regression

classification

Squared loss

Cross-entropy loss

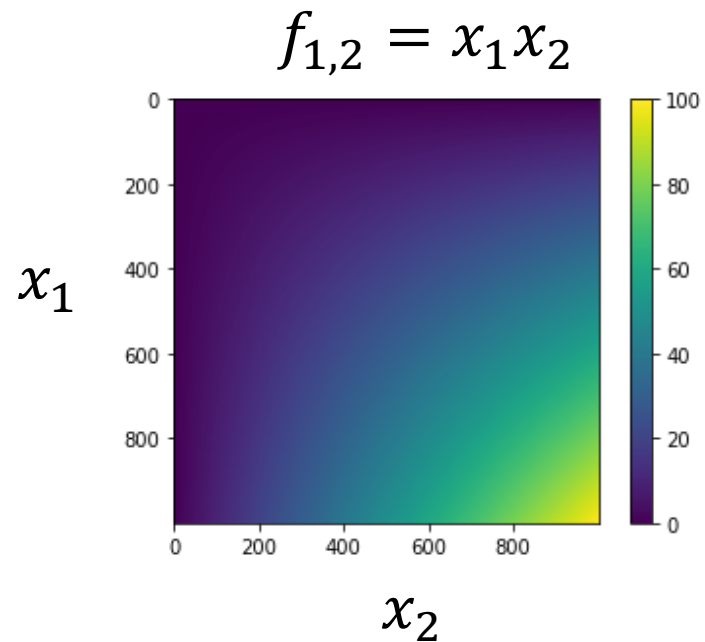
$$(y - F(\mathbf{x}))^2$$

$$-y \log F(\mathbf{x}) - (1 - y) \log(1 - F(\mathbf{x}))$$

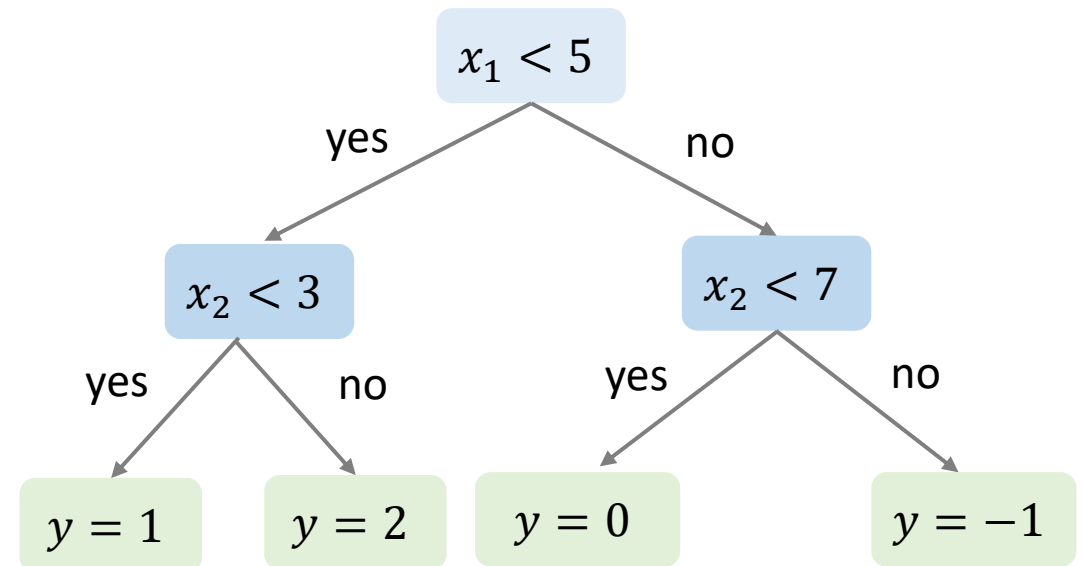
GA²M

- We have known how to learn shape functions for GAMs
- Applicable to two-dimensional shape functions $f_u, u = \{i, j\}$

Splines



Trees



Challenge

$$\sum f_i(x_i) + \sum f_{i,j}(x_i, x_j)$$

n features \longrightarrow $O(n^2)$ features interactions

How to find true
feature interactions?

Algorithm GA²M

1. $S \leftarrow \emptyset$ The set of the selected pairs
 2. $Z \leftarrow U_2$ The set of the remaining pairs
 3. **While** not converge **do**
 4. $F \leftarrow \arg \min_{F \in H_1 + \sum_{u \in S} H_u} \frac{1}{2} E \left[(y - F(\mathbf{x}))^2 \right]$
 5. $R \leftarrow y - F(\mathbf{x})$
 6. **for** all $u \in Z$ **do**
 7. $F_u \leftarrow E[R \mid x_u]$
 8. $u^* \leftarrow \arg \min_{u \in Z} \frac{1}{2} E[(R - f_u(x_u))^2]$
 9. $S \leftarrow S \cup \{u^*\}$
 10. $Z \leftarrow Z - \{u^*\}$
-

GA²M

Algorithm GA²M

1. $S \leftarrow \emptyset$ The set of the selected pairs
2. $Z \leftarrow U_2$ The set of the remaining pairs
3. **While** not converge **do**
4. $F \leftarrow \arg \min_{F \in H_1 + \sum_{u \in S} H_u} \frac{1}{2} E \left[(y - F(\mathbf{x}))^2 \right]$
5. $R \leftarrow y - F(\mathbf{x})$
6. **for** all $u \in Z$ **do**
7. $F_u \leftarrow E[R \mid x_u]$
8. $u^* \leftarrow \arg \min_{u \in Z} \frac{1}{2} E[(R - f_u(x_u))^2]$
9. $S \leftarrow S \cup \{u^*\}$
10. $Z \leftarrow Z - \{u^*\}$

The best additive model F so far in Hilbert space $H_1 + \sum_{u \in S} H_u$

Learning shape functions for all single features ($f_i(x_i)$) and the selected feature pairs ($f_{i,j}(x_i, x_j)$). When $S = \emptyset$, F is the GAM.

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Learning a shape function for each feature pair

GA²M

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-

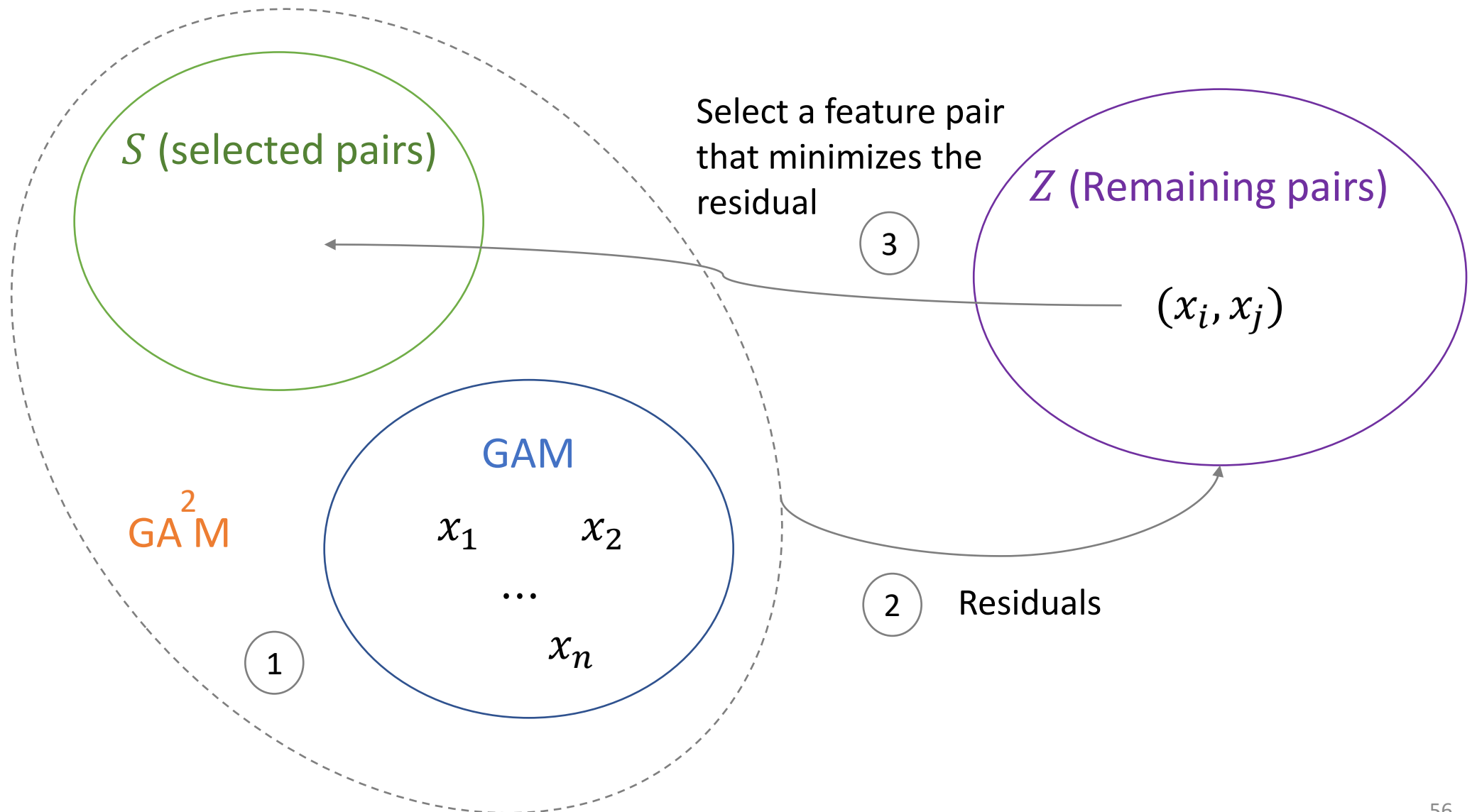
GA²M

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See a fast interaction detection algorithm in [Lou et al., 2013]

GA²M



Question?

Application

“Intelligible models for healthcare: Predicting pneumonia risk and hospital 30-day readmission”

Caruana et al., KDD 2015

Background

- In the mid 90's, a project was funded by Cost-Effective HealthCare (CEHC) to evaluate the application of machine learning to important problems in healthcare such as predicting pneumonia risk
- **Goal:** predict the probability of death (POD) for patients with pneumonia
- High-risk: patients could be admitted to the hospital
- Low-risk: patients were treated as outpatients

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Models

Logistic regression

Rule-based learning

k-nearest neighbor

Neural networks

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AUC=0.86 (Best performance)

...

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Models

Logistic regression

AUC=0.77 (safer to use on patients)

Rule-based learning

k-nearest neighbor

~~Neural networks~~

~~AUC=0.86 (Best performance)~~

...

Problem

The rule-based model learned a rule:

HasAsthama(x) \Rightarrow LowerRisk(x)

```
Rule-based models are interpretable  
if (chance_of_rain > 0.75)  
{ umbrella <- "yes" }  
else { umbrella <- "no" }
```

Problem

The rule-based model learned a rule:

$\text{HasAsthama}(x) \Rightarrow \text{LowerRisk}(x)$

counterintuitive



Problem

The rule-based model learned a rule:

$$\text{HasAsthama}(x) \Rightarrow \text{LowerRisk}(x)$$

counterintuitive



The model captures a true pattern in the training data:

Patients:
asthma +
pneumonia



Hospital (ICU)



The aggressive care
lowered the risk of
dying from pneumonia

Problem

The rule-based model learned a rule:

~~HasAsthama(x) \implies LowerRisk(x)~~

Asthmatics have much higher risk!

It would be dangerous if the model predicts low risk on patients who have not been hospitalized

Problem

How about other potential patterns?

Pregnancy \Rightarrow Lower Risk ?

Problem

How about other potential patterns?

Pregnancy \Rightarrow Lower Risk ?

**MUST understand ML models in healthcare.
Otherwise, models may hurt patients
because of true patterns in data!**

Generalized Additive Models

- Better prediction performance than logistic regression
(capture more data patterns)
- Interpretable

Case Study: Pneumonia Risk

- There are 46 features describing each patient
- Bagged trees with gradient boosting

<i>Patient-history findings</i>			
chronic lung disease	-	age	C
re-admission to hospital	-	gender	-
admitted through ER	-	diabetes mellitus	-
admitted from nursing home	-	asthma	-
congestive heart failure	-	cancer	-
ischemic heart disease	-	number of diseases	C
cerebrovascular disease	-	history of seizures	-
chronic liver disease	-	renal failure	-
history of chest pain	-		
<i>Physical examination findings</i>			
diastolic blood pressure	C	wheezing	-
gastrointestinal bleeding	-	stridor	-
respiration rate	C	heart murmur	-
altered mental status	-	temperature	C
heart rate	C		
<i>Laboratory findings</i>			
liver function tests	-	BUN level	C
glucose level	C	creatinine level	C
potassium level	C	albumin level	C
hematocrit	C	WBC count	C
percentage bands	C	pH	C
pO2	C	pCO2	C
sodium level	C		
<i>Chest X-ray findings</i>			
positive chest x-ray	-	lung infiltrate	-
pleural effusion	-	pneumothorax	-
cavitation/empyema	-	chest mass	-
lobe or lung collapse	-		

Prediction Performance

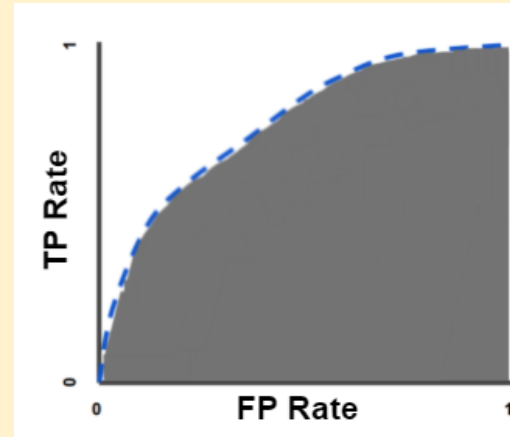
AUC for different learning methods

Model	Pneumonia
Logistic Regression	0.8432
GAM	0.8542
GA ² M	0.8576
Random Forests	0.8460
LogitBoost	0.8493

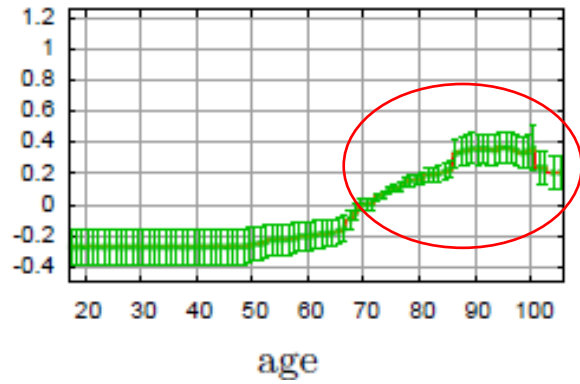
AUC: Area Under the ROC Curve

$$TPR = \frac{TP}{TP + FN}$$

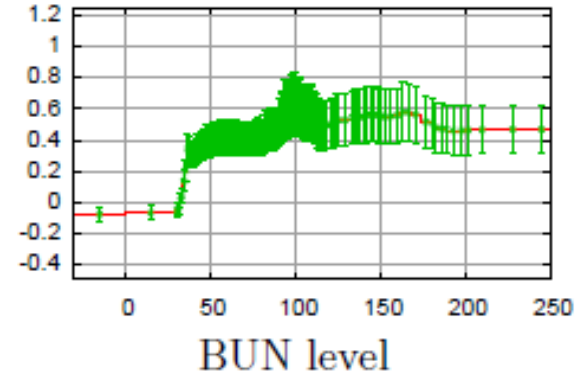
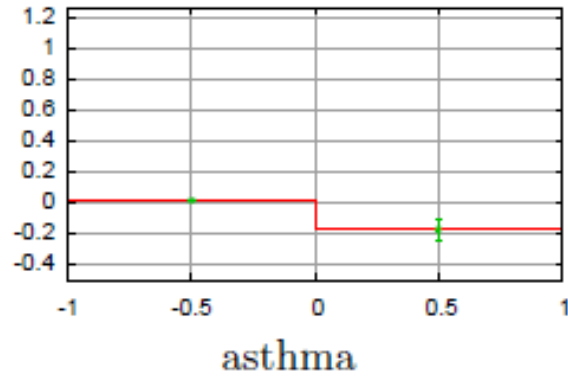
$$FPR = \frac{FP}{FP + TN}$$



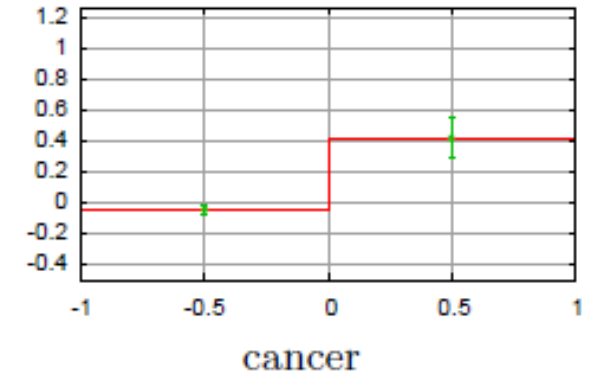
Interpretation



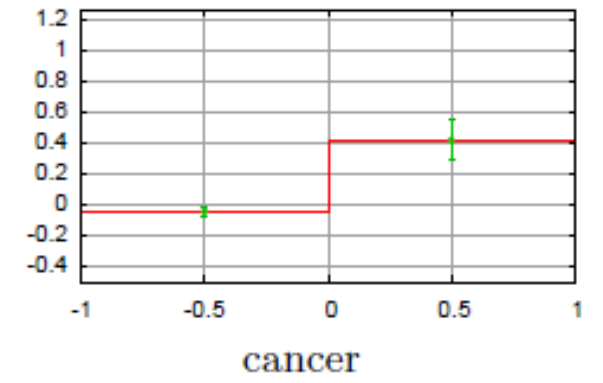
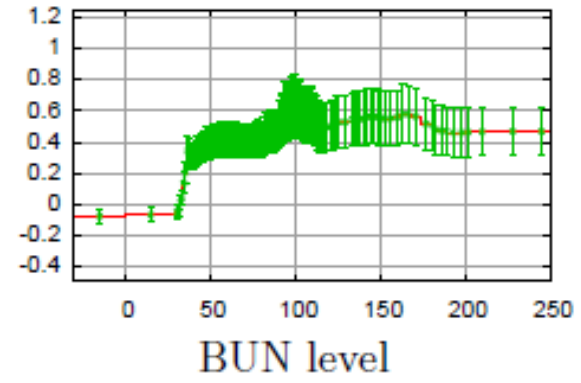
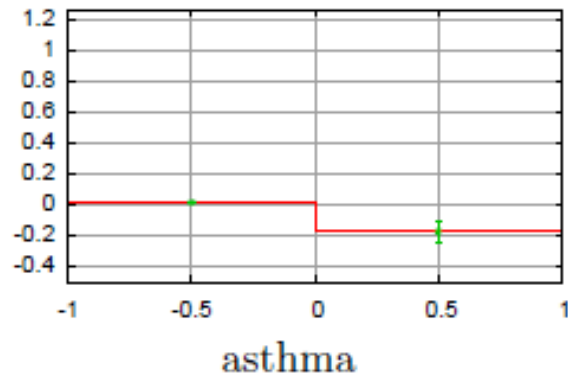
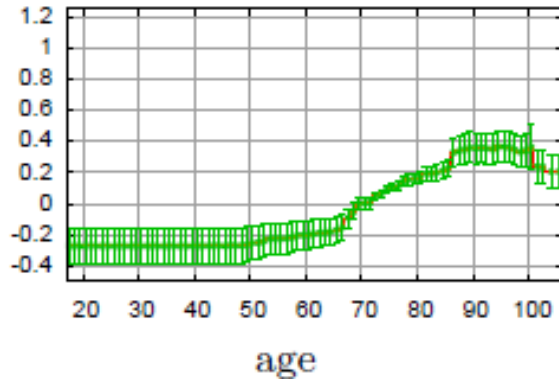
Older people have higher risk



(Blood Urea Nitrogen)



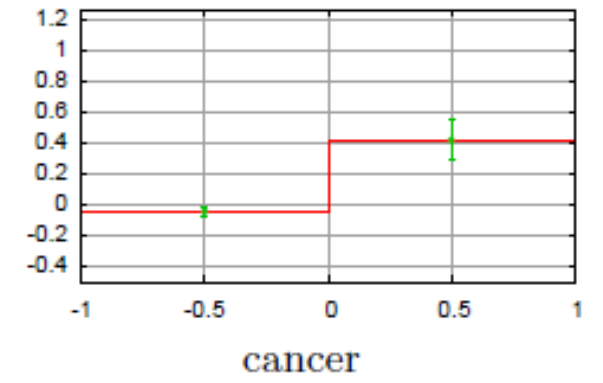
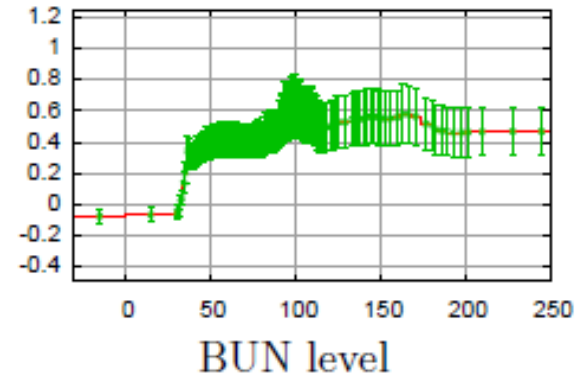
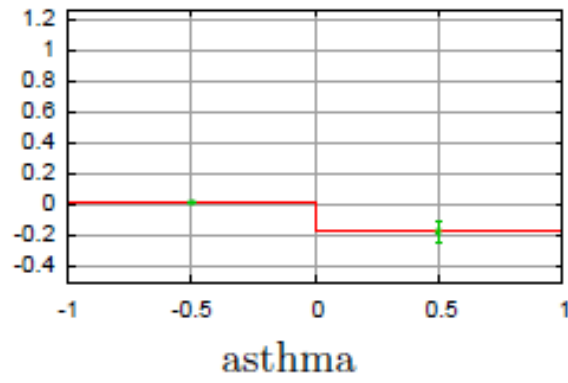
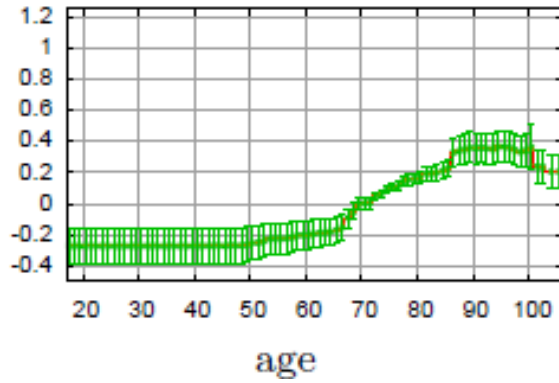
Interpretation



(Blood Urea Nitrogen)

GAMs also found the pattern: asthma lowers the risk

Interpretation

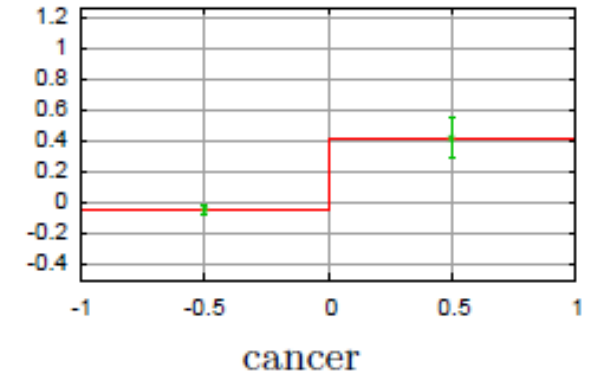
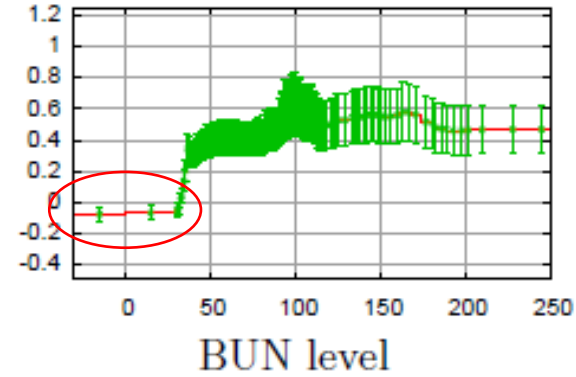
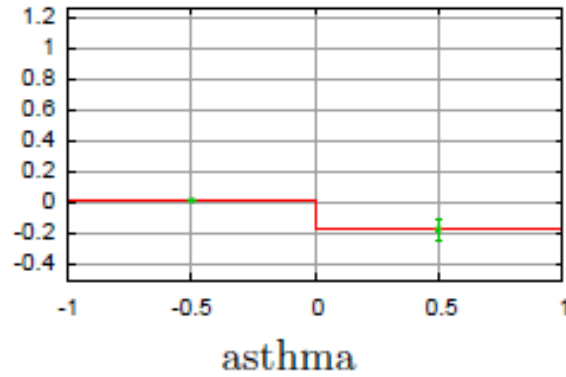
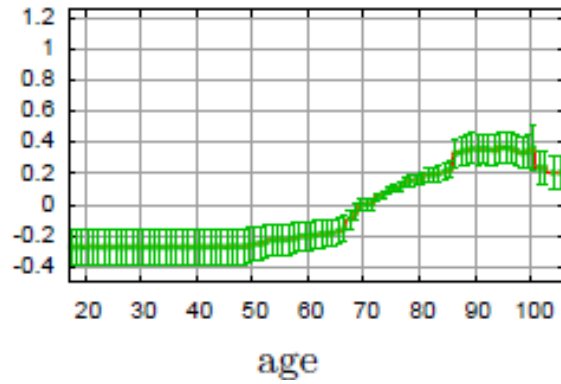


GAMs also found the pattern: asthma lowers the risk



Repair: eliminate this term

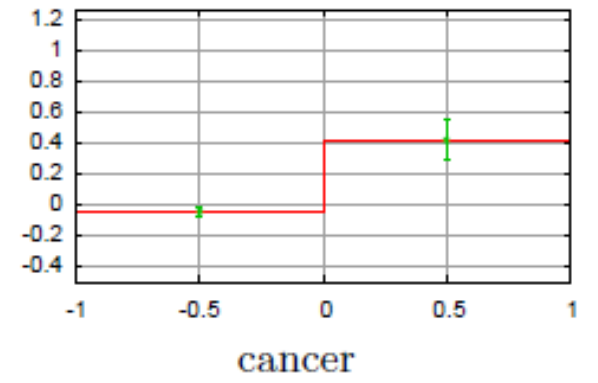
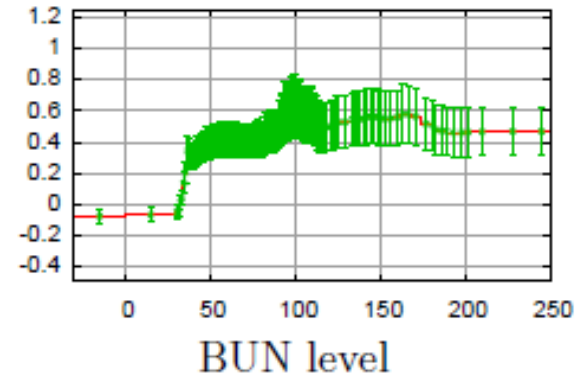
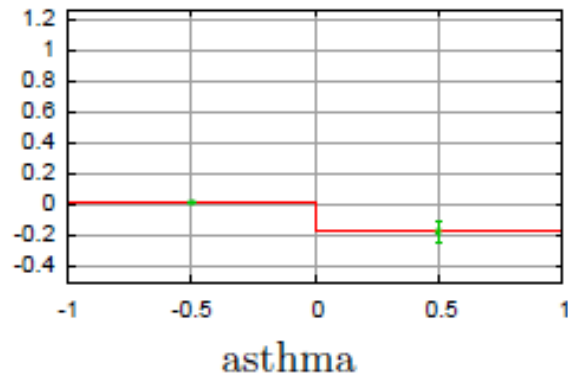
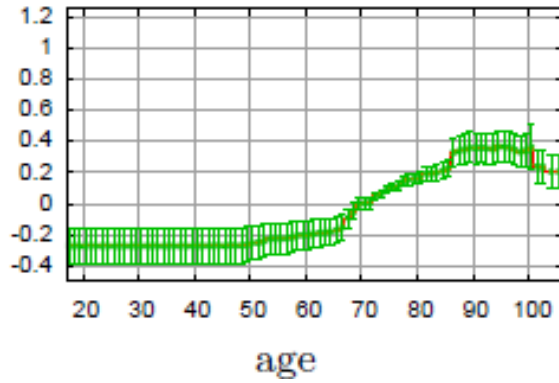
Interpretation



(Blood Urea Nitrogen)

Most patients have BUN=0 because, as in many medical datasets, if the variable is not measured or assumed normal it is coded as 0

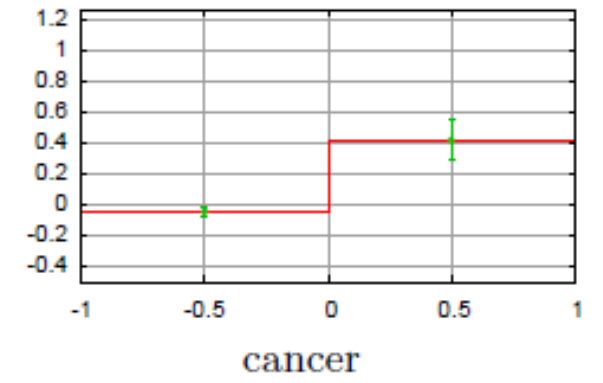
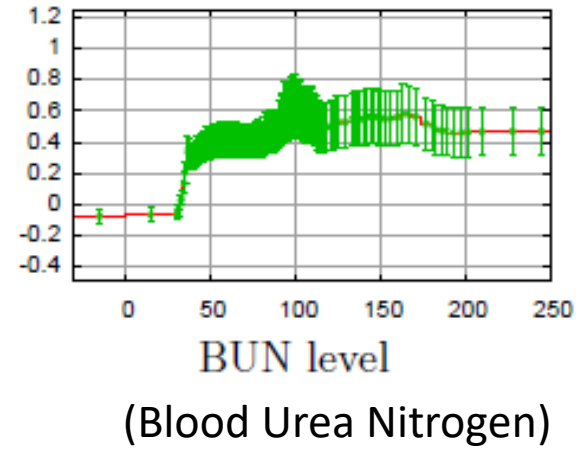
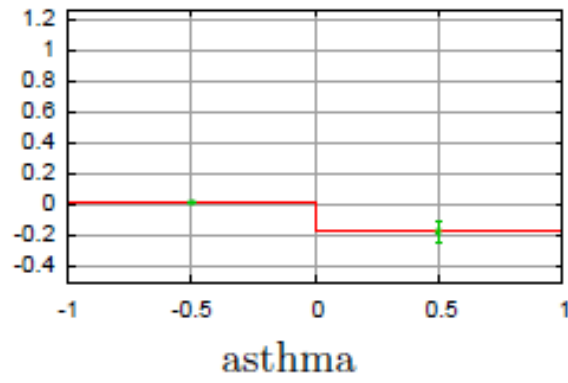
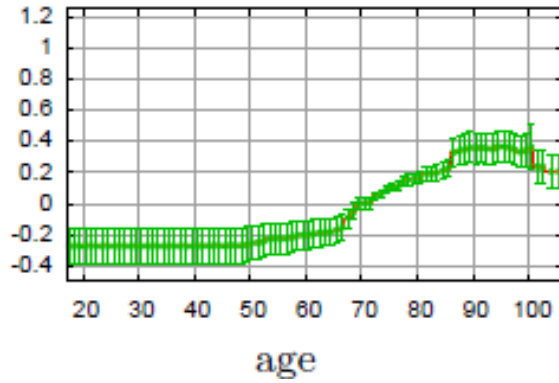
Interpretation



(Blood Urea Nitrogen)

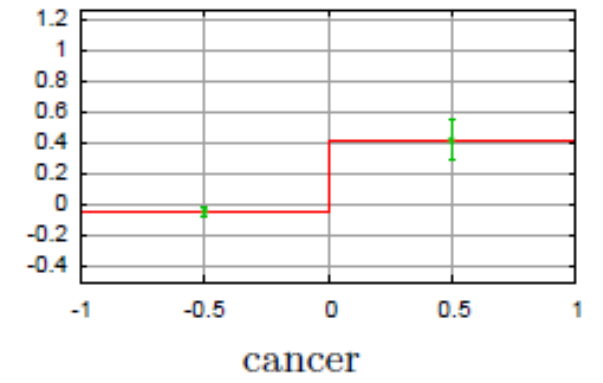
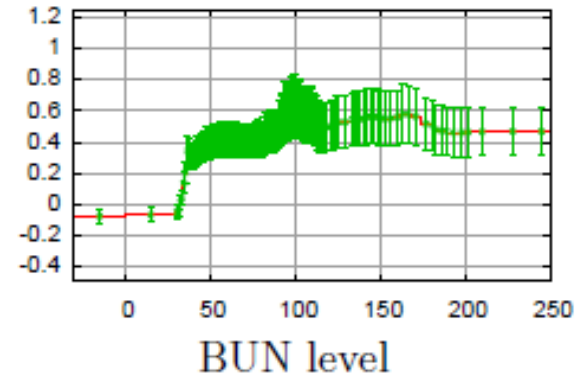
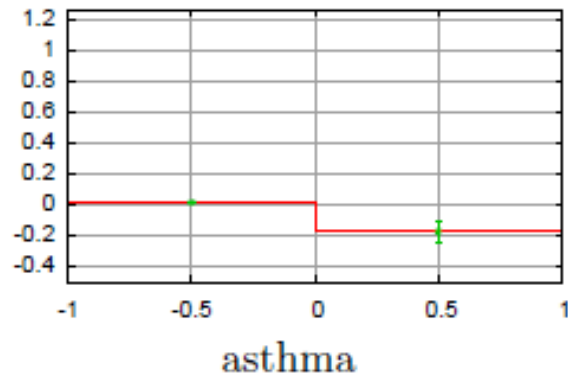
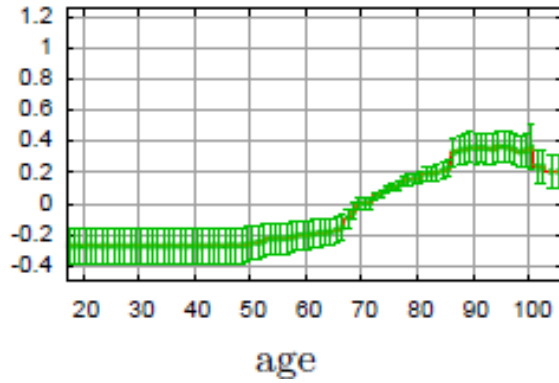
BUN levels below 30 appear to be low risk, while levels from 50-200 indicate higher risk

Interpretation

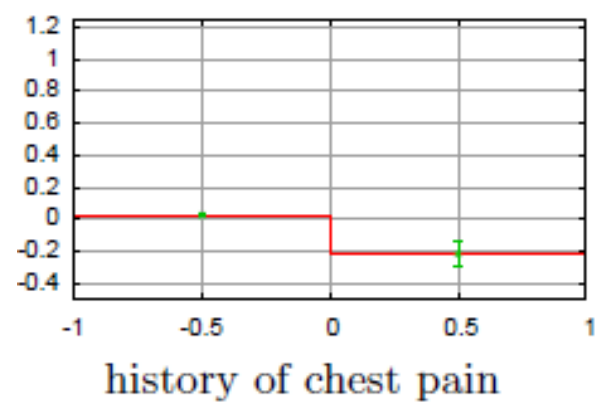
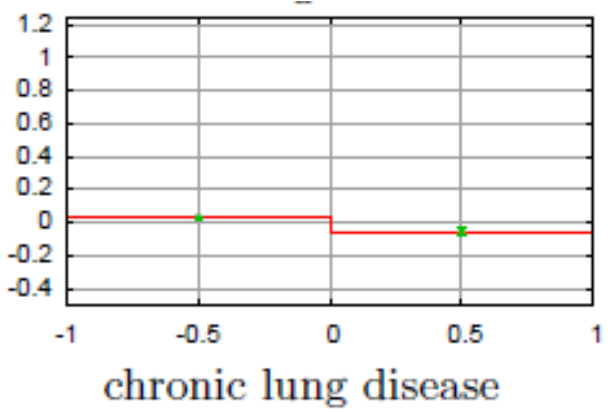


Having cancer significantly increases the risk of dying from pneumonia

Interpretation

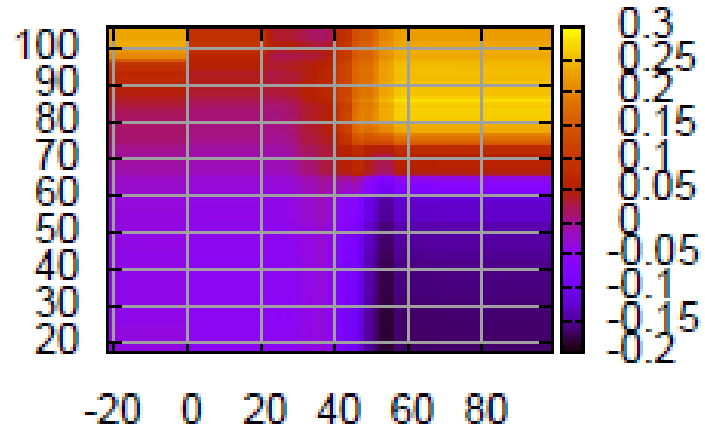


(Blood Urea Nitrogen)

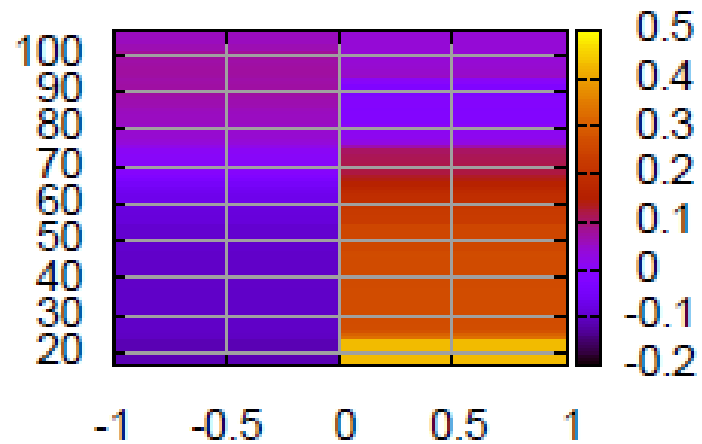


Chronic lung disease and a history of chest pain both lower risk (similar problem as asthma)

Interpretation



age vs. respiration rate



age vs. cancer

Old people with high respiration rate have the highest risk

- Risk is highest for the youngest patients
- It declines for patients who acquire cancer later in life
- For patients without cancer, risk rises as expected with age

Takeaway

- If a model contains a modest number of terms (e.g., less than 50), it is best to show terms in the model to experts in the order they are most familiar with
- When the number of terms grows large, it is best to provide a well-defined ordering of the terms for a patient (from terms that increase risk most to terms that decrease risk most)

Question?

Reference

- Lou, Yin, Rich Caruana, and Johannes Gehrke. "Intelligible models for classification and regression." *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2012.
- Lou, Yin, et al. "Accurate intelligible models with pairwise interactions." *Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2013.
- Caruana, Rich, et al. "Intelligible models for healthcare: Predicting pneumonia risk and hospital 30-day readmission." *Proceedings of the 21th ACM SIGKDD international conference on knowledge discovery and data mining*. 2015.