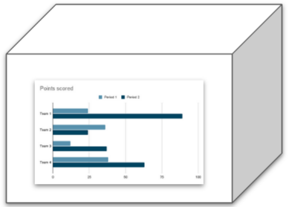
# Interpretable Machine Learning

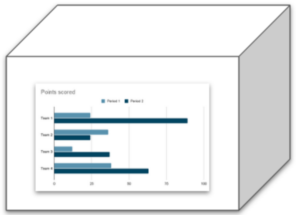
## Inherently Interpretable Models - Motivation



**Learning goals**

- Why should we use interpretable models?
- Advantages and disadvantages of interpretable models

Interpretable Machine Learning
Inherently Interpretable Models - Motivation



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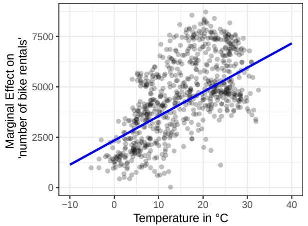
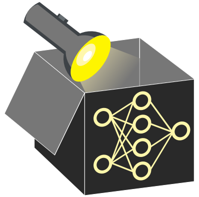
# MOTIVATION

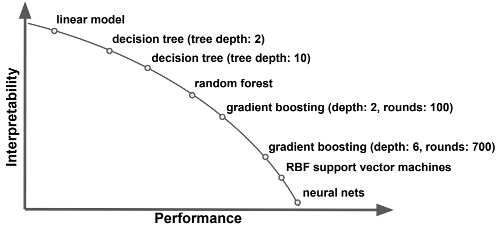
- Achieving interpretability by using interpretable models is the most straightforward approach
- Classes of models deemed interpretable:
  - (Generalized) linear models (LM, GLM)
  - Generalized additive models (GAM)
  - Decision trees
  - Rule-based learning
  - Model-based / component-wise boosting
  - ...



⇝ LM provides straightforward interpretation

- Often there is a trade-off between interpretability and model performance



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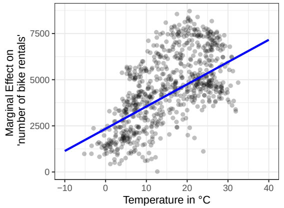


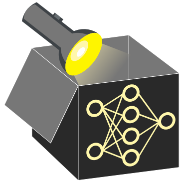

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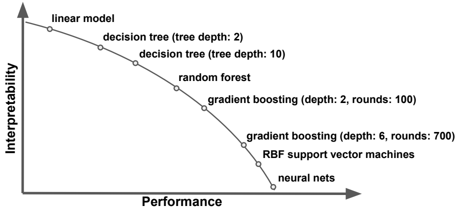

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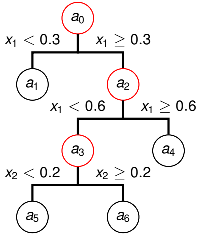
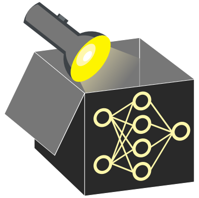
- Interpretable models are transparent by design, making many model-agnostic explanation methods unnecessary
  $\rightsquigarrow$ Eliminates an extra source of estimation error





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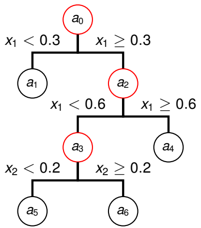


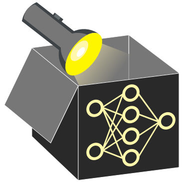

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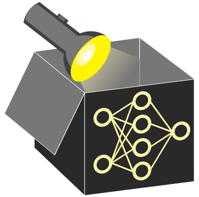

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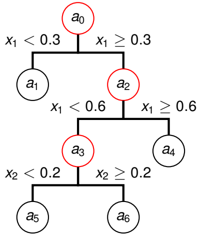


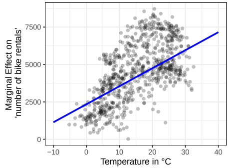




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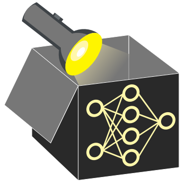

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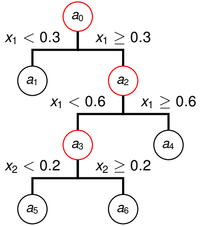


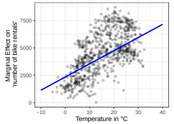

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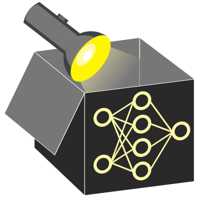

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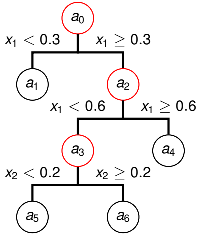


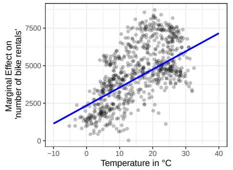




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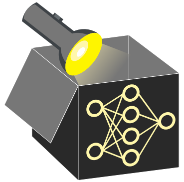

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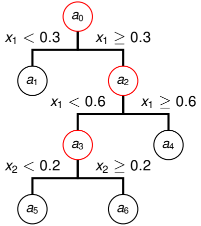

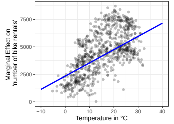

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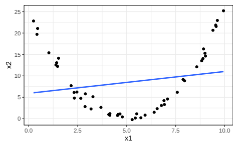
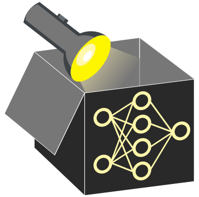
  ⇝ If assumptions are wrong, models may perform bad





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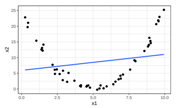

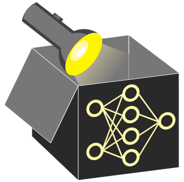

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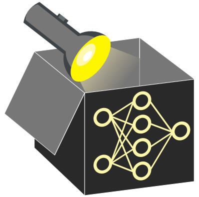

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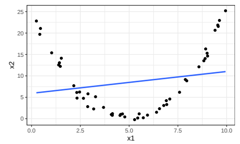


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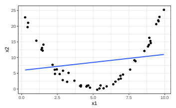

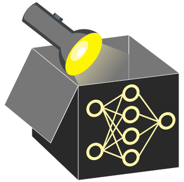

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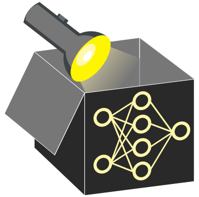

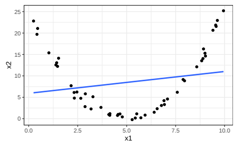


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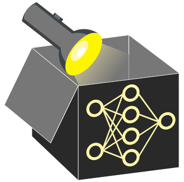

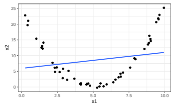

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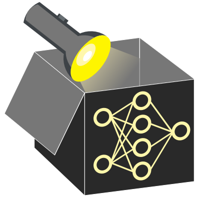

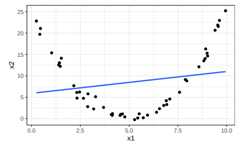


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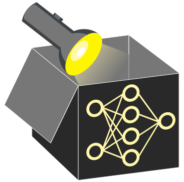

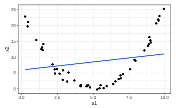

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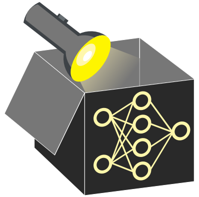

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  - Built-in interpretation ⇒ fewer risks from misleading post-hoc explanations
  - Good performance possible with effort on preprocessing / feat. engineering
  - But interpretability depends on meaning of created features
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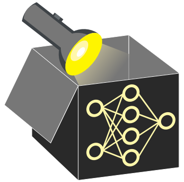

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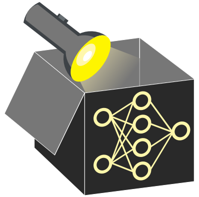

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  - Applies to image, text, or sensor data where features must be learned
  - Manual extraction of interpretable features is difficult
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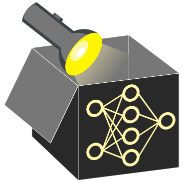

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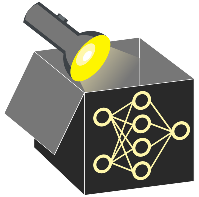

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- Increase complexity only if necessary to meet performance requirements
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- Choose the simplest model with sufficient accuracy $\rightsquigarrow$ Occam's razor

**Bike Data, 4-fold CV**

| Model | RMSE | $R^2$ |
|---|---|---|
| LM | 800.15 | 0.83 |
| Tree | 981.83 | 0.74 |
| Random Forest | 653.25 | 0.88 |
| Boosting (tuned) | 638.42 | 0.89 |



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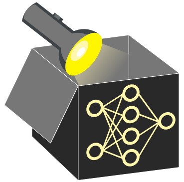

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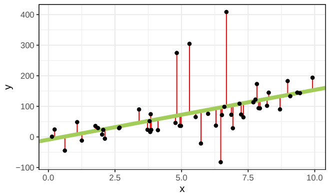
# Interpretable Machine Learning

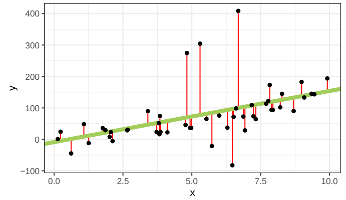
## Linear Regression Model




### Learning goals

- LM basics and assumptions
- Interpretation of main effects in LM
- What are significant features?


Interpretable Machine Learning
Linear Regression Model



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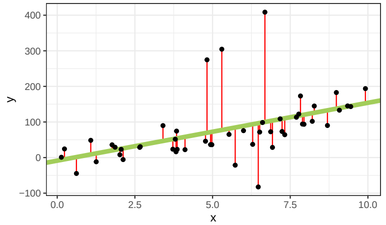


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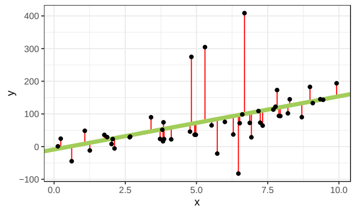



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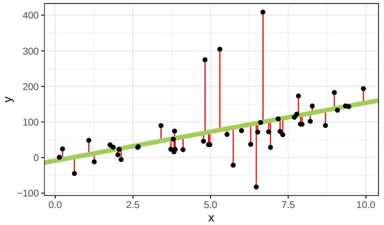


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**Properties and assumptions** ▸ Faraway (2002), Ch. 7 ▸ Checking assumptions in R & Python

- **Linear** relationship between features and target



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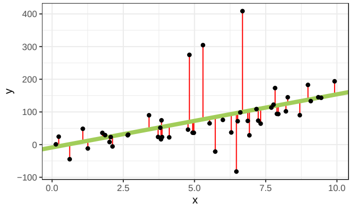


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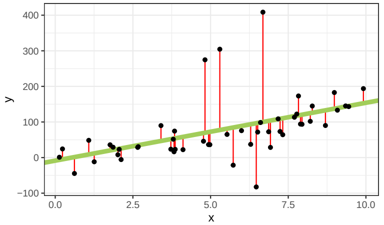


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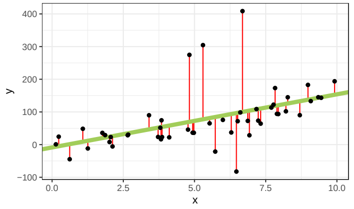


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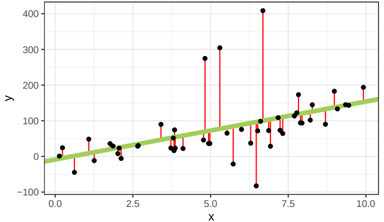


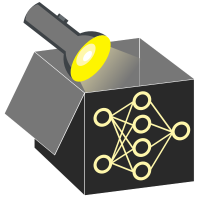

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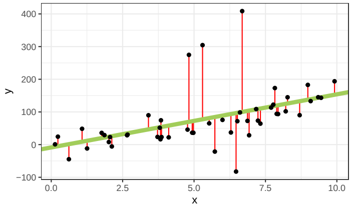


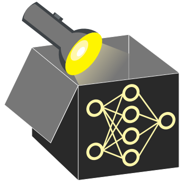

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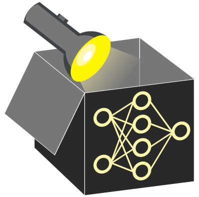

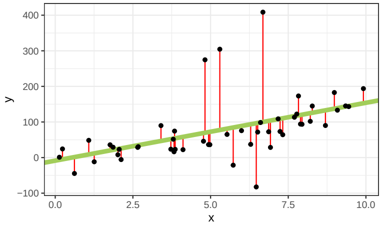


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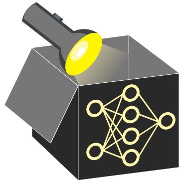

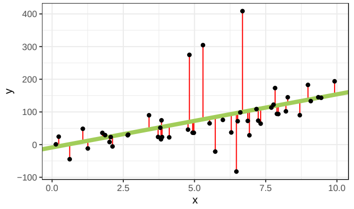


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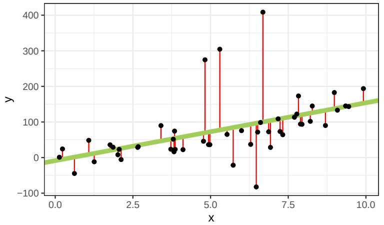


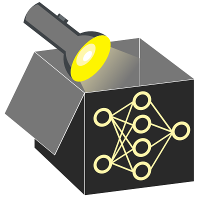

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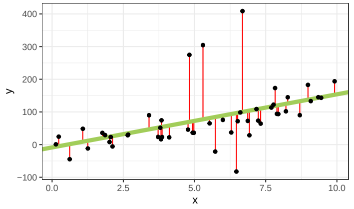


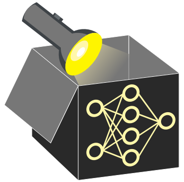

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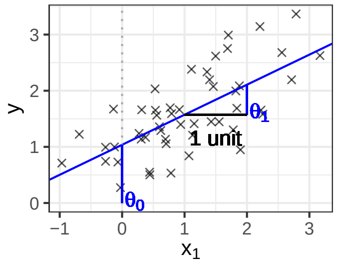





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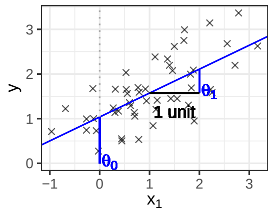

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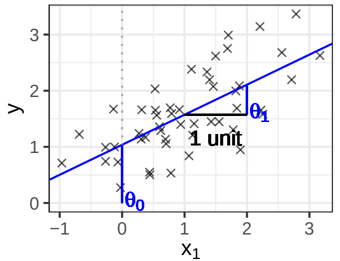




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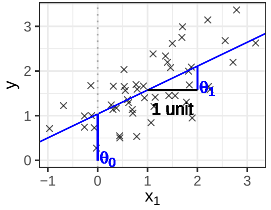

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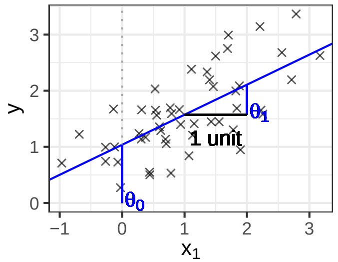





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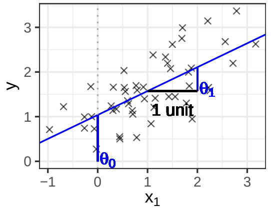

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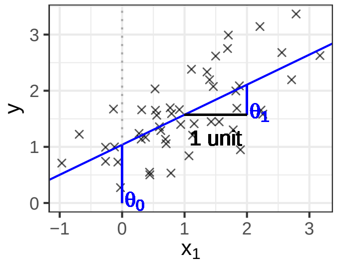




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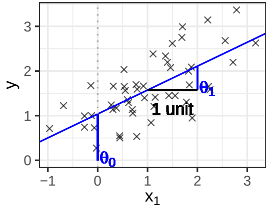

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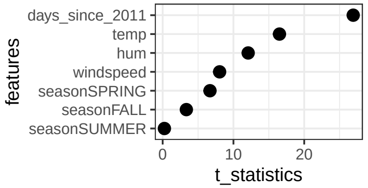


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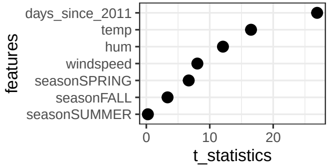


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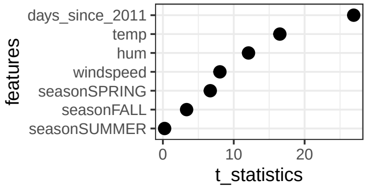


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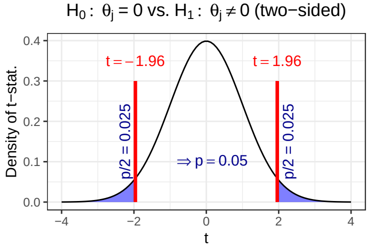





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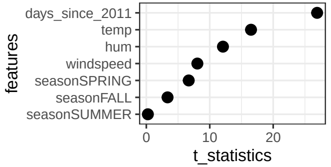



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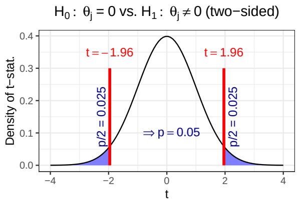
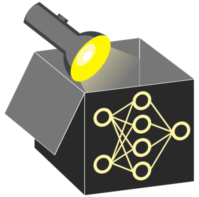
- **p-value**: probability of obtaining a more extreme test statistic assuming $H_0$ is correct (here: $\theta_j = 0$, i.e., feat. $j$ not significant) $\rightsquigarrow$ High $|t|$ $\Rightarrow$ small p-val. (speak against $H_0$)

# EXAMPLE: LINEAR REGRESSION - MAIN EFFECTS

**Bike data**: predict no. of rented bikes using 4 numeric, 1 categorical feat. (season)



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| | Weights | SE | t-stat. | p-val. |
|---|---|---|---|---|
| (Intercept) | 3229.3 | 220.6 | 14.6 | 0.00 |
| seasonSPRING | 862.0 | 129.0 | 6.7 | 0.00 |
| seasonSUMMER | 41.6 | 170.2 | 0.2 | 0.81 |
| seasonFALL | 390.1 | 116.6 | 3.3 | 0.00 |
| temp | 120.5 | 7.3 | 16.5 | 0.00 |
| hum | -31.1 | 2.6 | -12.1 | 0.00 |
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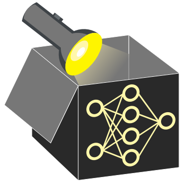

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\begin{aligned}
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**Interpretation:**

- **Intercept**: If all feature values are 0 (and season is `WINTER` $\hat{=}$ reference cat.), the expected number of bike rentals is $\hat{\theta}_0 = 3229.3$



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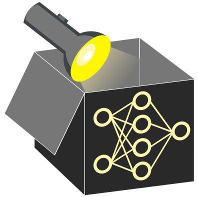

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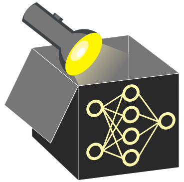

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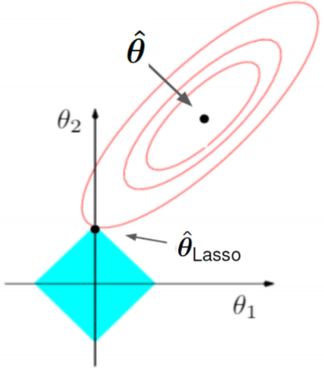
# Interpretable Machine Learning

# Extensions of Linear Regression Models




**Learning goals**

- Inclusion of high-order and interaction effects
- Regularization via LASSO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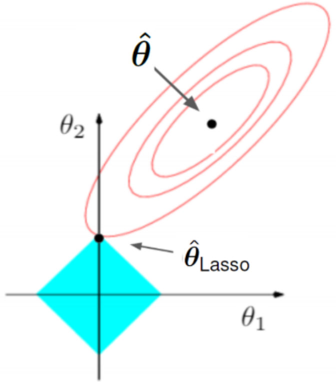


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# INTERACTION AND HIGH-ORDER EFFECTS

LM Equation: $y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p + \epsilon$

Equation above can be extended (polynomial regression) by including

- **high-order effects** which have their own weights
  $\rightsquigarrow$ e.g., quadratic effect: $\theta_{x_j^2} \cdot x_j^2$
- **interaction effects** as the product of multiple feat.
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**Bike Data**

| Method | $R^2$ | adj. $R^2$ |
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Implications of including high-order and interaction effects:

- Both make the model more flexible but also less interpretable
  $\rightsquigarrow$ More weights to interpret
- Both need to be specified manually (inconvenient and sometimes infeasible)
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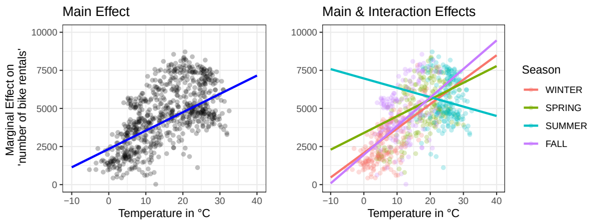
# EXAMPLE: INTERACTION EFFECT

**Example**: Interaction between `temp` and `season` will affect marginal effect of `temp`




| | Weights |
|---|---|
| (Intercept) | 3453.9 |
| seasonSPRING | 1317.0 |
| seasonSUMMER | 4894.1 |
| seasonFALL | -114.2 |
| temp | 160.5 |
| hum | -37.6 |
| windspeed | -61.9 |
| days_since_2011 | 4.9 |
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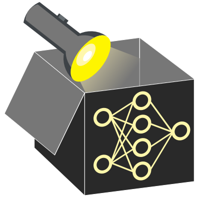



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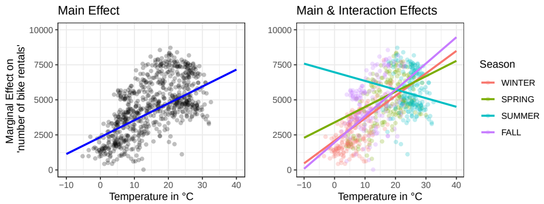



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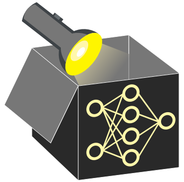

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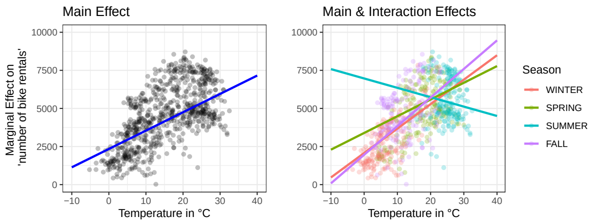


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**Interpretation**: If `temp` increases by 1 °C, bike rentals

- increase by 160.5 in `WINTER` (reference)



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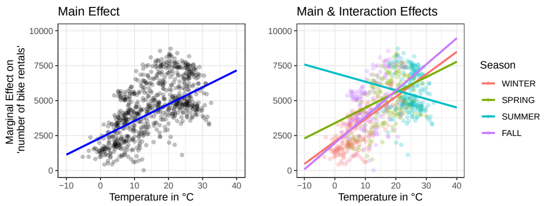


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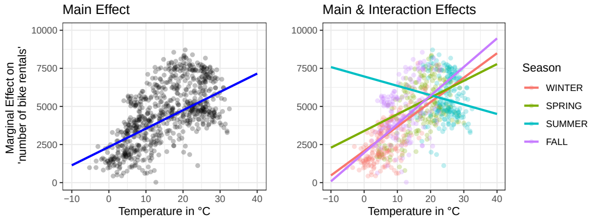


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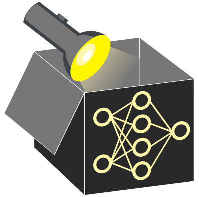

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- increase by 160.5 in `WINTER` (reference)
- increase by 109.8 (= 160.5 - 50.7) in `SPRING`



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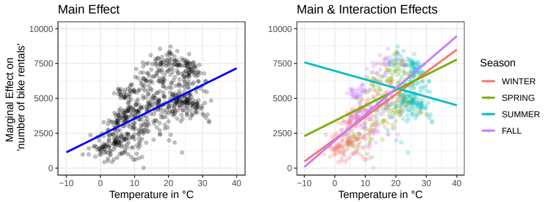


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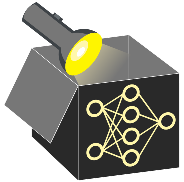

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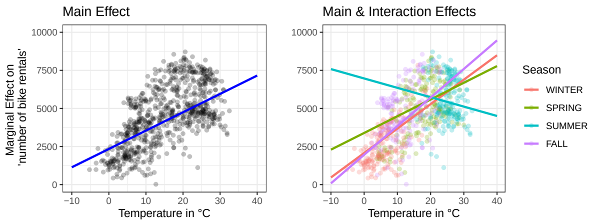
- increase by 160.5 in `WINTER` (reference)
- increase by 109.8 (= 160.5 - 50.7) in `SPRING`

# EXAMPLE: INTERACTION EFFECT

**Example**: Interaction between `temp` and `season` will affect marginal effect of `temp`




| | Weights |
|---|---|
| (Intercept) | 3453.9 |
| seasonSPRING | 1317.0 |
| seasonSUMMER | 4894.1 |
| seasonFALL | -114.2 |
| temp | 160.5 |
| hum | -37.6 |
| windspeed | -61.9 |
| days_since_2011 | 4.9 |
| seasonSPRING:temp | -50.7 |
| seasonSUMMER:temp | -222.0 |
| seasonFALL:temp | 27.2 |

**Interpretation**: If `temp` increases by 1 °C, bike rentals

- increase by 160.5 in `WINTER` (reference)
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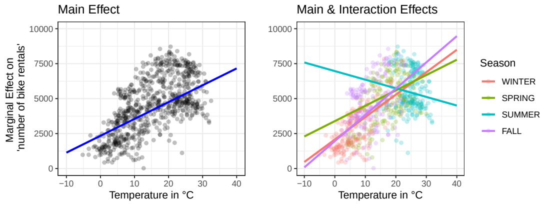
- decrease by -61.5 (= 160.5 - 222) in `SUMMER`



# EXAMPLE: INTERACTION EFFECT

**Ex.**: Interaction between `temp` and `season` will affect marginal effect of `temp`





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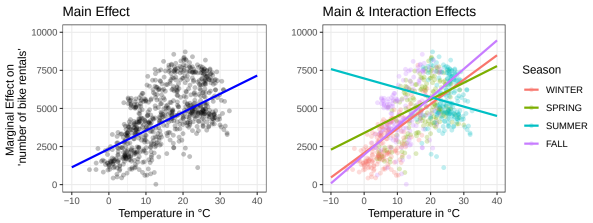


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- increase by 187.7 (= 160.5 + 27.2) in `FALL`



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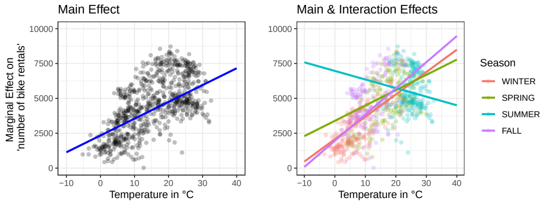


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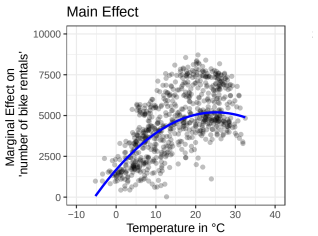
# EXAMPLE: QUADRATIC EFFECT

**Example**: Adding quadratic effect for `temp`




| | Weights |
|---|---|
| (Intercept) | 3094.1 |
| seasonSPRING | 619.2 |
| seasonSUMMER | 284.6 |
| seasonFALL | 123.1 |
| hum | -36.4 |
| windspeed | -65.7 |
| days_since_2011 | 4.7 |
| temp | 280.2 |
| temp$^2$ | -5.6 |

**Interpretation**: Not linear anymore!

- `temp` depends on two weights: $280.2 \cdot x_{temp} - 5.6 \cdot x_{temp}^2$



# EXAMPLE: QUADRATIC EFFECT

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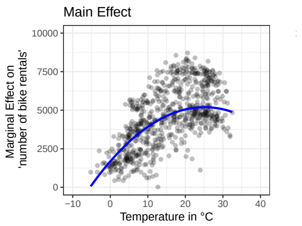


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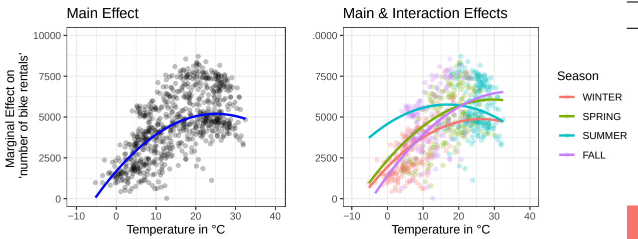
# EXAMPLE: QUADRATIC EFFECT

**Example**: Adding quadratic effect for `temp` (left) and interaction with `season` (right)




| | Weights |
|---|---|
| (Intercept) | 3802.1 |
| seasonSPRING | -1345.1 |
| seasonSUMMER | -6006.3 |
| seasonFALL | -681.4 |
| hum | -38.9 |
| windspeed | -64.1 |
| days_since_2011 | 4.8 |
| temp | 39.1 |
| temp$^2$ | 8.6 |
| seasonSPRING:temp | 407.4 |
| seasonSPRING:temp$^2$ | -18.7 |
| seasonSUMMER:temp | 801.1 |
| seasonSUMMER:temp$^2$ | -27.2 |
| seasonFALL:temp | 217.4 |
| seasonFALL:temp$^2$ | -11.3 |

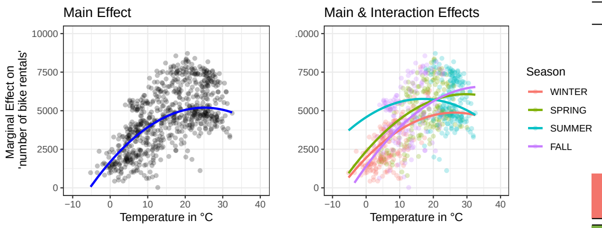
**Interpretation**: Not linear anymore!

- `temp` depends on multiple weights due to `season`:
  - $\rightsquigarrow$ `WINTER`: $39.1 \cdot x_{temp} + 8.6 \cdot x^2_{temp}$
  - $\rightsquigarrow$ `SPRING`: $(39.1+407.4) \cdot x_{temp} + (8.6-18.7) \cdot x^2_{temp}$
  - $\rightsquigarrow$ `SUMMER`: $(39.1+801.1) \cdot x_{temp} + (8.6-27.2) \cdot x^2_{temp}$
  - $\rightsquigarrow$ `FALL`: $(39.1+217.4) \cdot x_{temp} + (8.6-11.3) \cdot x^2_{temp}$



# EXAMPLE: QUADRATIC EFFECT

**Ex.**: Adding quadratic effect for `temp` (left) and interaction with `season` (right)




| | Weights |
|---|---|
| (Intercept) | 3802.1 |
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| seasonFALL | -681.4 |
| hum | -38.9 |
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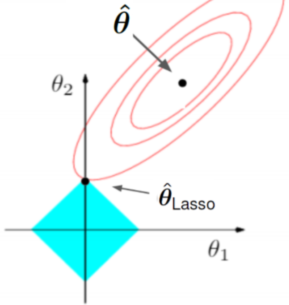
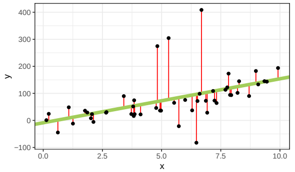
# REGULARIZATION VIA LASSO ▸ Tibshirani (1996)

- LASSO adds an $L_1$-norm penalization term ($\lambda||\theta||_1$) to least squares optimization problem
  - ⇝ Shrinks some feature weights to zero (feature selection)
  - ⇝ Sparser models (fewer features): more interpretable
- Penalization parameter $\lambda$ must be chosen (e.g., by CV)

$$min_\theta \left( \underbrace{\frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \mathbf{x}^{(i)\top}\theta)^2}_{\text{Least square estimate for LM}} + \lambda||\theta||_1 \right)$$



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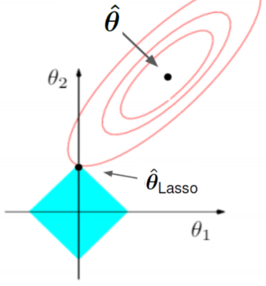
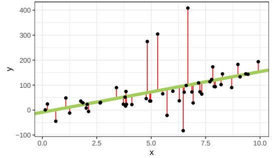
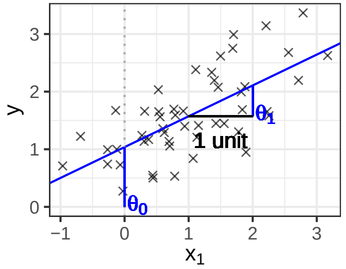


# REGULARIZATION VIA LASSO ▸ Tibshirani (1996)

**Example** (interpretation of weights analogous to LM):

- LASSO with main effects and interaction `temp` with `season`
- $\lambda$ is chosen $\rightsquigarrow$ 6 selected features ($\neq 0$)
- LASSO shrinks weights of single categories separately (due to dummy encoding)
  $\rightsquigarrow$ No feature selection of whole categorical features (only w.r.t. category levels)
  $\rightsquigarrow$ Solution: group LASSO ▸ Yuan and Lin (2006)




| | Weights |
|---|---|
| (Intercept) | 3135.2 |
| seasonSPRING | 767.4 |
| seasonSUMMER | 0.0 |
| seasonFALL | 0.0 |
| temp | 116.7 |
| hum | -28.9 |
| windspeed | -50.5 |
| days_since_2011 | 4.8 |
| seasonSPRING:temp | 0.0 |
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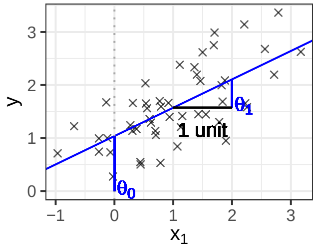



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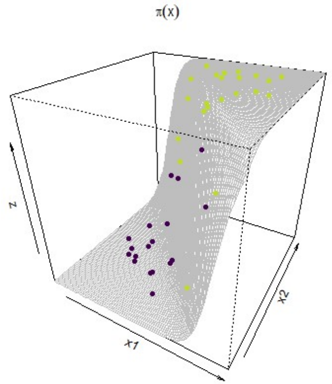
# Interpretable Machine Learning

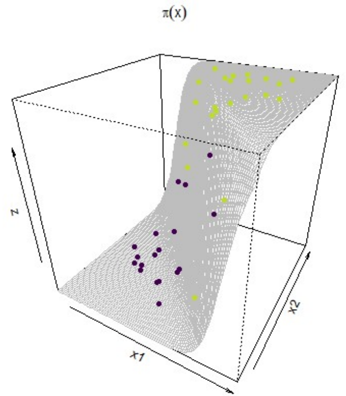
## Generalized Linear Models




**Learning goals**

- Definition of GLMs
- Logistic regression as example
- Interpretation in logistic regression

# Interpretable Machine Learning
## Generalized Linear Models (GLMs)




**Learning goals**

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- Logistic regression as example
- Interpretation in logistic regression

# GENERALIZED LINEAR MODEL (GLM) ▸ Nelder and Wedderburn 1972

**Problem**: Target variable given feat. not always normally dist. ⇝ LM not suitable

- Target is binary (e.g., disease classification)
  ⇝ Bernoulli / Binomial distribution
- Target is count variable
  (e.g., number of sold products)
  ⇝ Poisson distribution
- Time until an event occurs
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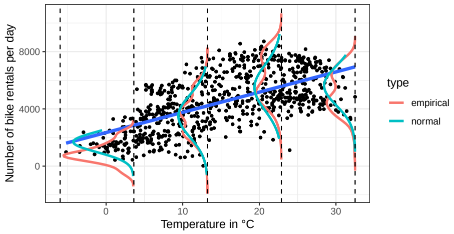


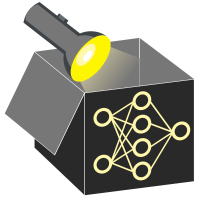



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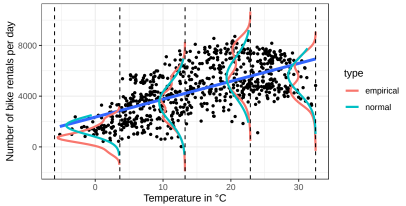


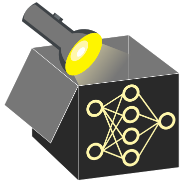

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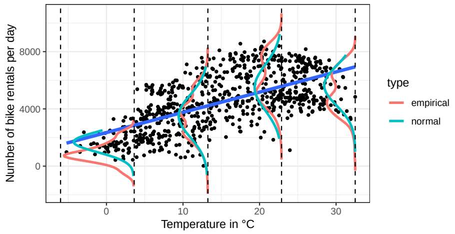


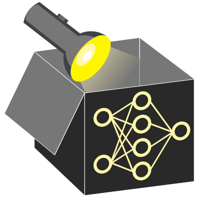

**Solution**: GLMs - extend LMs by allowing other distributions from exponential family

$$g(\mathbb{E}(y \mid \mathbf{x})) = \mathbf{x}^\top \boldsymbol{\theta} \;\Leftrightarrow\; \mathbb{E}(y \mid \mathbf{x}) = g^{-1}(\mathbf{x}^\top \boldsymbol{\theta})$$

- Link function $g$ links linear predictor $\mathbf{x}^\top\boldsymbol{\theta}$ to expectation of distribution of $y \mid \mathbf{x}$
  ⇝ LM is special case: Gaussian distribution for $y \mid \mathbf{x}$ with $g$ as identity function
- Link function $g$ and distribution need to be specified
- High-order and interaction effects can be manually added as in LMs
- Note: Interpretation of weights depend on link function and distribution



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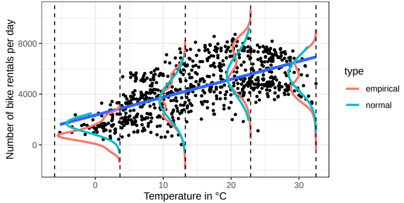


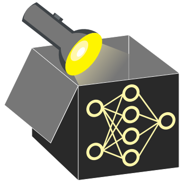

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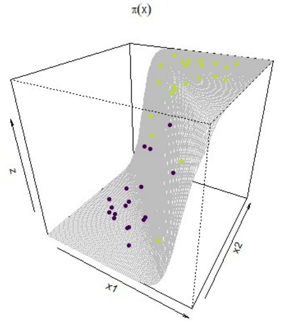
# GLM - LOGISTIC REGRESSION

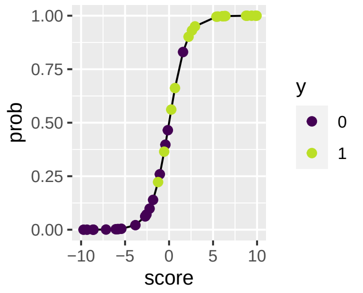
- Logistic regression $\hat{=}$ GLM with Bernoulli distribution and logit link function:

$$g(x) = \log\left(\frac{x}{1-x}\right) \Rightarrow g^{-1}(x) = \frac{1}{1+\exp(-x)}$$

- Models probabilities for binary classification by

$$\pi(\mathbf{x}) = \mathbb{E}(y \mid \mathbf{x}) = P(y=1) = g^{-1}(\mathbf{x}^\top \boldsymbol{\theta}) = \frac{1}{1+\exp(-\mathbf{x}^\top \boldsymbol{\theta})}$$



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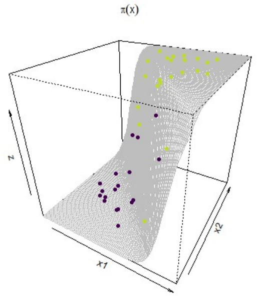

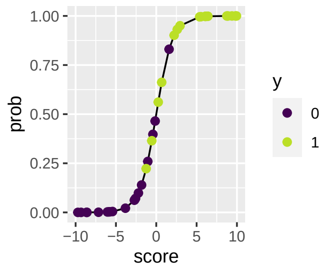

# GLM - LOGISTIC REGRESSION

- Typically, we set the threshold to 0.5 to predict classes, e.g.,
  - Class 1 if $\pi(\mathbf{x}) > 0.5$
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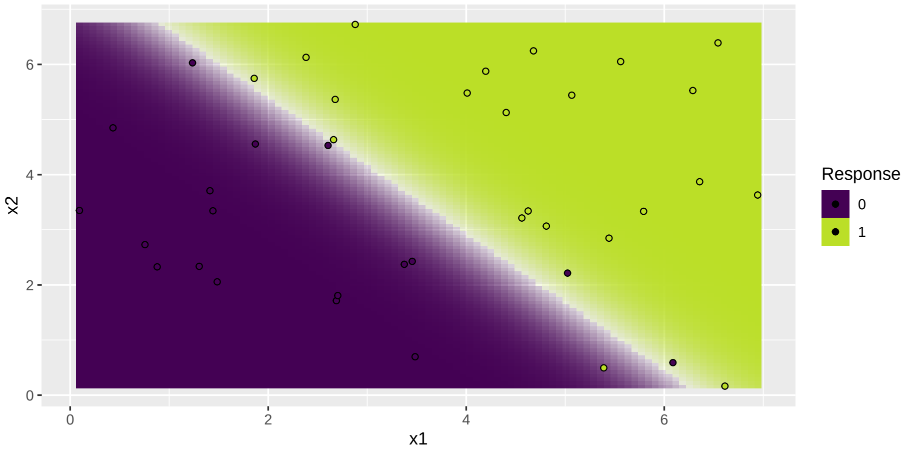





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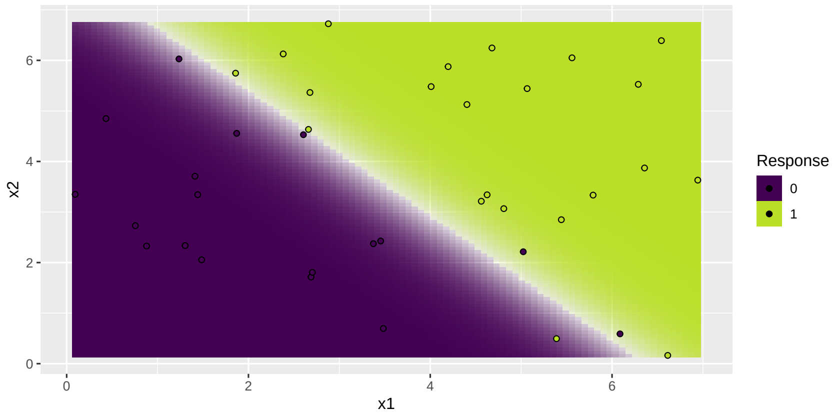

# GLM - LOGISTIC REGRESSION - INTERPRETATION

- **Recall:** Odds is ratio of two probabilities, odds ratio compares ratio of two odds
- Weights $\theta_j$ are interpreted linear as in LM (but w.r.t. log-odds)
  $\rightsquigarrow$ difficult to comprehend

$$\textit{log-odds} = \log\left(\frac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})}\right) = \log\left(\frac{P(y=1)}{P(y=0)}\right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_p x_p$$

**Interpretation:**
Changing $x_j$ by one unit, changes log-odds of class 1 compared to class 0 by $\theta_j$



# GLM - LOG. REGRESSION - INTERPRETATION

- **Recall:** Odds is ratio of two probabilities, odds ratio is ratio of two odds
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  $\rightsquigarrow$ difficult to comprehend

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# GLM - LOGISTIC REGRESSION - INTERPRETATION

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- Odds for class 1 vs. class 0: $\textit{odds} = \dfrac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})} = \exp(\theta_0 + \theta_1 x_1 + \ldots + \theta_p x_p)$
- Instead of interpreting changes w.r.t. log-odds, *odds ratio* is more common

$$= \frac{\textit{odds}_{x_j+1}}{\textit{odds}} = \frac{\exp(\theta_0 + \theta_1 x_1 + \ldots + \theta_j(x_j+1) + \ldots + \theta_p x_p)}{\exp(\theta_0 + \theta_1 x_1 + \ldots + \theta_j x_j + \ldots + \theta_p x_p)} = \exp(\theta_j)$$

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# GLM - LOGISTIC REGRESSION - EXAMPLE

- Create a binary target variable for bike rental data:
  - Class 1: “high number of bike rentals” $>$ 70% quantile (i.e., `cnt` $>$ 5531)
  - Class 0: “low to medium number of bike rentals” (i.e., `cnt` $\leq$ 5531)
- Fit a logistic regression model (GLM with Bernoulli distribution and logit link)

| | Weights | SE | p-value |
|---|---|---|---|
| (Intercept) | -8.52 | 1.21 | 0.00 |
| seasonSPRING | 1.74 | 0.60 | 0.00 |
| seasonSUMMER | -0.86 | 0.77 | 0.26 |
| seasonFALL | -0.64 | 0.55 | 0.25 |
| temp | 0.29 | 0.04 | 0.00 |
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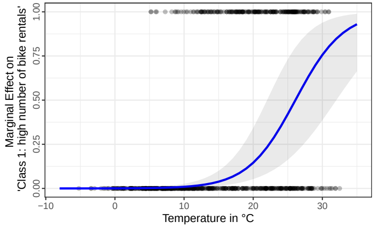


### Interpretation

- If $\texttt{temp}$ increases by $1°C$, odds ratio for class 1 increases by factor $\exp(0.29) = 1.34$ compared to class 0, c.p. ($\hat{=}$ “high number of bike rentals” now 1.34 times more likely)



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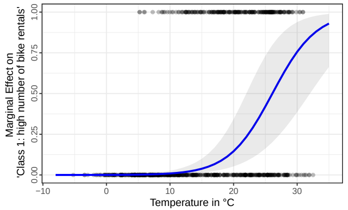


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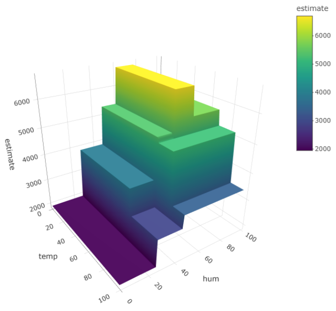
# Interpretable Machine Learning

# Rule-based Models




**Learning goals**

- Decision trees
- RuleFit
- Decision rules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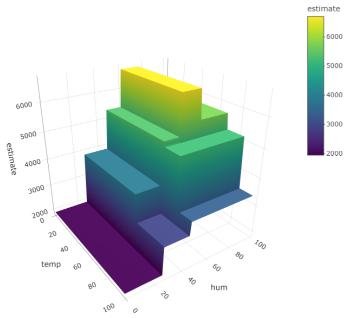

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**Idea**: Partition data into axis-aligned regions via greedy search for feature cut points (minimizing a split criterion), then predict a constant mean $c_m$ in each leaf region $\mathcal{R}_m$:

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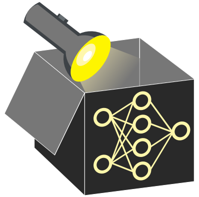

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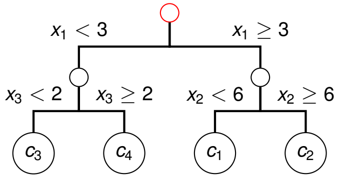
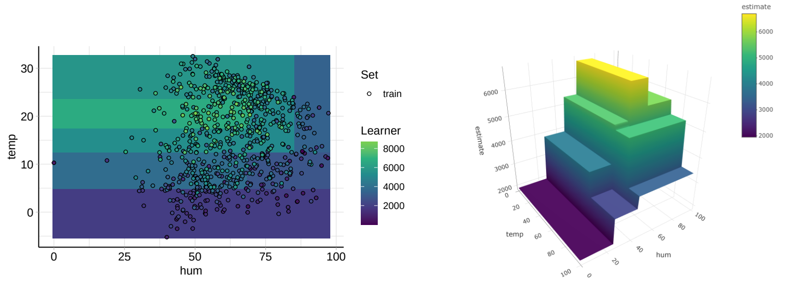



- Applicable to regression and classification
- Models interactions and non-linear effects
- Handles mixed feature spaces & missing values



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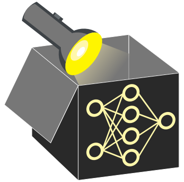

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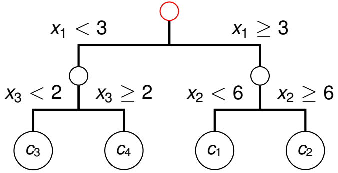


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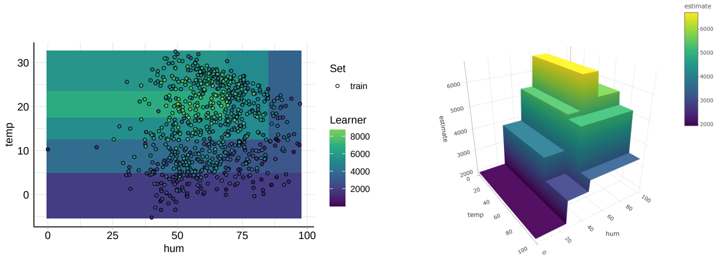

# INTERPRETATION OF TREE-BASED MODELS

- Interpretation via path of decision rules along tree branches
- **Feature importance** (quantifies how often and how usefully $x_j$ is used):
  - For each split on feature $x_j$, record the decrease in the split criterion
  - Aggregate this over the tree: sum or average over all splits involving $x_j$
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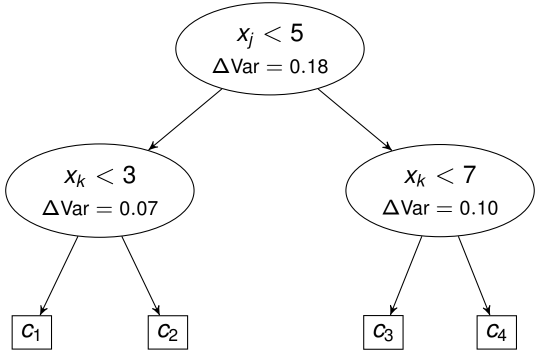


- Each $\Delta$Var is assigned to the splitting feature
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  $x_j$: $0.18$
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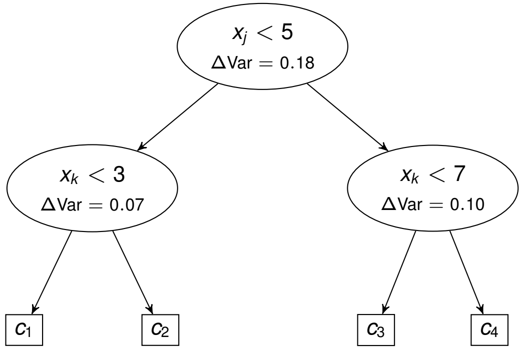


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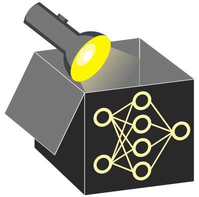

- Fit decision tree with tree depth of 3 on bike data
- E.g., mean prediction for the first 105 days since 2011 is 1798
  $\rightsquigarrow$ Applies to $\hat{=}$15% of the data (leftmost branch)
- `days_since_2011`: highest feature importance (explains most of variance)

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|---|---|
| days_since_2011 | 79.53 |
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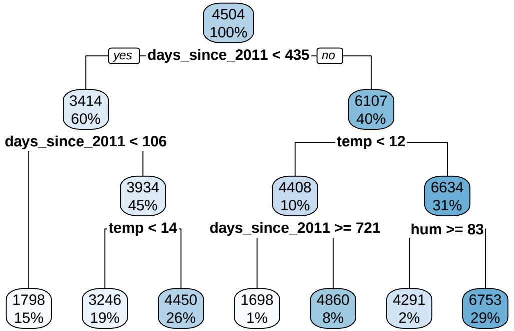




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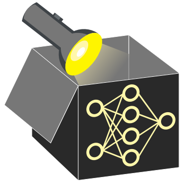

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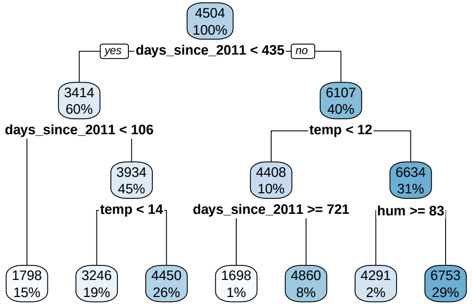

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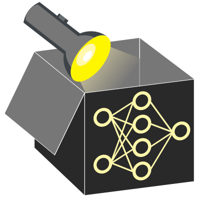

**Problems** with CART (Classification and Regression Trees):

1. Selection bias towards high-cardinal/continuous features
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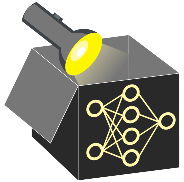

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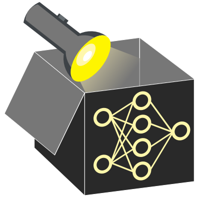

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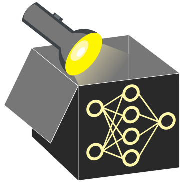

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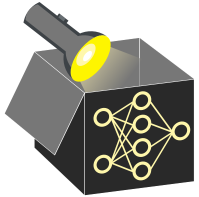

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**Example (selection bias)**:
Simulate data ($n = 200$) with $Y \sim N(0, 1)$ and 3 features of different cardinality independent from $Y$ (repeat 500 times):

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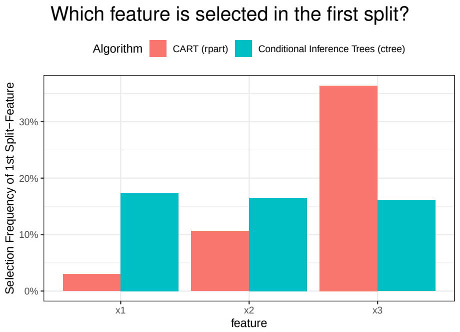




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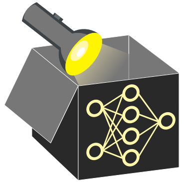

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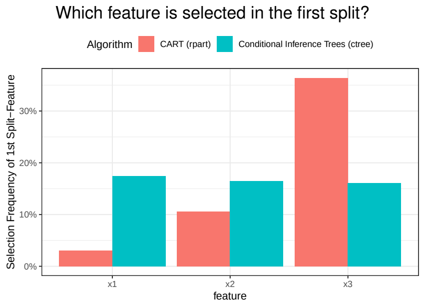

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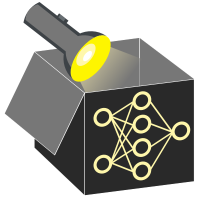

Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Parametric model (e.g. LM instead of constant) can be fitted in leave nodes
- Significance of split (p-value) given in each node
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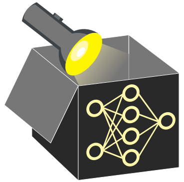

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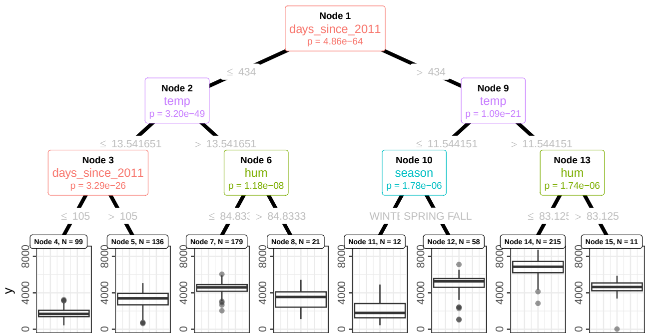


Train error (MSE):
758,844.0 (`ctree`)
742,244.4 (`mob`)



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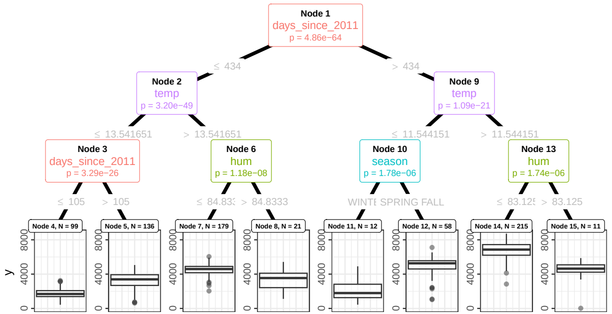
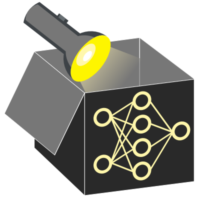


Train MSE:
758,844 (`ctree`)
742,244 (`mob`)

# UNBIASED RECURSIVE PARTITIONING



Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Parametric model (e.g. LM instead of constant) can be fitted in leave nodes
- Significance of split (p-value) given in each node
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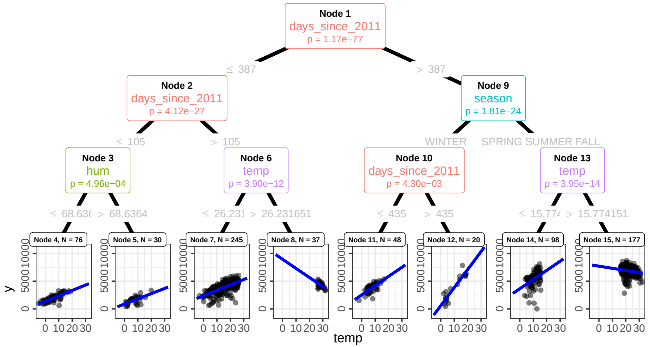
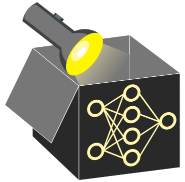
**Example** (`mob`): Bike data (linear model with `temp` in final nodes)




Train error (MSE):
758,844.0 (`ctree`)
742,244.4 (`mob`)



# UNBIASED RECURSIVE PARTITIONING



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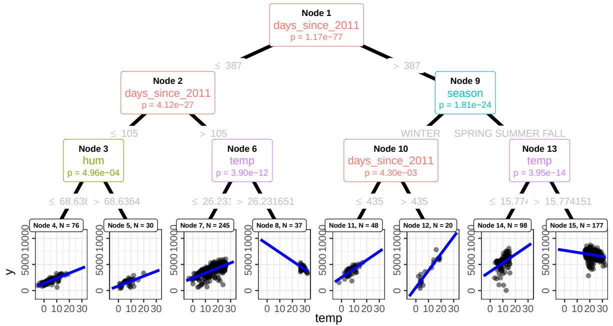


Train MSE:
758,844 (`ctree`)
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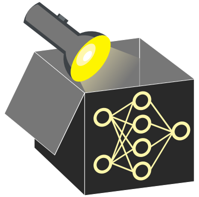
# OTHER RULE-BASED MODELS

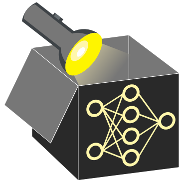


## Decision Rules ▸ Holte 1993

- Flat list of simple "if – then" statements
  ⇝ very intuitive and easy-to-interpret
- Mainly devised for classification
  (support for regression is limited)
- Numeric features are typically discretised

| | | |
|---|---|---|
| IF $x_1 \leq 2.3$ AND $x_4 = $ "A" | THEN | y = 1 |
| ELSE IF $x_2 > 5.0$ | THEN | y = 2 |
| ELSE | | y = 3 |





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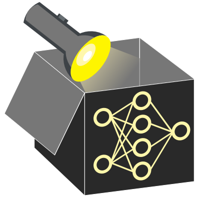
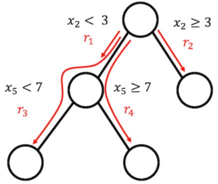


## RuleFit ▸ Friedman & Popescu 2008

- Extract binary rules $r_m(\mathbf{x}) \in \{0, 1\}$ from many shallow trees (one per root-to-leaf path)
- Fit an $L_1$-regularized LM
  $\hat{f}(\mathbf{x}) = \beta_0 + \sum_m \beta_m r_m(\mathbf{x}) + \sum_j \gamma_j x_j$
- Regularization retains only a few rules
  $\Rightarrow$ sparse, non-linear, interaction-aware
- Coefficients relate to rule/feature importance




▸ Molnar 2022

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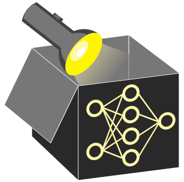


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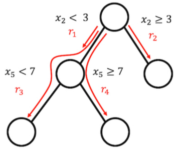


▸ Molnar 2022