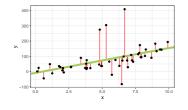
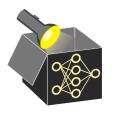
Interpretable Machine Learning

Extensions of Linear Regression Models



Learning goals

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



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: $\theta_{x_i^2} \cdot x_i^2$
- **interaction effects** as the product of multiple feat. \rightsquigarrow e.g., 2-way interaction: $\theta_{x_i,x_i} \cdot x_i \cdot x_i$

Bike Data		
Method	R^2	adj. <i>R</i> ²
Simple LM	0.85	0.84
High-order	0.87	0.87
Interaction	0.96	0.93



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: $\theta_{x_i^2} \cdot x_j^2$
- **interaction effects** as the product of multiple feat. \rightsquigarrow e.g., 2-way interaction: $\theta_{x_i,x_i} \cdot x_i \cdot x_i$

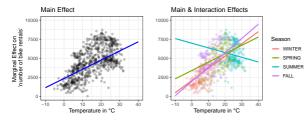
Bil	ke Data	
Method	R^2	adj. <i>R</i> 2
Simple LM	0.85	0.84
High-order	0.87	0.87
Interaction	0.96	0.93
•		

Implications of including high-order and interaction effects:

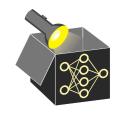
- Both make the model more flexible but also less interpretable
 → More weights to interpret
- Both need to be specified manually (inconvenient and sometimes infeasible)
 Other ML models learn them often automatically
- Marginal effect of a feature cannot be interpreted by single weights anymore
 → Feature x_i occurs multiple times (with different weights) in equation



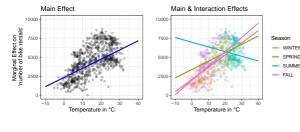
Example: Interaction between temp and season will affect marginal effect of temp



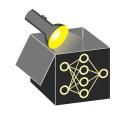
	Weights
(Intercept)	3453.9
seasonSPRING	1317.0
seasonSUMMER	4894.1
seasonFALL	-114.2
temp	160.5
hum	-37.6
windspeed	-61.9
days_since_2011	4.9
seasonSPRING:temp	-50.7
seasonSUMMER:temp	-222.0
seasonFALL:temp	27.2



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



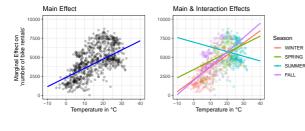
		Weights
	(Intercept)	3453.9
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	temp	160.5
	hum	-37.6
	windspeed	-61.9
	days_since_2011	4.9
	seasonSPRING:temp	-50.7
	seasonSUMMER:temp	-222.0
	seasonFALL:temp	27.2



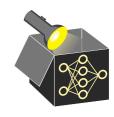
Interpretation: If temp increases by 1 °C, bike rentals

• increase by 160.5 in WINTER (reference)

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



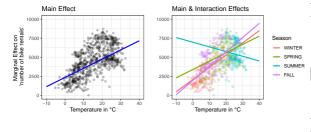
	Weights
(Intercept)	3453.9
seasonSPRING	1317.0
seasonSUMMER	4894.1
seasonFALL	-114.2
temp	160.5
hum	-37.6
windspeed	-61.9
days_since_2011	4.9
seasonSPRING:temp	-50.7
seasonSUMMER:temp	-222.0
seasonFALL:temp	27.2



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

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

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



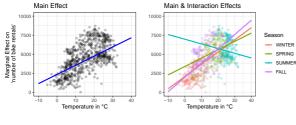
	Weights
(Intercept)	3453.9
seasonSPRING	1317.0
seasonSUMMER	4894.1
seasonFALL	-114.2
temp	160.5
hum	-37.6
windspeed	-61.9
days_since_2011	4.9
seasonSPRING:temp	-50.7
seasonSUMMER:temp	-222.0
seasonFALL:temp	27.2



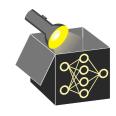
Interpretation: If temp increases by 1 °C, bike rentals

- increase by 160.5 in WINTER (reference)
- increase by 109.8 (= 160.5 50.7) in SPRING
- decrease by -61.5 (= 160.5 222) in SUMMER

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



		Weights
	(Intercept)	3453.9
	seasonSPRING	1317.0
R	seasonSUMMER	4894.1
G FR	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

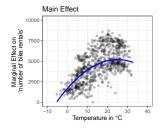


Interpretation: If temp increases by 1 °C, bike rentals

- increase by 160.5 in WINTER (reference)
- increase by 109.8 (= 160.5 50.7) in SPRING
- \bullet decrease by -61.5 (= 160.5 222) in SUMMER
- increase by 187.7 (= 160.5 + 27.2) in FALL

EXAMPLE: QUADRATIC EFFECT

Example: Adding quadratic effect for temp



Interpretation: Not linear anymore!

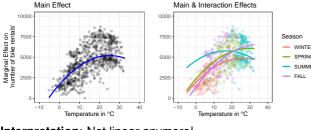
• temp depends on two weights: $280.2 \cdot x_{temp} - 5.6 \cdot x_{temp}^2$

	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



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
2	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:temp2

-11.3

Interpretation: Not linear anymore!

• temp depends on multiple weights due to season:

→ WINTER: 39.1 ·
$$x_{temp}$$
 + 8.6 · x_{temp}^2
→ SPRING: (39.1+407.4) · x_{temp} + (8.6-18.7) · x_{temp}^2
→ SUMMER:

$$(39.1+801.1) \cdot x_{temp} + (8.6-27.2) \cdot x_{temp}^2$$

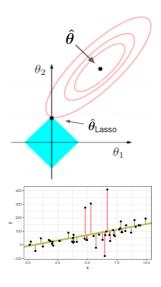
 $\rightsquigarrow \text{FALL:} (39.1+217.4) \cdot x_{temp} + (8.6-11.3) \cdot x_{temp}^2$



REGULARIZATION VIA LASSO Tibshirani (1996)

- LASSO adds an L₁-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 λ must be chosen (e.g., by CV)

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



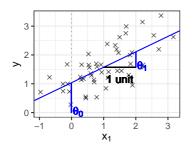


REGULARIZATION VIA LASSO Tibshirani (1996)



Example (interpretation of weights analogous to LM):

- LASSO with main effects and interaction temp with season
- λ is chosen \rightsquigarrow 6 selected features (\neq 0)
- LASSO shrinks weights of single categories separately (due to dummy encoding)
 - → No feature selection of whole categorical features (only w.r.t. category levels)
 - → 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
seasonSUMMER:temp	0.0
seasonFALL:temp	30.2

