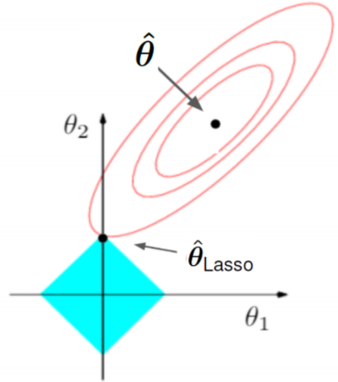
Interpretable Machine Learning

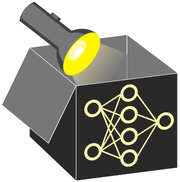
Extensions of Linear Regression Models



Learning goals

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

INTERACTION AND HIGH-ORDER EFFECTS



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

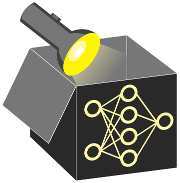
Equation above can be extended (polynomial regression) by including

- **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.
  $\rightsquigarrow$ e.g., 2-way interaction: $\theta_{x_i, x_j} \cdot x_i \cdot x_j$

Bike Data

Method	R^2	adj. R^2
Simple LM	0.85	0.84
High-order	0.87	0.87
Interaction	0.96	0.93

INTERACTION AND HIGH-ORDER EFFECTS



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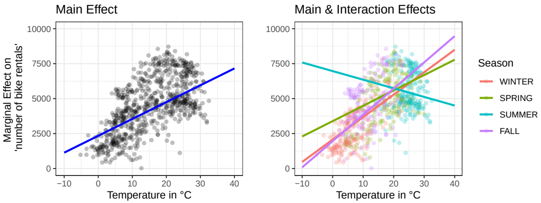
Implications of including high-order and interaction effects:

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

EXAMPLE: INTERACTION EFFECT

Ex.: 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

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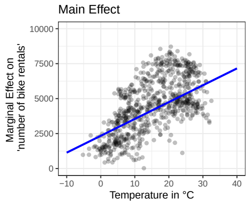

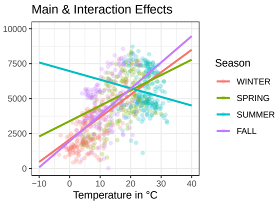

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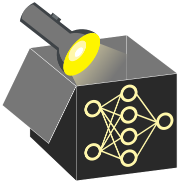

Interpretation: If `temp` increases by 1 °C, bike rentals

- increase by 160.5 in `WINTER` (reference)

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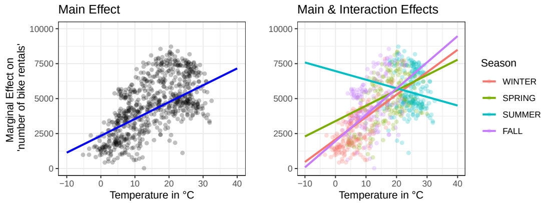

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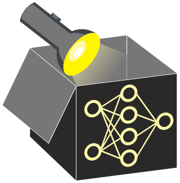
- increase by 160.5 in `WINTER` (reference)
- increase by 109.8 (= 160.5 - 50.7) in `SPRING`

EXAMPLE: INTERACTION EFFECT



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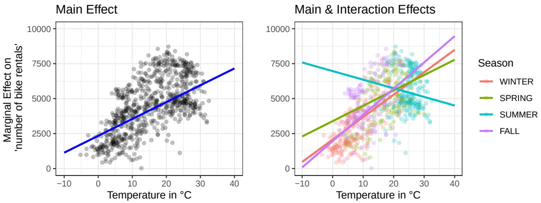

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- decrease by -61.5 (= 160.5 - 222) in `SUMMER`

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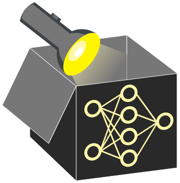

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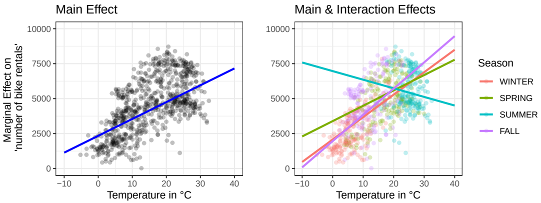

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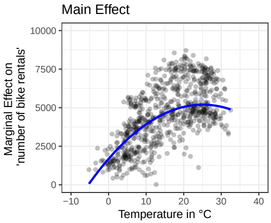
Interpretation: If `temp` increases by 1 °C,
bike rentals

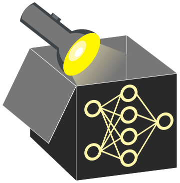
- increase by 160.5 in `WINTER` (reference)
- increase by 109.8 (= 160.5 - 50.7) in `SPRING`
- decrease by -61.5 (= 160.5 - 222) in `SUMMER`
- increase by 187.7 (= 160.5 + 27.2) in `FALL`

EXAMPLE: QUADRATIC EFFECT

Ex.: 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

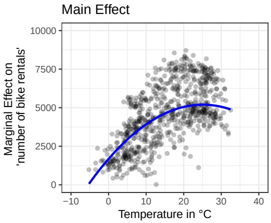


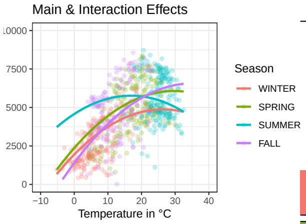
Interpretation: Not linear anymore!

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

EXAMPLE: QUADRATIC EFFECT

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



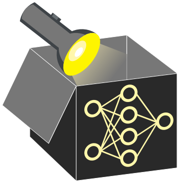


	Weights
(Intercept)	3802.1
seasonSPRING	-1345.1
seasonSUMMER	-6006.3
seasonFALL	-681.4
hum	-38.9
windspeed	-64.1
days_since_2011	4.8
temp	39.1
$temp^2$	8.6
seasonSPRING:temp	407.4
seasonSPRING:$temp^2$	-18.7
seasonSUMMER:temp	801.1
seasonSUMMER:$temp^2$	-27.2
seasonFALL:temp	217.4
seasonFALL:$temp^2$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

Interpretation: Not linear anymore!

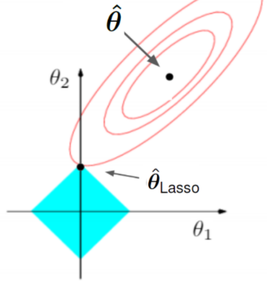
- `temp` depends on multiple weights due to `season`:
  $\leadsto$ `WINTER`:
  $39.1 \cdot x_{temp} + 8.6 \cdot x_{temp}^2$
  $\leadsto$ `SPRING`:
  $(39.1+407.4) \cdot x_{temp} + (8.6-18.7) \cdot x_{temp}^2$
  $\leadsto$ `SUMMER`:
  $(39.1+801.1) \cdot x_{temp} + (8.6-27.2) \cdot x_{temp}^2$
  $\leadsto$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

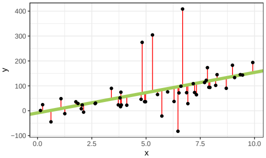
REGULARIZATION VIA LASSO ▸ TIBSHIRANI



- 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 λ must be chosen (e.g., by CV)

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

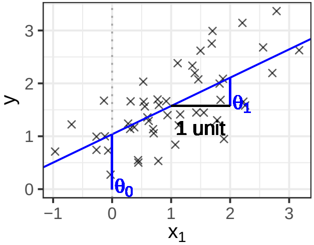




REGULARIZATION VIA LASSO ▸ TIBSHIRANI

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)
  $\rightsquigarrow$ 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
seasonSUMMER:temp	0.0
seasonFALL:temp	30.2