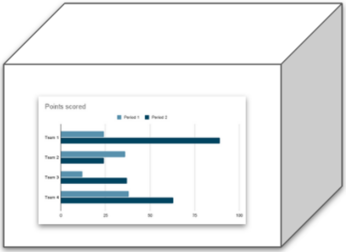
Interpretable Machine Learning

Linear Regression Model



Learning goals

- Interpretation of main effects in LM
- Inclusion of high-order and interaction effects
- Regularization via LASSO

LINEAR REGRESSION

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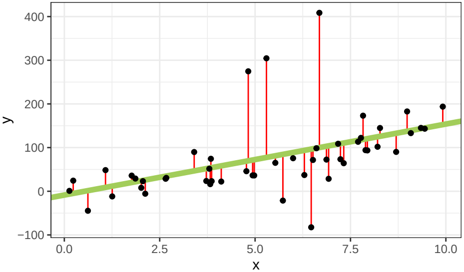

- y: target / output
- ϵ: remaining error / residual (e.g., due to noise)
- θ_j: weight of input feature x_j (with intercept θ_0)
  $\rightsquigarrow$ model consists of $p+1$ weights

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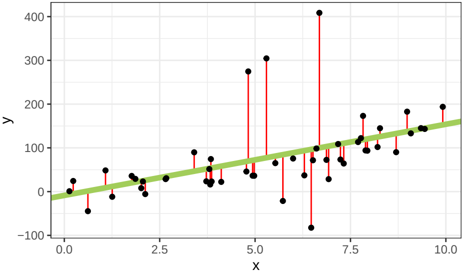

Properties and assumptions

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

- **Linear** relationship between features and target

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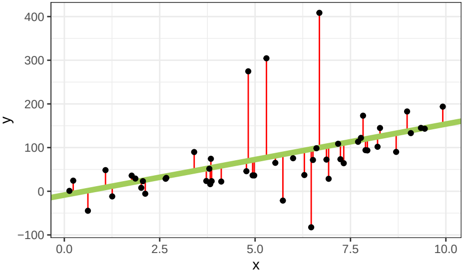

Properties and assumptions

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- ϵ and $y|\mathbf{x}$ are **normally** distributed with **constant variance** (homoscedastic)
  $\rightsquigarrow \epsilon \sim N(0, \sigma^2) \;\Rightarrow\; (y|\mathbf{x}) \sim N(\mathbf{x}^\top\theta, \sigma^2)$
  $\rightsquigarrow$ if violated, inference-based metrics (e.g., p-values) are invalid

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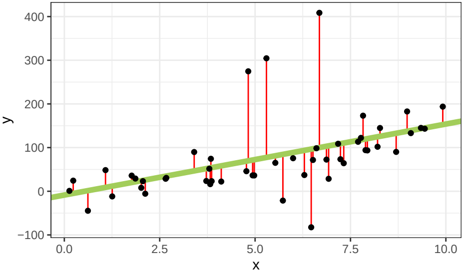

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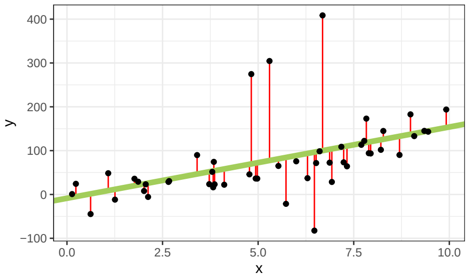

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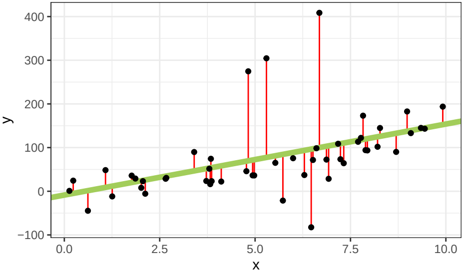

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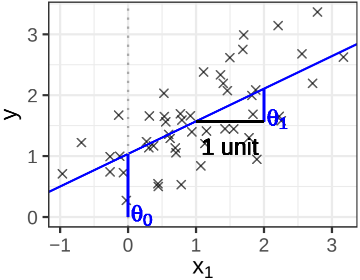
  $\leadsto$ if violated, inference-based metrics (e.g., p-values) are invalid
- Independence of observations (e.g., no repeated measurements)
- Independence of features x_j with error term ϵ
- No or little multicollinearity (i.e., no strong feature correlations)

LINEAR REGRESSION - INTERPRETATION

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p + \epsilon = \mathbf{x}^\top \theta + \epsilon$$

Interpretation of weights (**feature effects**) depend on type of feature:

- **Numerical** x_j: Increasing x_j by one unit changes outcome by θ_j, ceteris paribus (c.p.) (*ceteris paribus* means "everything else held constant".)



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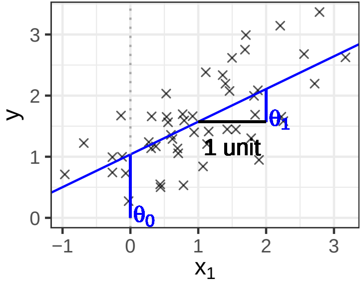

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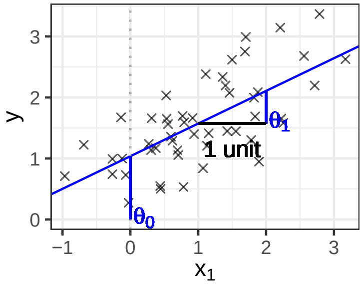
- **Categorical** x_j **with** L **categories**: Create $L - 1$ one-hot-encoded features $x_{j,1}, \ldots, x_{j,L-1}$ (each having its own weight), left out category is reference ($\hat{=}$ dummy encoding)
  $\rightsquigarrow$ Interpretation: Outcome changes by $\theta_{j,l}$ for category l compared to reference cat., c.p.



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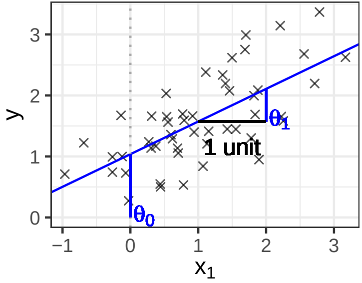
- **Intercept** θ_0: Expected outcome if all feature values are set to 0



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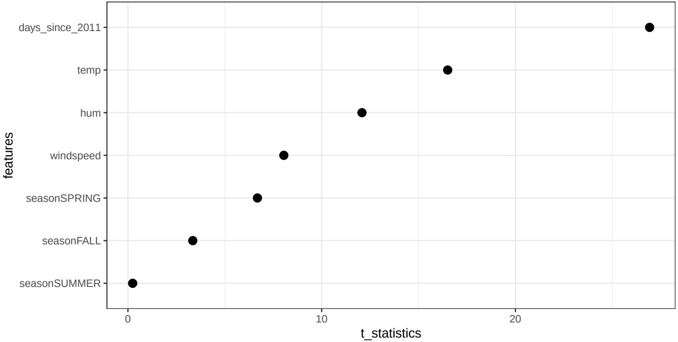
Feature importance:

- Absolute t-statistic value: $\hat{\theta}_j$ scaled with its standard error ($SE(\hat{\theta}_j) \hat{=}$ reliability of the estimate)

$$|t_{\hat{\theta}_j}| = \left| \frac{\hat{\theta}_j}{SE(\hat{\theta}_j)} \right|$$

- High values indicate important (i.e. significant) features



EXAMPLE: LINEAR REGRESSION - MAIN EFFECTS

Bike data: predict number of rented bikes using 4 numeric and 1 categorical feature (season)

$$\hat{y} = \hat{\theta}_0 + \hat{\theta}_1 \mathbb{1}_{x_{season}=SPRING} + \hat{\theta}_2 \mathbb{1}_{x_{season}=SUMMER} + \hat{\theta}_3 \mathbb{1}_{x_{season}=FALL} + \hat{\theta}_4 x_{temp} + \hat{\theta}_5 x_{hum} + \hat{\theta}_6 x_{windspeed} + \hat{\theta}_7 x_{days\_since\_2011}$$

	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
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- **Interpretation categorical**: Rentals in `SPRING` are by $\hat{\theta}_1 = 862$ higher than in `WINTER`, c.p.
- **Interpretation numerical**: Rentals increase by $\hat{\theta}_4 = 120.5$ if `temp` increases by 1 °C, c.p.

LINEAR REGRESSION - INTERACTION AND HIGH-ORDER EFFECTS

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

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
Higher-order	0.87	0.87
Interaction	0.96	0.93

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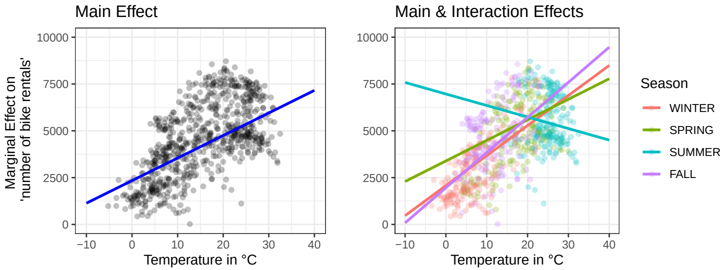
Implications of including high-order and interaction effects:

- 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)
  $\rightsquigarrow$ Other ML models learn them often automatically
- Marginal effect of a feature cannot be interpreted by single weights anymore
  $\rightsquigarrow$ Feature x_j occurs multiple times (with different weights) in equation

EXAMPLE: LINEAR REGRESSION - INTERACTION EFFECT

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



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seasonSUMMER	4894.1
seasonFALL	-114.2
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hum	-37.6
windspeed	-61.9
days_since_2011	4.9
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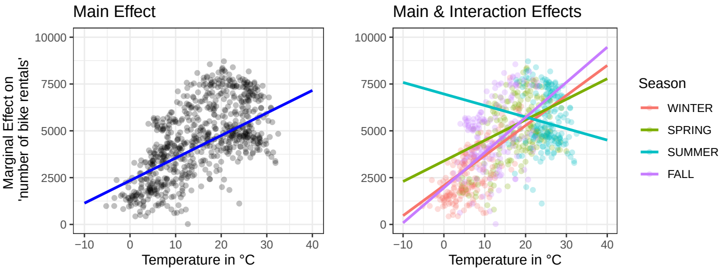

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Interpretation: If `temp` increases by 1 °C, bike rentals

- increase by 160.5 in `WINTER` (reference)

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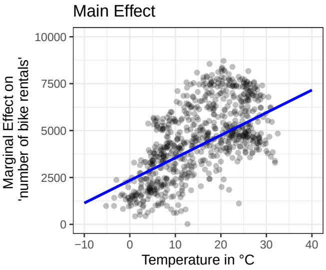

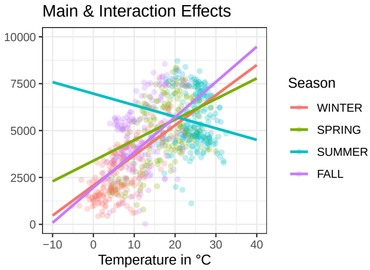

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Interpretation: If `temp` increases by 1 °C, bike rentals

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

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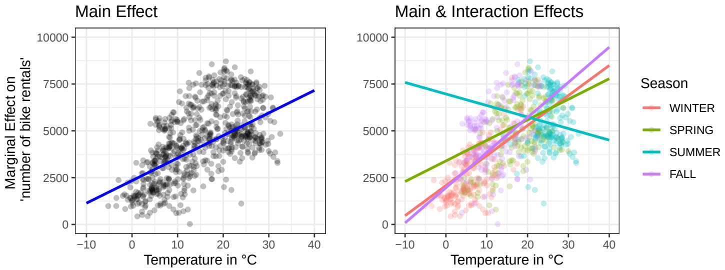

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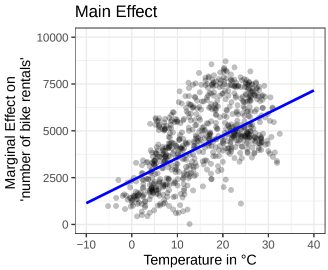
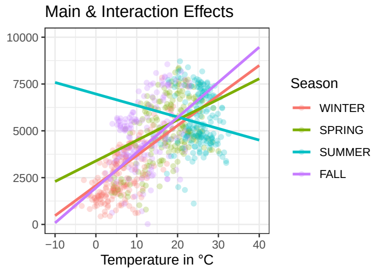
Interpretation: If `temp` increases by 1 °C, bike rentals

- 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`

EXAMPLE: LINEAR REGRESSION - INTERACTION EFFECT

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





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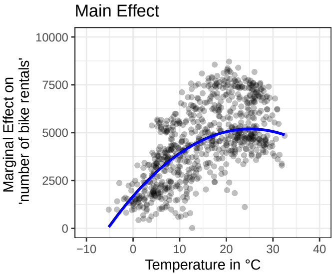
Interpretation: If `temp` increases by 1 °C, bike rentals

- 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: LINEAR REGRESSION - QUADRATIC EFFECT

Example: Adding quadratic effect for `temp`



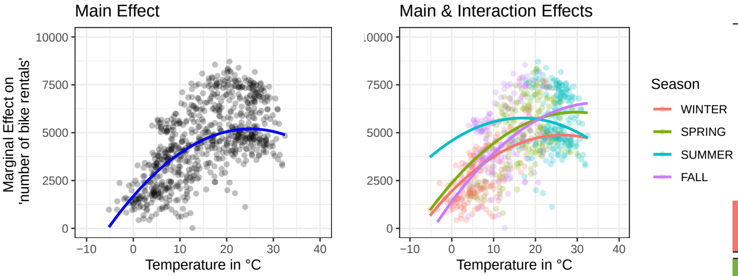
	Weights
(Intercept)	3094.1
seasonSPRING	619.2
seasonSUMMER	284.6
seasonFALL	123.1
hum	-36.4
windspeed	-65.7
days_since_2011	4.7
temp	280.2
temp^2	-5.6

Interpretation: Not linear anymore!

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

EXAMPLE: LINEAR REGRESSION - QUADRATIC EFFECT

Example: Adding quadratic effect for `temp` (left) and an 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

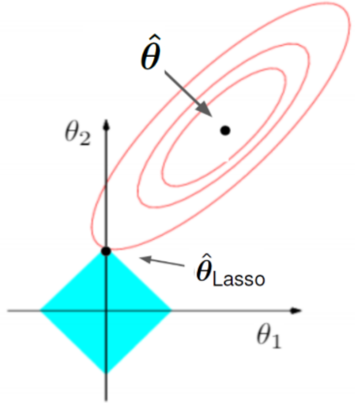
Interpretation: Not linear anymore!

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

REGULARIZATION VIA LASSO ▸ Tibshirani (1996)

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

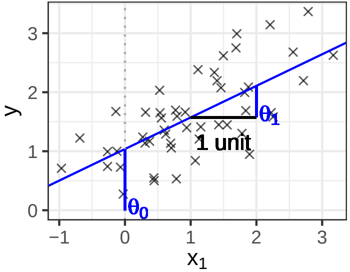
$$min_\theta \left(\underbrace{\frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \mathbf{x}^{(i)\top}\theta)^2}_{\text{Least square estimate for LM}} + \lambda||\theta||_1 \right)$$



REGULARIZATION VIA LASSO ▸ Tibshirani (1996)

Example (interpretation of weights analogous to LM):

- LASSO with main effects and interaction `temp` with `season`
- λ is chosen such that 6 features are selected (not zero)
- For categorical features, LASSO shrinks weights of single categories separately (due to dummy encoding)
  $\rightsquigarrow$ No feature selection of whole categorical features
  $\rightsquigarrow$ 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