

INTRODUCTION



TO STATISTICAL LEARNING

Introduction to Statistical Learning

Linear Models - Part B - Class 4

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Extending the linear model

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Categorical features with k levels

When $k = 2$:

- If x indicates whether person “has tattoos” or “no tattoos”
- Define: $x_i = \begin{cases} 1 & \text{if person } i \text{ has tattoos,} \\ 0 & \text{otherwise.} \end{cases}$
- Model: $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$
- Meaning: $\beta_0 = E(y|\text{no tattoos})$ $\beta_1 = E(y|\text{has tattoos}) - E(y|\text{no tattoos})$

 Question: how would you test if “tattoo” has effect on y ?

 Question: what if $x_i = \begin{cases} 1 & \text{if person } i \text{ has tattoos} \\ -1 & \text{otherwise.} \end{cases}$

Categorical features with k levels: $k > 2$

- If x is a person's profession (carpenter, gardener, or teacher)

(i)

Question: what if we just had $x_i = \begin{cases} 0 & \text{if person } i \text{ is a teacher} \\ 1 & \text{if person } i \text{ is a carpenter} \\ 2 & \text{if person } i \text{ is a gardener} \end{cases}$

- Define $k - 1$ indicators:

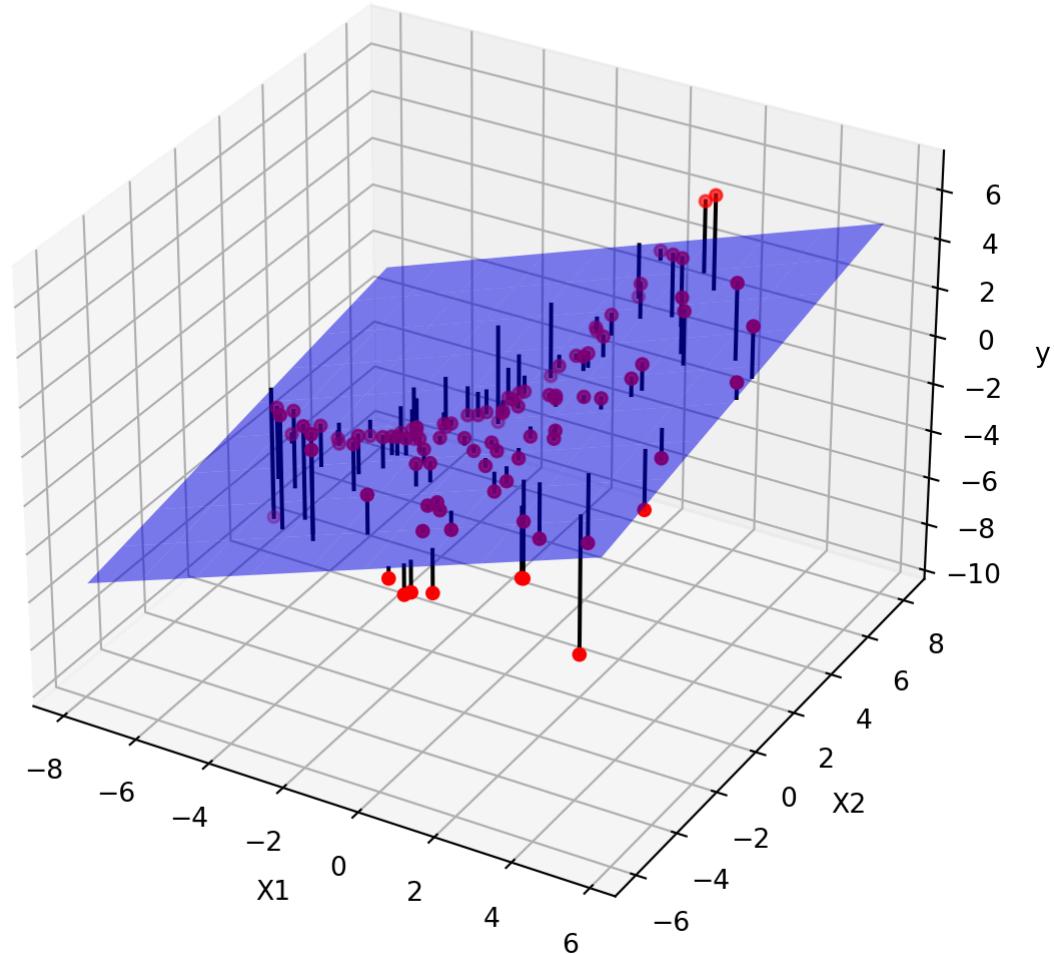
$$x_{i1} = \begin{cases} 1 & \text{if person } i \text{ is a carpenter,} \\ 0 & \text{otherwise.} \end{cases}, x_{i2} = \begin{cases} 1 & \text{if person } i \text{ is a gardener,} \\ 0 & \text{otherwise.} \end{cases}$$

- Why $k - 1$ indicators?
- Model: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \varepsilon_i$
- Meaning:
 $\beta_1 = E(y|\text{carpenter}) - E(y|\text{teacher}); \quad \beta_2 = E(y|\text{gardener}) - E(y|\text{teacher})$

(i)

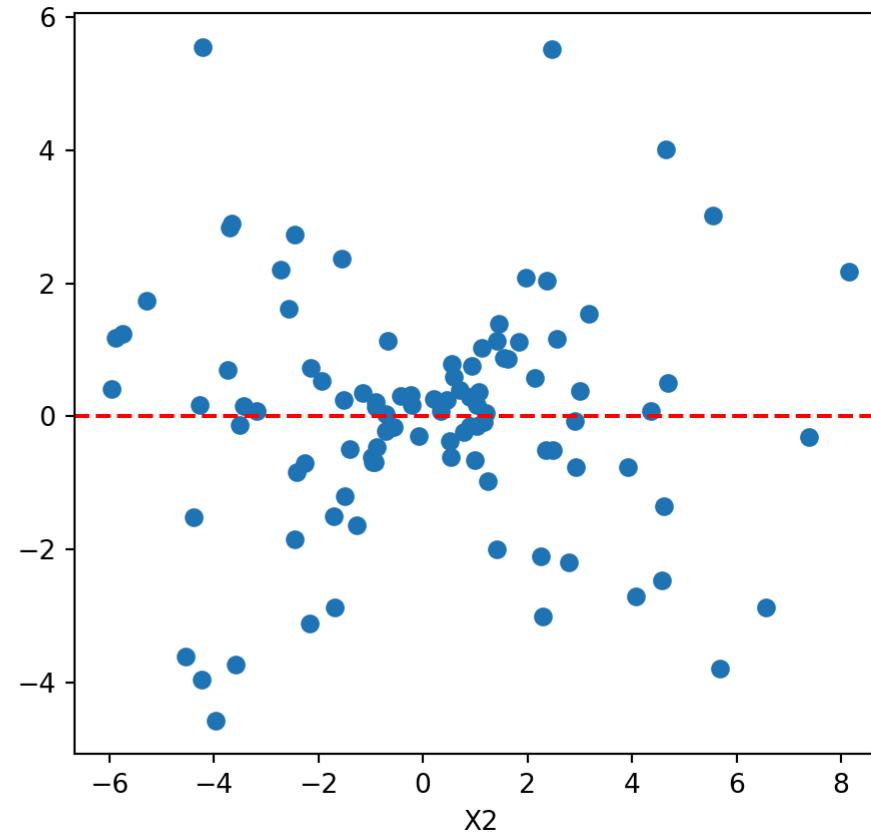
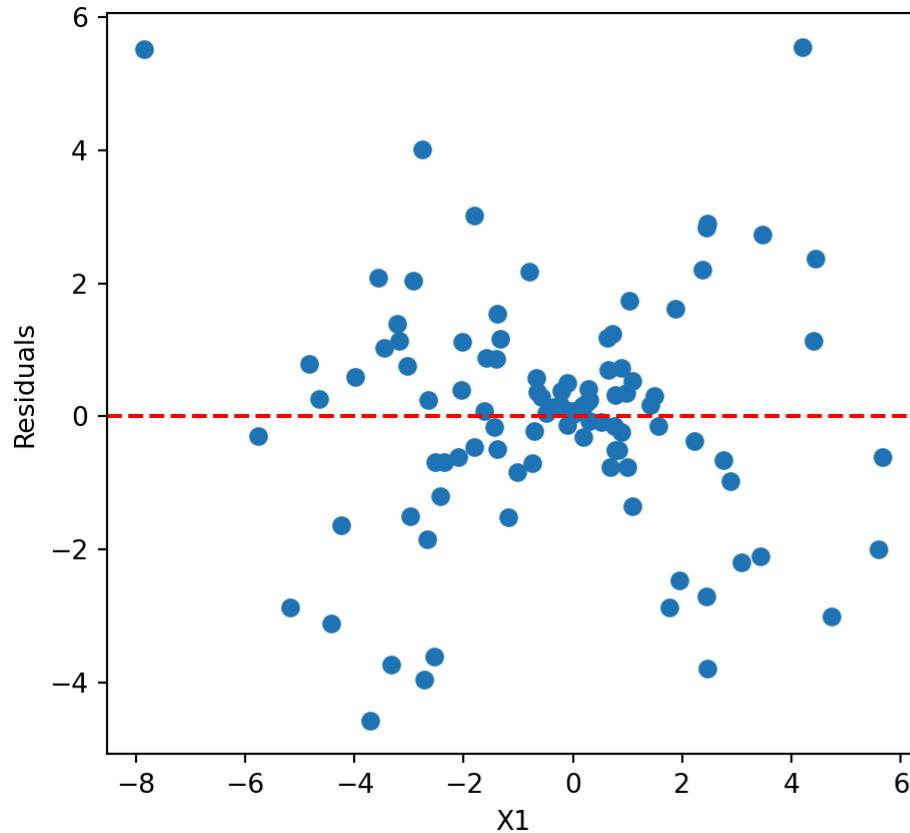
Question: how would you test if "profession" has effect on y ?

Interactions



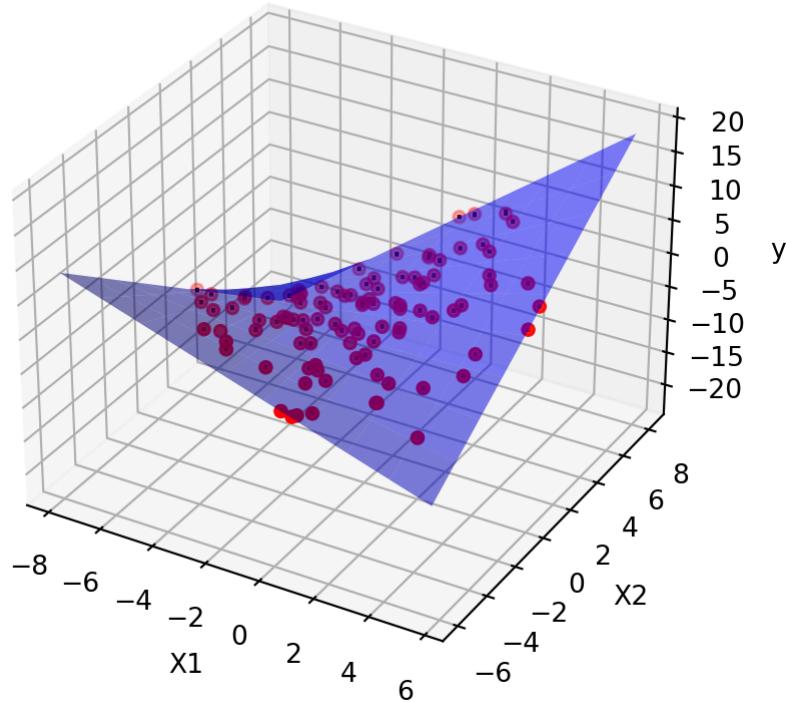
A multiplicative effect?

Interactions: residuals plots



Consider adding an interaction term to the model: $x_1 \cdot x_2$

Interactions: adding an interaction term

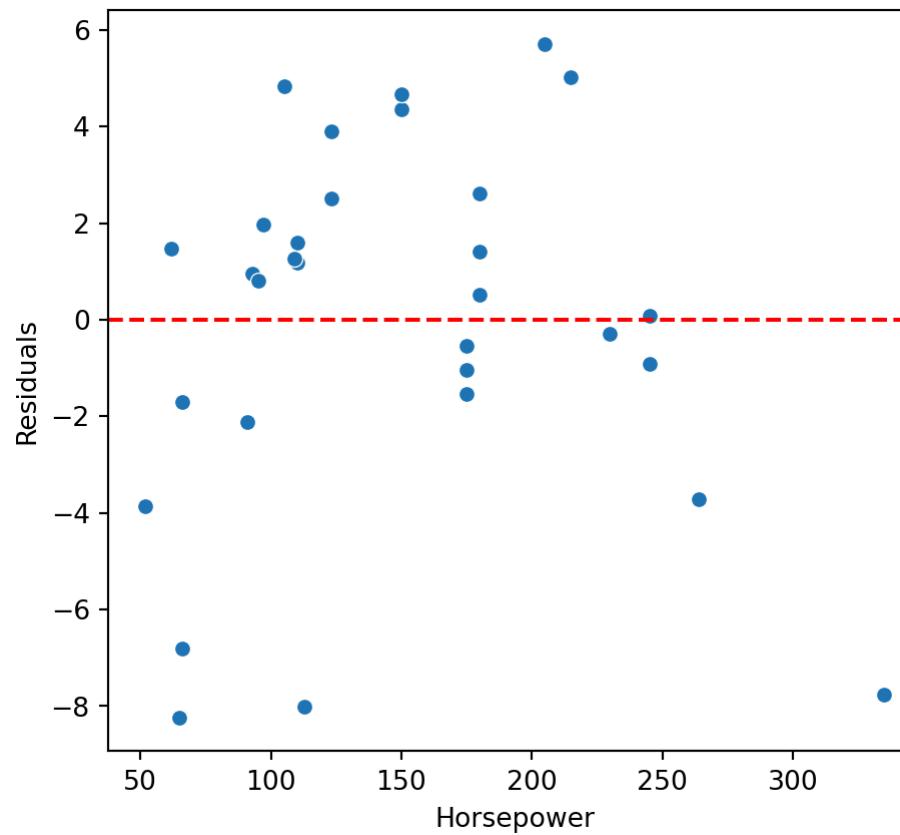
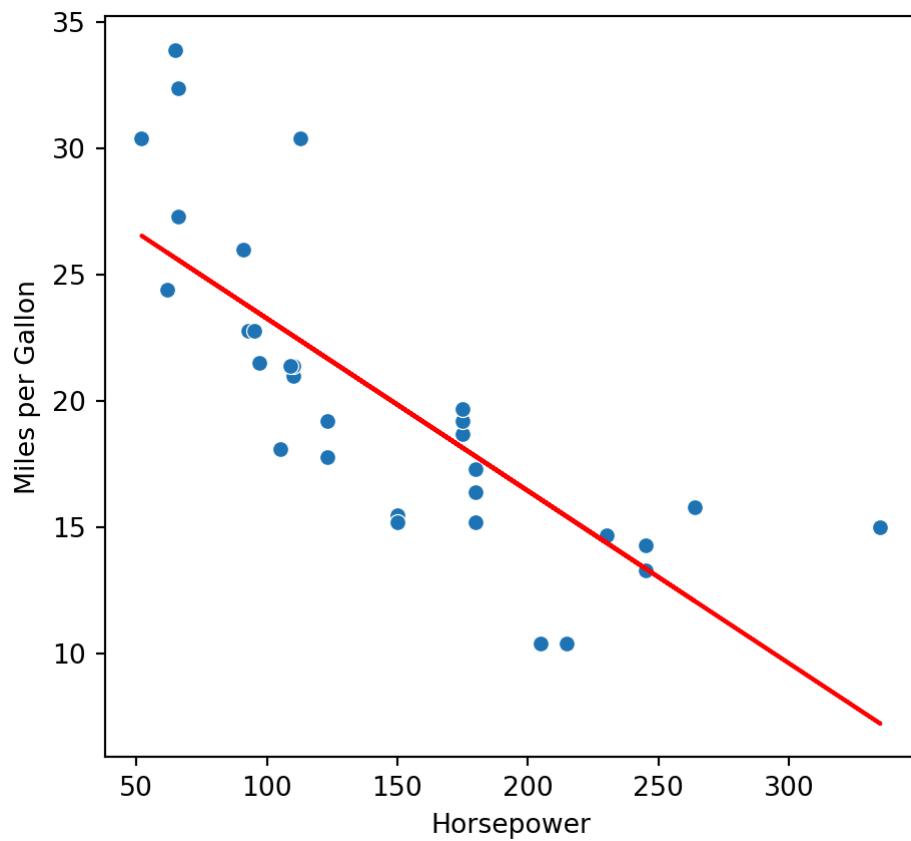


$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i1} + \beta_3 x_{i1} \cdot x_{i2} + \varepsilon_i$$



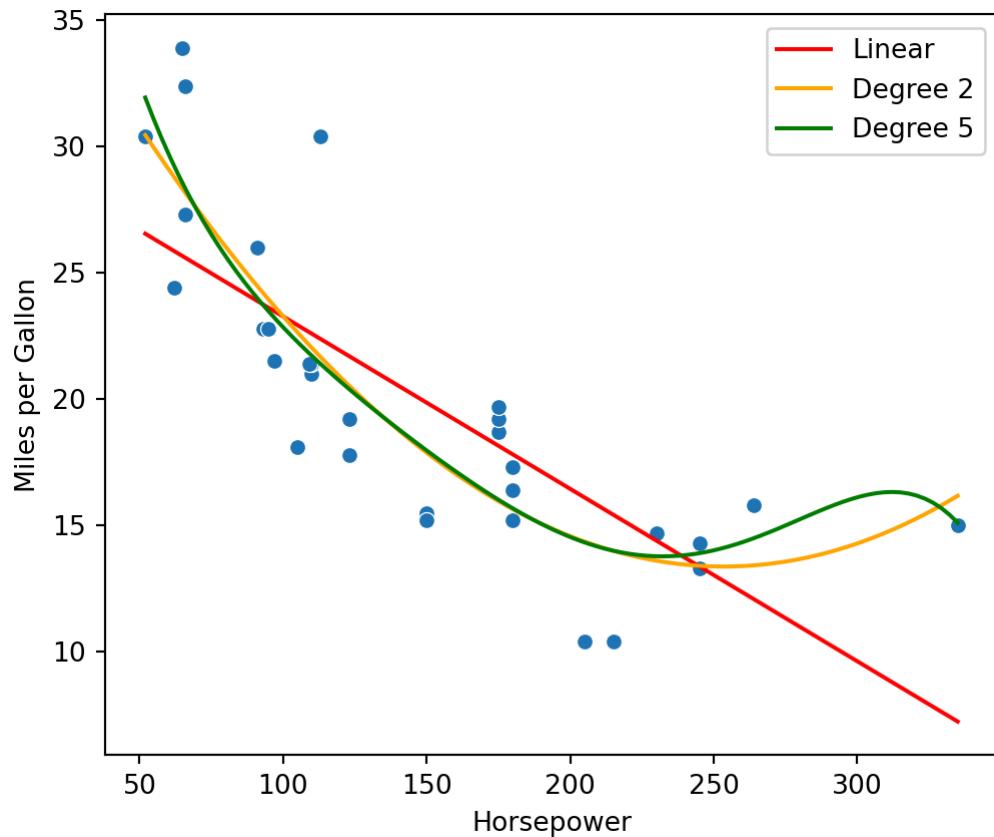
Note: in multiplicative models we usually add the features without interactions to the model (“main effects”), even if their P-value is not small.

Non-linear relations



Consider adding polynomial terms x_1^2, x_1^3, \dots

Plynomial regression: Beware 1



Plynomial regression: Beware 1

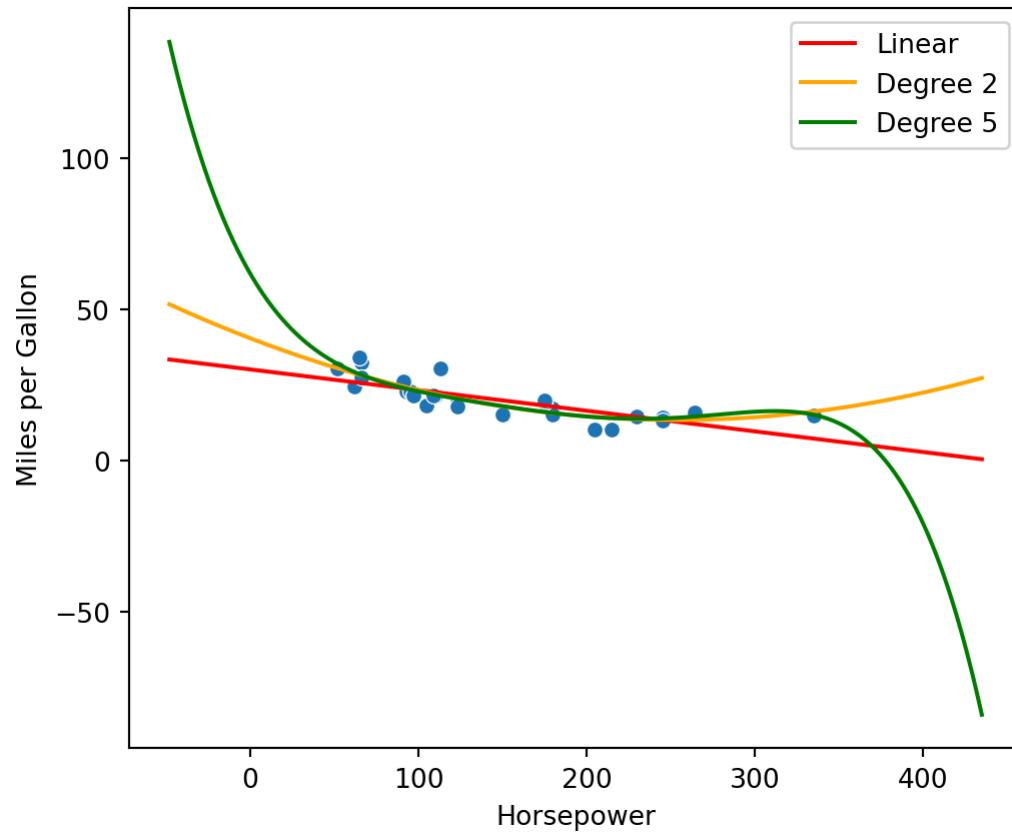
Quadratic:

	coef	std err	t	P> t	[0.025	0.975]
const	40.4091	2.741	14.744	0.000	34.804	46.015
x1	-0.2133	0.035	-6.115	0.000	-0.285	-0.142
x2	0.0004	9.84e-05	4.275	0.000	0.000	0.001

Cubic:

	coef	std err	t	P> t	[0.025	0.975]
const	44.2249	5.961	7.419	0.000	32.015	56.435
x1	-0.2945	0.118	-2.500	0.019	-0.536	-0.053
x2	0.0009	0.001	1.328	0.195	-0.000	0.002
x3	-8.701e-07	1.2e-06	-0.722	0.476	-3.34e-06	1.6e-06

Plynomial regression: Beware 2



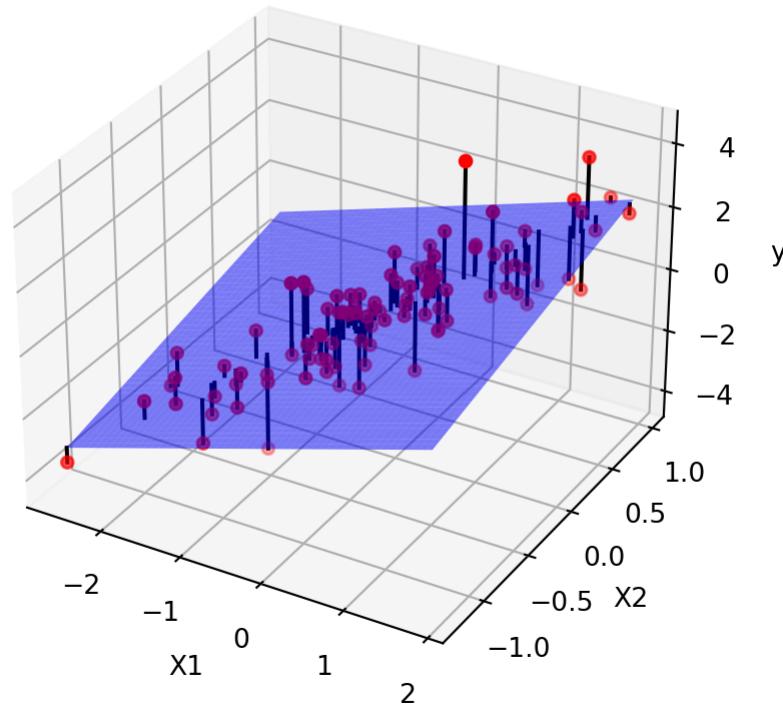
Other issues with linear regression

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Why “not significant”?



	coef	std err	t	P> t	[0.025	0.975]
const	0.0886	0.108	0.819	0.415	-0.126	0.303
X1	0.7875	0.568	1.386	0.169	-0.340	1.915
X2	0.8772	1.144	0.767	0.445	-1.393	3.147

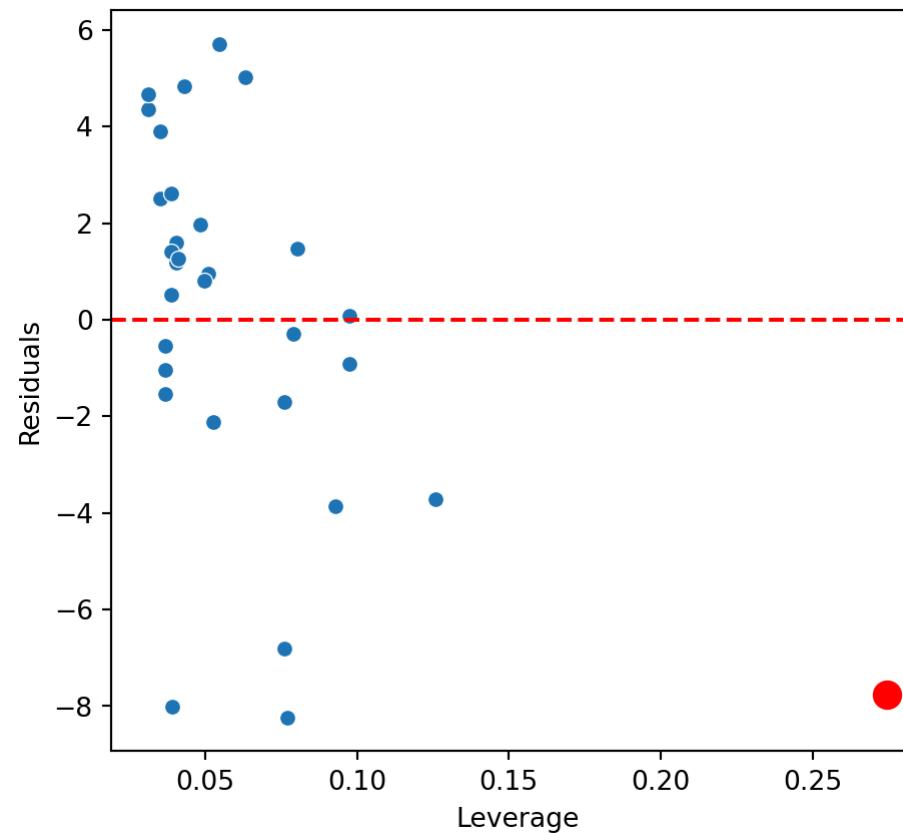
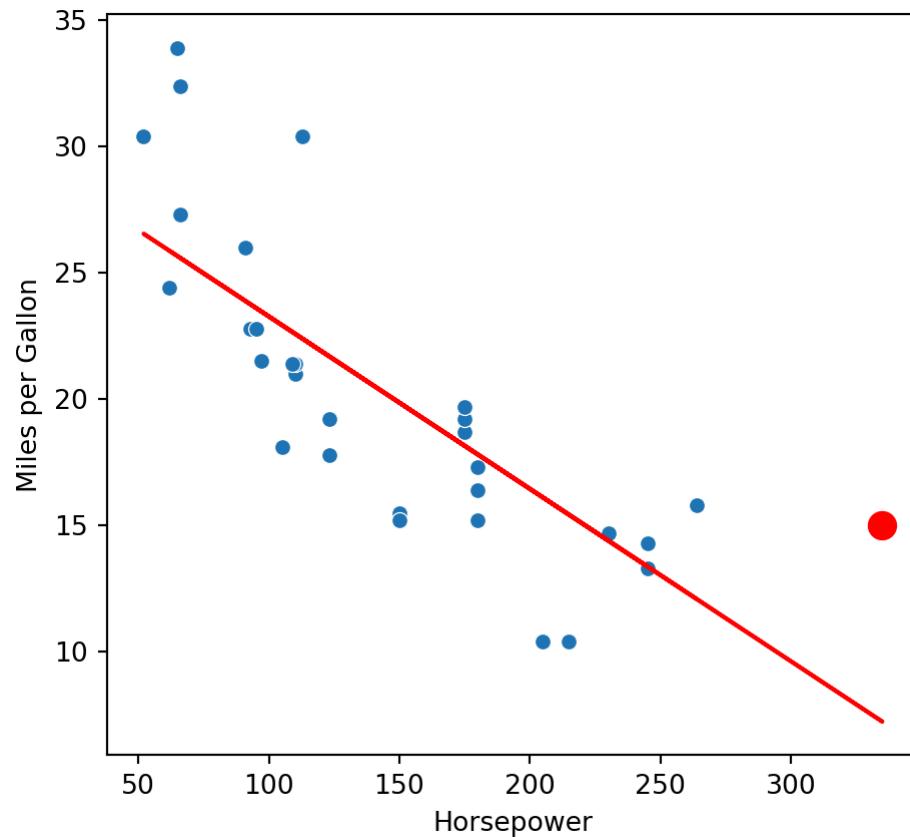
Collinearity

- Collinearity is when a feature is in the span of other features
- Usually it is not exactly in the span but near the span
- In the case of exact collinearity: the matrix $X^T X$ is singular, no unique solution
- In the case of approximate collinearity:
 - If $X_1 \approx X_2$, then:
 $y = X_1; \quad y = X_2; \quad y = \frac{1}{2}X_1 + \frac{1}{2}X_2; \quad y = 1000X_1 - 999X_2$ are the same models!
 - the solution is not numerically stable
 - $SE(\hat{\beta})$ grows, t_{obs} value decreases, feature is “masked” in inference
- Explore your data with a correlation matrix, many other metrics

High-leverage and Outlier observations

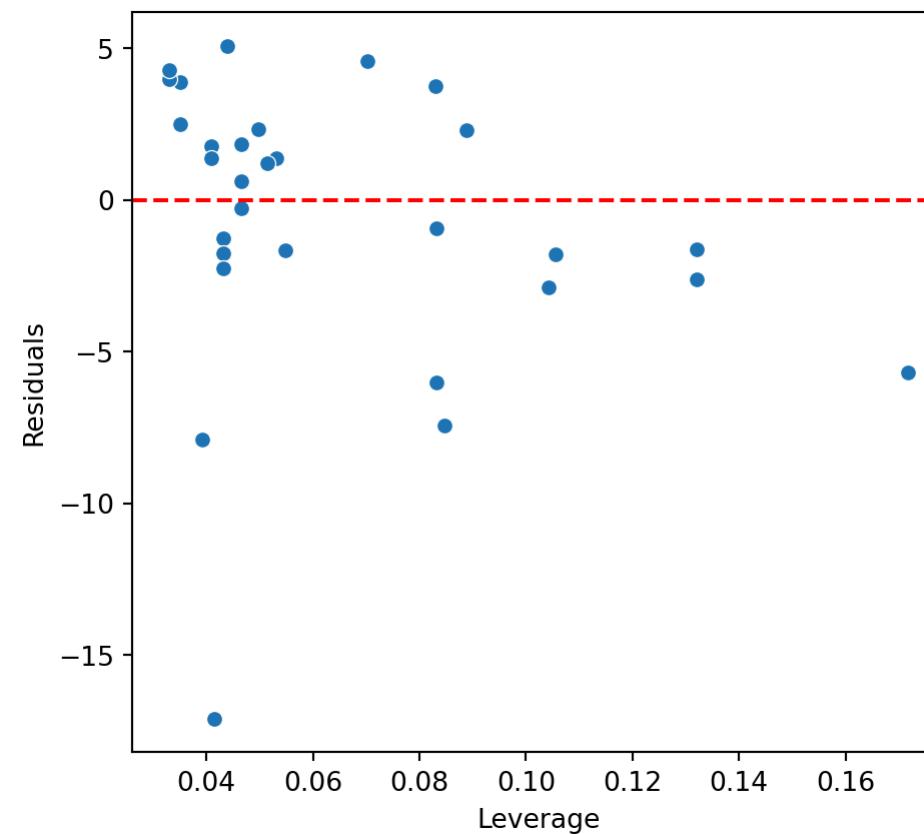
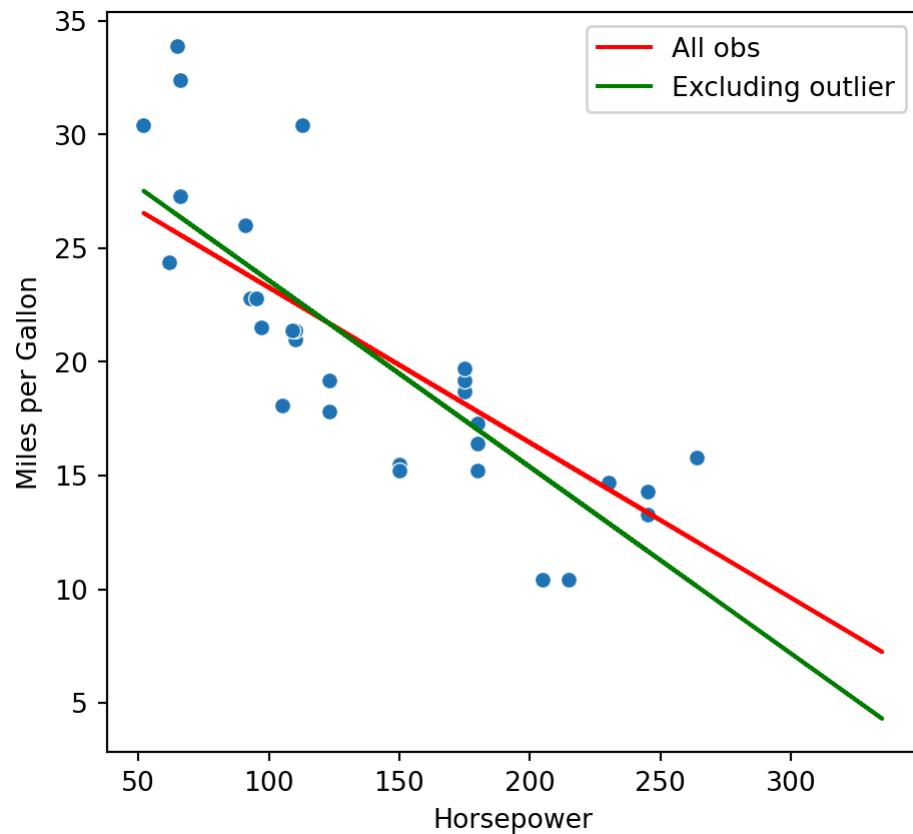
- An observation with high leverage has an extreme x value
- For simple linear regression: $h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum(x_i - \bar{x})^2}$
- Observations with large $h_i \Rightarrow$ large effect on $SE(\hat{\beta})$
- If such an observation also has an unusual y – an outlier \Rightarrow the model changes a lot if removed

High-leverage and Outlier observations



Consider removing (careful!).

Excluding high-leverage + outlier



Logistic Regression

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What about classification?

- Let's start with the simplest (and most important) case of two-class classification:
 - Sick vs. healthy
 - Buy vs. won't buy
 - Dog vs. cat
- As before, we have $T = (\mathbf{X}, \mathbf{y})$ a sample of size n
- For now, keep assuming $x \in \mathbb{R}^p$ is numeric
- Can we use the OLS mechanism we have built to build a classification model?
- For sure we can, if we encode $y = \text{sick} \Rightarrow y = 1$, $y = \text{healthy} \Rightarrow y = 0$, we have numeric y

What is wrong with using OLS for classification?

- If we encode y as above what is $E(y|x)$? It is $P(y = \text{sick} | \text{data})$ — a clearly interesting quantity
- Problem: as a probability, $0 \leq P(y = \text{sick} | \text{data}) \leq 1$. But model predictions $x^T \hat{\beta}$ can fall outside the legal range!
- Another problem: can we make the model assumptions of normal ε ? No — because y can only be 0 or 1
- The idea: try to create an approach that is similar to OLS, but more fitting for classification, taking into account the limited range of values and the need for a sensible statistical model

Logistic regression

- Deals with the two problems above
- We start from assuming a model:

$$\log \frac{P(y = 1|x)}{P(y = 0|x)} = \log \frac{P(y = 1|x)}{1 - P(y = 1|x)} = \text{logit}(P(y = 1|x)) = x^T \beta$$

- Notice that now all values are legal:

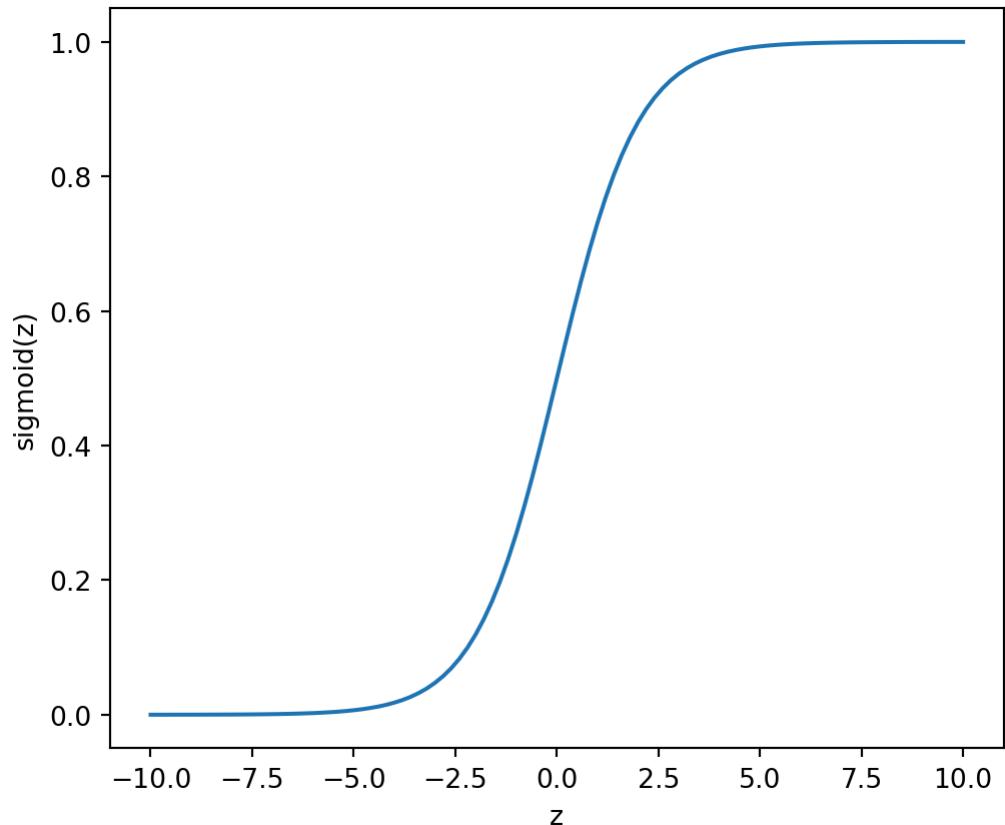
$$0 \leq P(y = 1|x) \leq 1 \Leftrightarrow -\infty \leq \log \frac{P(y = 1|x)}{P(y = 0|x)} \leq \infty.$$

The Sigmoid function

Another way of writing this:

$$P(y = 1|x) = \text{sigmoid}(x^T \beta) = \frac{\exp(x^T \beta)}{1 + \exp(x^T \beta)}$$

$$P(y = 0|x) = 1 - P(y = 1|x) = \frac{1}{1 + \exp(x^T \beta)}$$



Fitting a logistic regression

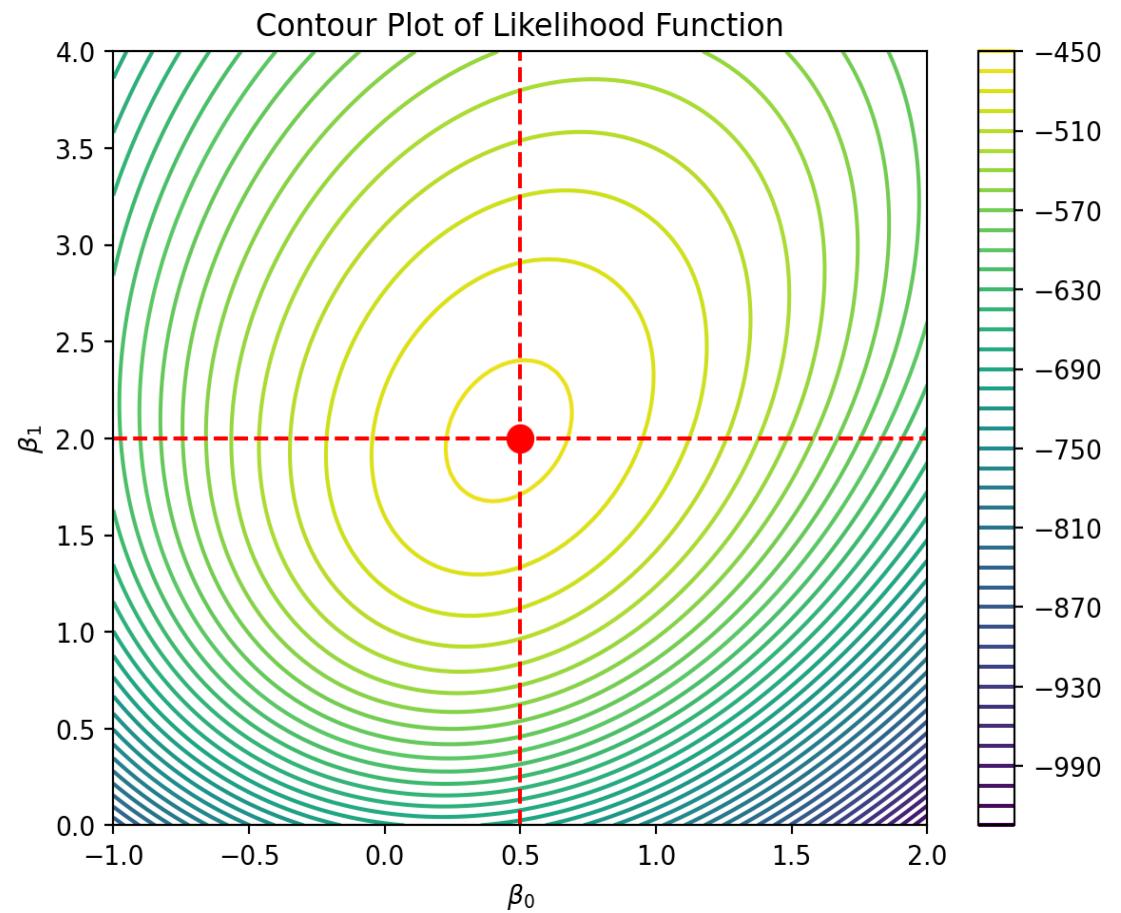
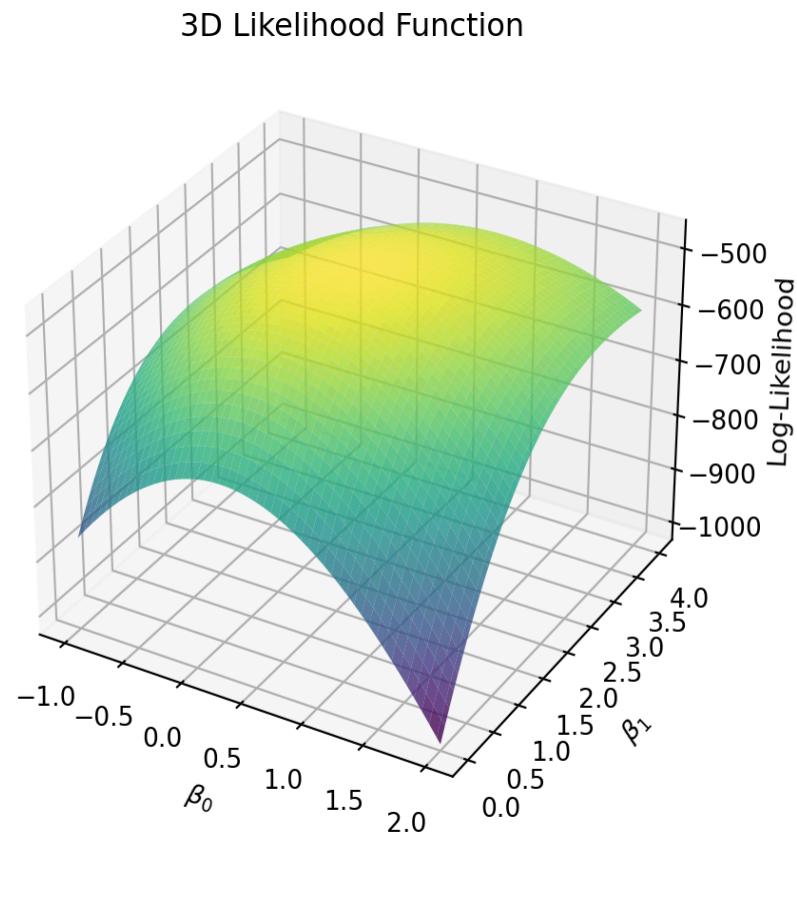
- Given training data T , we want to find the best coefficients $\hat{\beta}$
- This is done by maximum likelihood, finding β to maximize:

$$L(\beta|X, y) = \prod_{i=1}^n P(y_i|x_i; \beta) = \prod_{i=1}^n P(y_i = 1|x_i; \beta)^{y_i} P(y_i = 0|x_i; \beta)^{1-y_i}$$

$$\max_{\beta} \prod_{i=1}^n \left(\frac{\exp(x_i^T \beta)}{1 + \exp(x_i^T \beta)} \right)^{y_i} \left(\frac{1}{1 + \exp(x_i^T \beta)} \right)^{1-y_i}$$

- The solution is $\hat{\beta}$, the logistic regression coefficients estimates

Logistic Regression Likelihood



Prediction and interpretation of coefficients

- Predicting on $x \in Te$:

$$P(\widehat{y=1}|x) = \frac{\exp(x^T \hat{\beta})}{1 + \exp(x^T \hat{\beta})} \Rightarrow \hat{y} = \begin{cases} 1 & \text{if } P(\widehat{y=1}|x) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

- We can write our model as:

$$\log \frac{P(y=1|x)}{P(y=0|x)} = x^T \beta$$

- The expression on the left is called the *log odds*: log of the ratio of “positive” vs “negative” probability
- Interpretation: β_j is the change in the log odds from a change of 1 unit in x_j .
- For example, if $\beta_j = 1$ then when $x_j = 1$ vs $x_j = 0$ the log odds increase by 1, and the odds increase **times** $e = 2.72$

Example: SAHeart

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Example: South African Hearth Disease Data

```

      sbp  tobacco   ldl  adiposity famhist typea  obesity alcohol \
row.names
1       160     12.00  5.73    23.11 Present    49   25.30  97.20
2       144      0.01  4.41    28.61 Absent     55   28.87   2.06
3       118      0.08  3.48    32.28 Present    52   29.14   3.81
4       170      7.50  6.41    38.03 Present    51   31.99  24.26
5       134     13.60  3.50    27.78 Present    60   25.99  57.34

      age   chd
row.names
1       52     1
2       63     1
3       46     0
4       58     1
5       49     1

```

No. of train rows: 369, no. train of cols: 9

No. of test rows: 93, no. test of cols: 9

no. of obs in train y: 369

no. of obs in test y: 93

SAHeart: LR with statsmodels

Optimization terminated successfully.

Current function value: 0.513971

Iterations 6

Logit Regression Results

Dep. Variable:	chd	No. Observations:	369			
Model:	Logit	Df Residuals:	359			
Method:	MLE	Df Model:	9			
Date:	Wed, 06 Nov 2024	Pseudo R-squ.:	0.1994			
Time:	17:15:45	Log-Likelihood:	-189.66			
converged:	True	LL-Null:	-236.90			
Covariance Type:	nonrobust	LLR p-value:	2.041e-16			
	coef	std err	z	P> z	[0.025	0.975]
const	-5.3373	1.478	-3.612	0.000	-8.234	-2.441
sbp	0.0081	0.006	1.262	0.207	-0.004	0.021
tobacco	0.0563	0.029	1.926	0.054	-0.001	0.114
ldl	0.1676	0.064	2.599	0.009	0.041	0.294
adiposity	0.0273	0.033	0.823	0.411	-0.038	0.092
typea	0.0411	0.014	3.005	0.003	0.014	0.068
obesity	-0.0820	0.049	-1.661	0.097	-0.179	0.015

SAHeart: LR Test Performance

	pred:no	pred:yes
true:no	52	7
true:yes	15	19

Accuracy: 0.76, Misclassification loss: 0.24

Classification Model Evaluation

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Measuring Classification Performance

- Different errors have different costs/value.
- Summarize performance in different ways that capture different types of errors:

		Pred		
Real	Pos	Neg	Total	
Pos	TP	FN	P	
Neg	FP	TN	N	
Total	\hat{P}	\hat{N}		

$P = \sum_{i=n+1}^{n+m} y_i$ number of positive examples, similarly N .

$\hat{P} = \sum_{i=n+1}^{n+m} \hat{y}_i$ number of positive predictions, similarly \hat{N} .

$TP = \sum_{i=n+1}^{n+m} y_i \hat{y}_i$ number of true positives, $FP = \hat{P} - TP$

$TN = \sum_{i=n+1}^{n+m} (1 - y_i)(1 - \hat{y}_i)$ number of true negatives, $FN = \hat{N} - TN$

		Pred		
Real	Pos	Neg	Total	
Pos	TP	FN	P	
Neg	FP	TN	N	
Total	\hat{P}	\hat{N}	m	

Accuracy: $P(Correct) = (TN + TP)/m$

Prediction error: $P(Error) = (FN + FP)/m$

Precision+ (positive predictive value): $P(True+ | Pred+) = TP/\hat{P}$

Recall+ (sensitivity, true positive rate): $P(Pred+ | True+) = TP/P$

False positive rate: $P(Pred+ | True-) = FP/N$

Harmonic mean of precision and recall: $F_1 = 2 \times \frac{Precision \times Recall}{Precision + Recall}$

		pred:no	pred:yes	
	true:no	52	7	
	true:yes	15	19	
precision				
0	0.78	0.88	0.83	59
1	0.73	0.56	0.63	34
accuracy			0.76	93
macro avg	0.75	0.72	0.73	93
weighted avg	0.76	0.76	0.76	93

All is still based on that cutoff, 0.5!

Classification evaluation: different goals

We can think of several different prediction goals, all potentially important:

1. Classify correctly – make few (weighted) errors on test set or new prediction points
2. Predict probabilities well: $P(\widehat{y} = 1|x) \approx P(y = 1|x)$ for new points
3. Rank well: given multiple prediction points, predict which one is *more likely* to have $y = 1$.

These different tasks can reflect in the loss function / model evaluation task:

1. Correct classification: misclassification loss as above, also precision, recall etc.
2. Good probability prediction: using Bernoulli loss / likelihood:

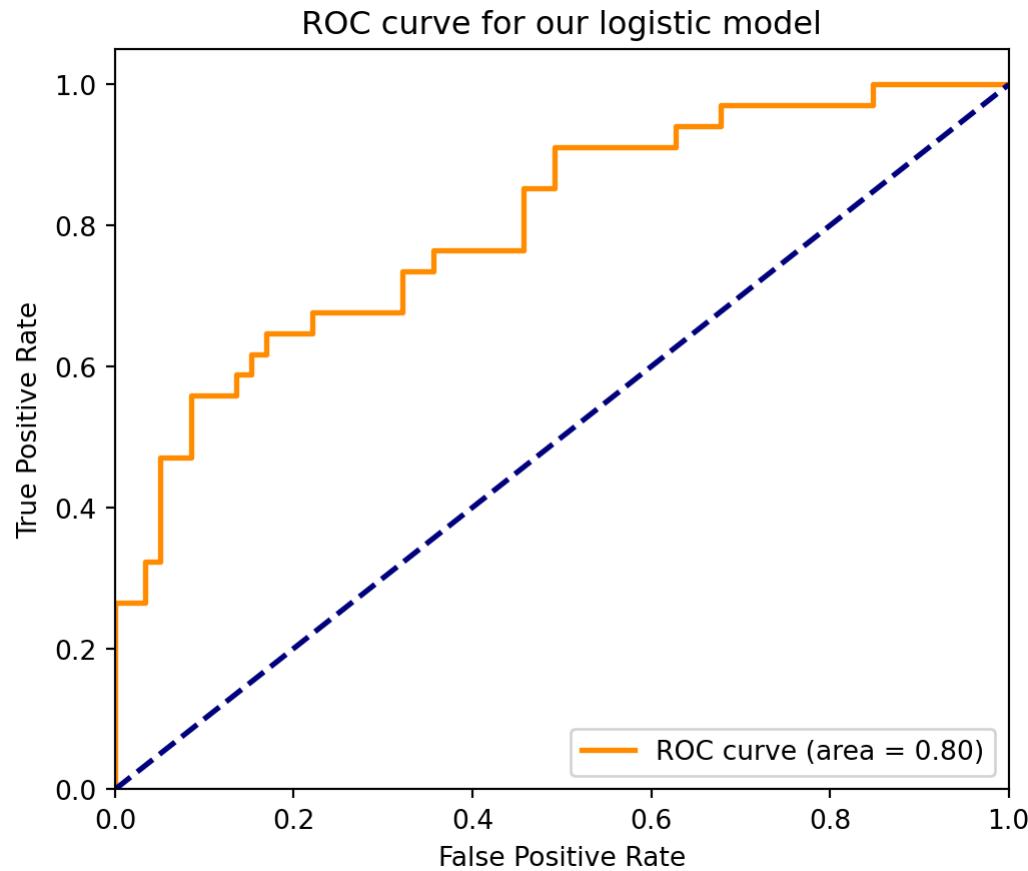
$$L(y, \hat{p}) = \hat{p}^y(1 - \hat{p})^{(1-y)}$$

3. How do we measure ranking performance of a model on a test set?

The ROC Curve

The idea: to evaluate ranking performance, do not set the threshold 0.5 but check what happens at all possible thresholds:

1. True positive rate: what % of the positive observations pass the threshold?
 2. False positive rate: what % of the negative observations pass the threshold?
- The ROC curve plots TPR vs FPR for all possible thresholds: if the model ranks well, for high thresholds we will have $FPR \approx 0$, while for low thresholds we will have $TPR \approx 1$
 - Note that even if $\widehat{P(y=1|x)}$ predicts probabilities badly, or even if the predictions are not in the range $[0, 1]$, the ranking can still be good



The Area Under the Curve (AUC)

- For a random ranking: $FPR \approx TPR$ at every threshold, so we are around the diagonal $x = y$:

$$AUC \approx 0.5$$

- For a perfect ranking model: at high thresholds, $FPR = 0$, at low thresholds $TPR = 1$, hence:

$$AUC = 1.$$

- Very nice interpretation of AUC: Assume the test set has m_1 ones ($y = 1$) and m_0 zeros, then AUC is the % of correctly ranked pairs with different response:

$$AUC = \frac{\# \{(i, j) : y_i = 0, y_j = 1 \text{ and } \hat{p}_i < \hat{p}_j\}}{m_1 \times m_0}$$