# High-Dimensional Statistics and Generalized Linear Models

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#### **Statistical Analysis and Document Mining**

Complementary Course, Master of Applied Mathematics in Grenoble

- Previous Episode: Discriminative Approaches for Classification Problems
  - Multiple logistic regression
  - Nearest-neighbour methods
  - High-dimensional data classification
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  - KNN learning algorithm
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  - The impact of high dimensionality on statistics is multiple!
- Generalized Linear Models
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  - Bikeshare data: linear regression
  - Bikeshare data: Poisson regression
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## Previous episode: multiple logistic regression

- We are given a training dataset  $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}, \ y_{[N]} \in [2] \equiv \mathcal{C},$  i.i.d. sampled from the true (but unknown) joint PDF of  $(\mathbf{X}, Y)$ .
- ? How to model relationship between  $p_c(\mathbf{X}) = \mathbb{P}(Y = c | \mathbf{X}), c \in \mathcal{C}$ , and  $\mathbf{X}$ ?
- Multiple logistic regression (MLR) takes the form  $p_2(\mathbf{X}) = 1 p_1(\mathbf{X})$ , and models the probability that Y belongs to a particular category instead Y,

$$\log\left(\frac{p_1(\mathbf{X})}{1-p_1(\mathbf{X})}\right) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p, \text{ or } p_1(\mathbf{X}) = \frac{\exp(\beta_0 + \sum_{p=1}^{P} \beta_p X_p)}{1 + \exp(\beta_0 + \sum_{p=1}^{P} \beta_p X_p)}.$$

**Training error:** using non-linear LS or maximum likelihood estimation (MLE), we obtain  $\widehat{\beta}$  and  $\widehat{r}_{\mathcal{D}}(\mathbf{x}_n) = \operatorname{argmax}_{c \in \mathcal{C}} p_c(\mathbf{x}_n)$  such that  $\forall n \in [N]$ ,

$$y_n pprox \widehat{r}_{\mathcal{D}}(\mathbf{x}_n)$$
, or equivalent,  $\mathcal{L}(\widehat{r}_{\mathcal{D}}, \mathcal{D}) \equiv \frac{1}{N} \sum_{n=1}^{N} \mathbb{1} \left[ y_n \neq \widehat{r}_{\mathcal{D}}(\mathbf{x}_n) \right] \approx 0.$  (1)

**? Test (generalization) error:** for any **new sample**  $(\mathbf{x}^*, y^*)$ , how we guarantee  $y^* \approx \hat{r}_D(\mathbf{x}^*)$ , or equivalent,  $\mathcal{L}(\hat{r}_D) \equiv \mathbb{E}_{\mathbf{X},Y} [\mathbb{1}(Y \neq \hat{r}_D(\mathbf{X}))] \approx 0$ ? (2)

# Previous episode: Cross-Validation for MLR

- Split the training dataset randomly into K folds so that we have  $\mathcal{D}_1 \cup \cdots \cup \mathcal{D}_K = \mathcal{D}$ , where  $\mathcal{D}_k$  denotes the indices of the observations in part k. There are  $N_k$  observations in part k: if N is a multiple of K, then  $N_k = N/K$ .
- ② For each  $k \in [K]$ , fit a model  $\hat{r}^{(-k)}(\mathbf{x}, \mathbf{m})$ , indexed by a tuning parameter (or a model)  $\mathbf{m} \in \mathcal{M}$ , on all samples from the training set except those in the kth fold.
- **3** Estimating test error  $\mathcal{L}(\hat{r}_{\mathcal{D}})$  via averaging the final resulting MSE estimates

$$\mathcal{L}(\widehat{r}_{\mathcal{D}}) \approx \underbrace{\frac{1}{K} \sum_{k=1}^{K}}_{\text{average over } K \text{ folds}} \underbrace{\left[ \frac{1}{N_k} \sum_{n \in \mathcal{D}_k} \mathbb{1}\left(y_n \neq \widehat{r}^{(-k)}(\mathbf{x}_n)\right) \right]}_{\text{Estimate test error for each fold}} \equiv \text{CV}(\widehat{r}, K, \mathbf{m}).$$

● Best data-driven model:  $\widehat{\mathbf{m}} \equiv \operatorname{argmin}_{\mathbf{m} \in \mathcal{M}} \operatorname{CV}(\widehat{r}, K, \mathbf{m})$ . K = ? Setting K = N yields N-fold or leave-one out cross-validation (LOOCV, **high variance**). A common better choice K = 5 or 10.

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# Previous episode: Nearest-neighbour methods

- We are given a **training dataset**  $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}, \ \underline{y_{[N]}} \in \mathcal{C} \subsetneq \mathbb{N},$  i.i.d. sampled from **the true (but unknown) joint PDF** of  $(\mathbf{X}, Y)$ .
- **3** How to model relationship between  $p_c(\mathbf{X}) = \mathbb{P}(Y = c | \mathbf{X}), c \in \mathcal{C}$ , and  $\mathbf{X}$ ?
- $\nearrow$  K-Nearest-neighbours (kNN) approximate the probability that Y belongs to a particular category instead Y,

$$\mathbb{P}(Y = c | \mathbf{X} = \mathbf{x}) \approx \frac{1}{K} \sum_{\mathbf{x}_n \in \mathcal{N}_K(\mathbf{x})} \mathbb{1}_{y = c}(y_n).$$

- kNN is a nonparametric classifier: it makes no assumptions about the data. → It can be very flexible but may not be optimal when we know something about the data.
- The hyper-parameter K usually chosen via cross-validation.
- ② It works well in low dimensions, but suffers from the curse of dimensionality. To be verified soon!

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## High-dimensional data classification

- We are given a **training dataset**  $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n \in [N]}, \ y_{[N]} \in \mathcal{C},$  i.i.d. sampled from **the true (but unknown) joint PDF** of  $(\mathbf{X}, Y)$ .
- In genomics and other areas of computational biology, the number of features P is much larger than the number of observations N, often written as  $P \gg N$ , where  $\mathbf{x}_n \in \mathbb{R}^P$ .
- **?** How to model relationship between  $p_c(\mathbf{X}) = \mathbb{P}(Y = c | \mathbf{X}), c \in \mathcal{C}$ , and  $\mathbf{X}$ ?
- Which is suitable for high-dimensional data: Discriminative approaches (CM5) or Generative approaches (CM6).
  - M-nearest neighbors (K-NN) (CM5),
  - 2 Logistic Regression (CM5),
  - 3 Linear Discriminant Analysis (CM5),
  - Naive Bayes classifier (CM6).

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# A synthetically generated Oil Flow data set<sup>1</sup>

- Representing N = 1000 data points (for each training, validation, and test sets) taken from a pipeline containing a mixture of oil, water, and gas.
- ightharpoonup Comprising a P=12-dimensional input vector consisting of measurements taken with gamma ray densitometers that measure the attenuation of gamma rays passing along narrow beams through the pipe.
- Each data point is labelled according to which of the three geometrical classes it belongs to:  $Y \in \{\text{Stratified}, \text{Annular}, \text{Homogeneous}\}$ , see Figure 1 for more details.

<sup>&</sup>lt;sup>1</sup>Bishop, C. M. and G. D. James (1993). *Analysis of multiphase flows using dual-energy gamma densitometry and neural networks*. Nuclear Instruments and Methods in Physics Research.

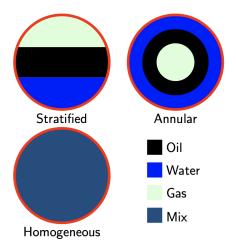


Figure 1: The three geometrical configurations of the oil, water, and gas phases used to generate the oil-flow data set. For each configuration, the proportions of the three phases can vary [Bishop, 2006, Figure A.2].

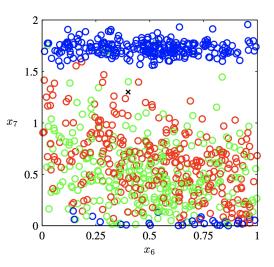
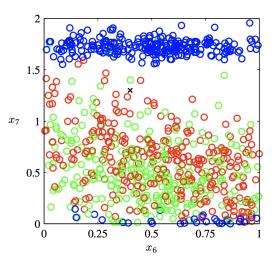
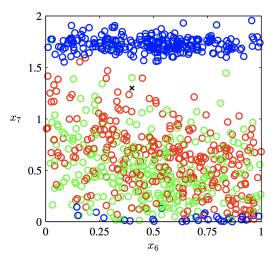


Figure 2: Scatter plot of the oil flow data for input variables  $x_6$  and  $x_7$ , in which red denotes the 'homogenous' class, green denotes the 'annular' class, and blue denotes the 'laminar' class. Our goal is to classify the new test point denoted by 'x'. [Bishop, 2006, Figure 1.19].

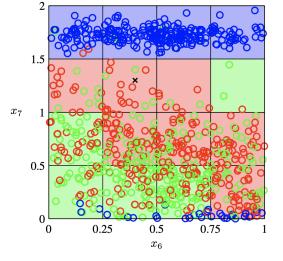


**Your intuitive solution** ... New test point denoted by ' $\times$ ' should be  $\mathbf{x}$ ,  $\times$  or  $\mathbf{x}$ ?



**Intuitive solution** the cross **x** is surrounded by numerous **red points**, and so we might suppose that it belongs to the **red class**. There are also plenty of green points nearby, so we might think that it could instead belong to the green class. It seems unlikely that it belongs to the blue class.

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KNN learning algorithm: divide the input space into regular cells and any new test point is assigned to the class that has a majority number of representatives in the same cell as the test point.

[Bishop, 2006, Figure 1.20]. A few potentially serious shortcomings ...

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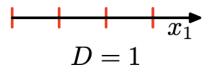
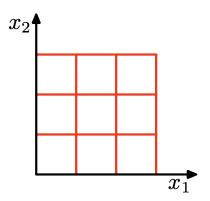
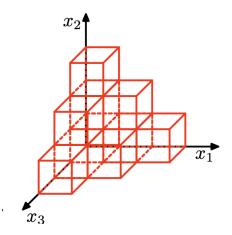


Illustration of the curse of dimensionality: number of cells  $= 3^1 = 3$  [Bishop, 2006, Figure 1.21].



**Illustration of the curse of dimensionality:** when P = 2, number of cells  $= 3^2 = 9$  [Bishop, 2006, Figure 1.21].



**Illustration of the curse of dimensionality:** when P = 3, number of cells  $= 3^3 = 27$  [Bishop, 2006, Figure 1.21].

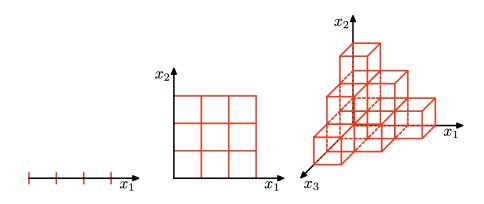


Illustration of the curse of dimensionality: exponentially large number of cells  $3^P$ , e.g.,  $3^{12} = 531441$  is that we would need an exponentially large quantity of training data in order to ensure that the cells are not empty [Bishop, 2006, Figure 1.21].

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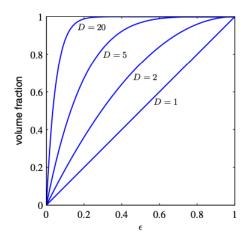
## Lost in the immensity of high-dimensional spaces

Our geometrical intuitions, formed through a life spent in a space of three dimensions, can fail badly when we consider spaces of higher dimensionality [Bishop, 2006].

Fraction of the volume of the sphere that lies between radius  $r=1-\epsilon$  and r=1 is given by

$$\frac{V_P(1)-V_P(1-\epsilon)}{V_P(1)}=1-(1-\epsilon)^P\longrightarrow 1 \text{ for large } P \text{ and small } \epsilon!$$

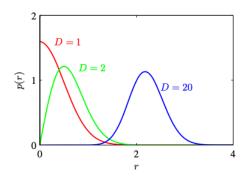
Here,  $V_P(1)$  is a volume of a sphere of radius r in  $P(\equiv D)$  dimensions.



in spaces of high dimensionality, most of the volume of a sphere is concentrated in a thin shell near the surface!

## Lost in the immensity of high-dimensional spaces

- Our geometrical intuitions, formed through a life spent in a space of three dimensions, can fail badly when we consider spaces of higher dimensionality [Bishop, 2006].
  - Behaviour of a Gaussian distribution in a high-dimensional space.
  - If we transform from Cartesian to polar coordinates, and then integrate out the directional variables, we obtain an expression for the density p(r) as a function of radius r from the origin.
  - Thus  $p(r)\delta r$  is the probability mass inside a thin shell of thickness  $\delta r$  located at radius r.



Plot of the probability density with respect to radius r of a Gaussian distribution for various values of the dimensionality  $P(\equiv D)$ .

[Bishop, 2006, Figure 1.23]. ANY comments ?

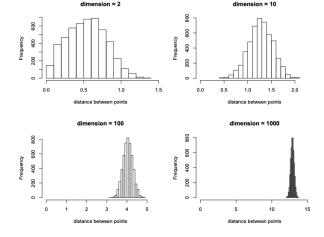
 **\stackrel{\*}{\triangleright}** For large  $P(\equiv D)$  most of the probability mass of a Gaussian is concentrated in a thin shell!

# Lost in the immensity of high-dimensional spaces

- → High-dimensional spaces are vast and data points are isolated in their immensity [Giraud, 2021].
  - So far, we have considered the situation where we want to explain a response variable  $Y \in \mathbb{R}$  by P variables  $X_1, ..., X_P \in [0, 1]$ . Assume that each variable  $X_p$  follows a uniform distribution on [0, 1].
  - If these variables are independent, then the variable  $X = (X_1, ..., X_p) \in [0, 1]^P$  follows a uniform distribution on the hypercube  $[0, 1]^P$ .
  - ullet Consider classical regression, given  $\epsilon_{[N]}$  independent and centered,

$$Y_n = f(\mathbf{X}_n) + \epsilon_n, \quad n \in [N] \text{ with } f : [0,1]^P \to \mathbb{R}.$$
 (3)

Assuming that the function f is smooth, it is natural to estimate f(x) by some average of the  $Y_n$  associated to the  $\mathbf{X}_n$  in the vicinity of x. The most simple version of this idea is the kNN estimator, where f(x) is estimated by the mean of the  $Y_n$  associated to the k points  $\mathbf{X}_n$ , which are the nearest from x!



Histograms of the pairwise-distances between N = 100 points sampled uniformly in the hypercube  $[0,1]^P$ , for P = 2,10,100, and 1000 [Giraud, 2021, Figure 1.3].

 $\stackrel{*}{\rightleftharpoons}$  For large P: (1) the minimal distance between two points increases, (2) all the points are at a similar distance from the others, so the notion of "nearest points" vanishes.

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- High-dimensional spaces are vast and data points are isolated in their immensity.
- The accumulation of small fluctuations in many different directions can produce a large global fluctuation.
- An event that is an accumulation of rare events may not be rare.
- Numerical computations and optimizations in high-dimensional spaces can be overly intensive.

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## Bikeshare data set: motivation example

We consider the Bikeshare data set. The response is bikers, the number of hourly users of a bike sharing program in Washington, DC. This response value is neither qualitative nor quantitative: instead, it takes on non-negative integer values, or counts.

Predicting bikers using the covariates mnth (month of the year), hr (hour of the day, from 0 to 23), workingday (an indicator variable that equals 1 if it is neither a weekend nor a holiday), temp (the normalized temperature, in Celsius), and weathersit (a qualitative variable that takes on one of four possible values: clear; misty or cloudy; light rain or light snow; or heavy rain or heavy snow.)

>	hea	d(Bi	kesh	ire)												
	sea	son	mnth	day	hr	holiday	weekday	workingday	weathersit	temp	atemp	hum	windspeed	casual	registered	bikers
1		1	Jan	1	0	0	6	0	clear	0.24	0.2879	0.81	0.0000	3	13	16
2		1	Jan	1	1	0	6	0	clear	0.22	0.2727	0.80	0.0000	8	32	40
3		1	Jan	1	2	0	6	0	clear	0.22	0.2727	0.80	0.0000	5	27	32
4		1	Jan	1	3	0	6	0	clear	0.24	0.2879	0.75	0.0000	3	10	13
5		1	Jan	1	4	0	6	0	clear	0.24	0.2879	0.75	0.0000	0	1	1
6		1	Jan	1	5	0	6	0	cloudy/misty	0.24	0.2576	0.75	0.0896	0	1	1

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```
> mod.lm2 <- lm(
     bikers ~ mnth + hr + workingday + temp + weathersit,
     data = Bikeshare
> summary(mod.lm2)
Call:
lm(formula = bikers ~ mnth + hr + workingday + temp + weathersit,
   data = Bikeshare)
Residuals:
   Min
            10 Median
                           3Q
                                  Max
-299.00 -45.70 -6.23 41.08 425.29
Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)
                          73.5974
                                      5.1322 14.340 < 2e-16 ***
mnth1
                          -46.0871
                                      4.0855 -11.281 < 2e-16 ***
                                      3.5391 -11.088 < 2e-16 ***
mnth2
                          -39.2419
mnth3
                          -29.5357
                                      3.1552 -9.361 < 2e-16 ***
mnth4
                           -4.6622
                                      2.7406 -1.701 0.08895 .
                                      2.8508 9.285 < 2e-16 ***
mnth5
                          26.4700
mnth6
                          21.7317
                                      3.4651 6.272 3.75e-10 ***
mnth7
                                      3.9084 -0.195 0.84530
                           -0.7626
mnth8
                                      3.5347 2.024 0.04295 *
                           7.1560
mnth9
                           20.5912
                                      3.0456
                                              6.761 1.46e-11 ***
mn+h10
                          29.7472
                                      2.6995 11.019 < 2e-16 ***
mnth11
                           14.2229
                                      2.8604
                                               4.972 6.74e-07 ***
```

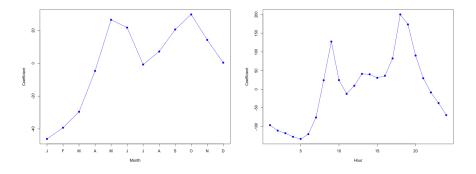
mnth11	14.2229	2.8604	4.972	6.74e-07	***
hr1	-96.1420	3.9554	-24.307	< 2e-16	***
hr2	-110.7213	3.9662	-27.916	< 2e-16	***
hr3	-117.7212	4.0165	-29.310	< 2e-16	***
hr4	-127.2828	4.0808	-31.191	< 2e-16	***
hr5	-133.0495	4.1168	-32.319	< 2e-16	***
hr6	-120.2775	4.0370	-29.794	< 2e-16	***
hr7	-75.5424	3.9916	-18.925	< 2e-16	***
hr8	23.9511	3.9686	6.035	1.65e-09	***
hr9	127.5199	3.9500	32.284	< 2e-16	***
hr10	24.4399	3.9360	6.209	5.57e-10	***
hr11	-12.3407	3.9361	-3.135	0.00172	**
hr12	9.2814	3.9447	2.353	0.01865	*
hr13	41.1417	3.9571	10.397	< 2e-16	***
hr14	39.8939	3.9750	10.036	< 2e-16	***
hr15	30.4940	3.9910	7.641	2.39e-14	***
hr16	35.9445	3.9949	8.998	< 2e-16	***
hr17	82.3786	3.9883	20.655	< 2e-16	
hr18	200.1249	3.9638	50.488	< 2e-16	***
hr19	173.2989	3.9561	43.806	< 2e-16	***
hr20	90.1138	3.9400	22.872	< 2e-16	***
hr21	29.4071	3.9362	7.471	8.74e-14	***
hr22	-8.5883	3.9332	-2.184	0.02902	*
hr23	-37.0194	3.9344	-9.409	< 2e-16	***
workingday	1.2696	1.7845	0.711	0.47681	
temp	157.2094	10.2612	15.321	< 2e-16	***
weathersitcloudy/misty	-12.8903			5.60e-11	
weathersitlight rain/snow	-66.4944	2.9652	-22.425	< 2e-16	***
 arTin Nauven High D	imensional Sta	tistics and GLM	1	Marc	h 07 20

```
hr20
                                    3.9400 22.872 < 2e-16 ***
                         90.1138
hr21
                         29.4071
                                    3.9362 7.471 8.74e-14 ***
hr22
                         -8.5883
                                    3.9332 -2.184 0.02902 *
hr23
                        -37.0194
                                    3.9344 -9.409 < 2e-16 ***
                          1.2696
                                    1.7845 0.711 0.47681
workingday
temp
                        157.2094
                                   10.2612 15.321 < 2e-16 ***
weathersitcloudy/misty -12.8903
                                    1.9643 -6.562 5.60e-11 ***
weathersitlight rain/snow -66.4944 2.9652 -22.425 < 2e-16 ***
weathersitheavy rain/snow -109.7446
                                   76.6674 -1.431 0.15234
```

---

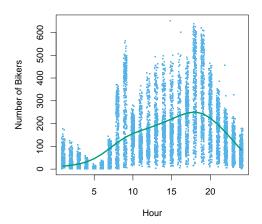
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 76.5 on 8605 degrees of freedom Multiple R-squared: 0.6745, Adjusted R-squared: 0.6731 F-statistic: 457.3 on 39 and 8605 DF, p-value: < 2.2e-16



A least squares linear regression model was fit to predict bikers in the Bikeshare data set. Left: The coefficients associated with the month of the year. Bike usage is highest in the spring and fall, and lowest in the winter. Right: The coefficients associated with the hour of the day. Bike usage is highest during peak commute times, and lowest overnight [James et al., 2021, Figure 4.13]

At first glance, fitting a linear regression model to the Bikeshare seems to provide reasonable and intuitive results.



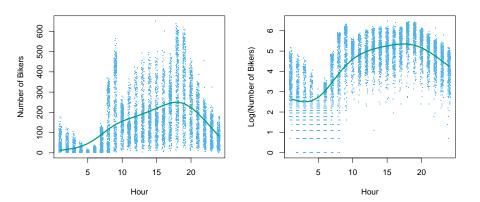
For the most part, as the **mean number of bikers increases**, so does **the variance in the number of bikers** [James et al., 2021, Figure 4.14].

**?** At first glance, fitting a linear regression model to the Bikeshare seems to provide reasonable and intuitive results.

#### Some issues

- 9.6% of the fitted values in the Bikeshare data set are negative: that is, the linear regression model predicts a negative number of users during 9.6% of the hours in the data set.
- ② Since  $\epsilon$  is a continuous-valued error term, response Y is necessarily continuous-valued (quantitative) but the response bikers is integer-valued.

The mean-variance relationship is a major violation of the assumptions of a linear model, which state that  $Y = \beta_0 + \sum_{p=1}^P X_p \beta_p + \epsilon$ , where  $\epsilon$  is a mean-zero error term with variance  $\sigma^2$  that is constant, and not a function of the covariates. For the most part, as the mean number of bikers increases, so does the variance in the number of bikers!



#### Some solutions

- **1** Transforming the response Y avoids the possibility of negative predictions, and it overcomes much of the heteroscedasticity in the untransformed data  $\log(Y) = \beta_0 + \sum_{p=1}^P X_p \beta_p + \epsilon$ . **BUT** Making predictions and inference in terms of the log of the response, rather than the response →challenges in interpretation!
- Poisson regression model provides a much more natural and elegant approach for this task! (See more in CC6).

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  - Curse of dimensionality for kNN
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  - The impact of high dimensionality on statistics is multiple!
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  - Bikeshare data: Poisson regression
  - Bikeshare data: linear regression and Poisson regression
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# Poisson Regression

**?** Definition of Poisson distribution: Suppose that a random variable Y takes on nonnegative integer values, Poisson, *i.e.*,  $Y \in \{0, 1, 2, ...\}$ . If Y follows the Poisson distribution, then

$$\mathbb{P}(Y=k) = \frac{e^{\lambda} \lambda^k}{k!} \text{ for } k = 0, 1, 2, \dots, \lambda > 0.$$
 (4)

Here,  $\mathbb{E}[Y] = \text{var}[Y] = \lambda$ .

**?** Definition of Poisson regression model:

$$\mathbb{E}[Y] = \lambda \equiv \lambda(X_1, \dots, X_P) = \exp(\beta_0 + \sum_{p=1}^P X_p \beta_p).$$
 (5)

MLE approach: we want to maximize MLE

$$I(\beta_0, \beta_1, \dots, \beta_P) = \prod_{n=1}^{N} \frac{e^{-\lambda(x_n)} \lambda(x_n)^{y_n}}{y_n!}, \quad \lambda(x_n) = \exp(\beta_0 + \sum_{p=1}^{P} x_{np} \beta_p).$$
 (6)

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  - Bikeshare data: Poisson regression
  - Bikeshare data: linear regression and Poisson regression
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```
> mod.lm2 <- lm(
     bikers ~ mnth + hr + workingday + temp + weathersit,
     data = Bikeshare
> summary(mod.lm2)
Call:
lm(formula = bikers ~ mnth + hr + workingday + temp + weathersit,
   data = Bikeshare)
Residuals:
   Min
            10 Median
                           3Q
                                  Max
-299.00 -45.70 -6.23 41.08 425.29
Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)
                          73.5974
                                      5.1322 14.340 < 2e-16 ***
mnth1
                          -46.0871
                                      4.0855 -11.281 < 2e-16 ***
                                      3.5391 -11.088 < 2e-16 ***
mnth2
                          -39.2419
mnth3
                          -29.5357
                                      3.1552 -9.361 < 2e-16 ***
mnth4
                           -4.6622
                                      2.7406 -1.701 0.08895 .
                                      2.8508 9.285 < 2e-16 ***
mnth5
                          26.4700
mnth6
                          21.7317
                                      3.4651 6.272 3.75e-10 ***
mnth7
                                      3.9084 -0.195 0.84530
                           -0.7626
mnth8
                                      3.5347 2.024 0.04295 *
                           7.1560
mnth9
                           20.5912
                                      3.0456
                                              6.761 1.46e-11 ***
mn+h10
                          29.7472
                                      2.6995 11.019 < 2e-16 ***
mnth11
                           14.2229
                                      2.8604
                                               4.972 6.74e-07 ***
```

```
> mod.pois <- alm(</pre>
     bikers ~ mnth + hr + workingday + temp + weathersit.
     data = Bikeshare, family = poisson
+
+
> summary(mod.pois)
Call:
alm(formula = bikers ~ mnth + hr + workingday + temp + weathersit.
    family = poisson, data = Bikeshare)
Deviance Residuals:
     Min
               10
                     Median
                                   30
                                            Max
         -3.3441
-20.7574
                    -0.6549
                               2.6999
                                        21.9628
Coefficients:
                          Estimate Std. Error z value Pr(>|z|)
                          4.118245
                                     0.006021 683.964 < 2e-16 ***
(Intercept)
                                    0.005907 -113.445 < 2e-16 ***
mnth1
                         -0.670170
mnth2
                         -0.444124
                                     0.004860 -91.379 < 2e-16 ***
mnth3
                         -0.293733
                                     0.004144 -70.886 < 2e-16 ***
                                                 6.888 5.66e-12 ***
mnth4
                          0.021523
                                     0.003125
mnth5
                          0.240471
                                     0.002916 82.462 < 2e-16 ***
mnth6
                          0.223235
                                     0.003554
                                                62.818 < 2e-16 ***
                                     0.004125 25.121 < 2e-16 ***
mnth7
                          0.103617
mnth8
                          0.151171
                                     0.003662 41.281 < 2e-16 ***
                                                75.281 < 2e-16 ***
mnth9
                          0.233493
                                     0.003102
mnth10
                          0.267573
                                     0.002785
                                                96.091 < 2e-16 ***
mnth11
                          0.150264
                                     0.003180
                                                47.248
                                                        < 2e-16 ***
```

mnth11	14.2229	2.8604	4.972	6.74e-07	***
hr1	-96.1420	3.9554	-24.307	< 2e-16	***
hr2	-110.7213	3.9662	-27.916	< 2e-16	***
hr3	-117.7212	4.0165	-29.310	< 2e-16	***
hr4	-127.2828	4.0808	-31.191	< 2e-16	***
hr5	-133.0495	4.1168	-32.319	< 2e-16	***
hr6	-120.2775	4.0370	-29.794	< 2e-16	***
hr7	-75.5424	3.9916	-18.925	< 2e-16	***
hr8	23.9511	3.9686	6.035	1.65e-09	***
hr9	127.5199	3.9500	32.284	< 2e-16	***
hr10	24.4399	3.9360	6.209	5.57e-10	***
hr11	-12.3407	3.9361	-3.135	0.00172	**
hr12	9.2814	3.9447	2.353	0.01865	*
hr13	41.1417	3.9571	10.397	< 2e-16	***
hr14	39.8939	3.9750	10.036	< 2e-16	***
hr15	30.4940	3.9910	7.641	2.39e-14	***
hr16	35.9445	3.9949	8.998	< 2e-16	***
hr17	82.3786	3.9883	20.655	< 2e-16	
hr18	200.1249	3.9638	50.488	< 2e-16	***
hr19	173.2989	3.9561	43.806	< 2e-16	***
hr20	90.1138	3.9400	22.872	< 2e-16	***
hr21	29.4071	3.9362	7.471	8.74e-14	***
hr22	-8.5883	3.9332	-2.184		
hr23	-37.0194	3.9344	-9.409	< 2e-16	***
workingday	1.2696	1.7845	0.711	0.47681	
temp	157.2094	10.2612	15.321	< 2e-16	***
weathersitcloudy/misty	-12.8903			5.60e-11	
weathersitlight rain/snow	-66.4944	2.9652	-22.425	< 2e-16	***
 arTin Nauven High D	imensional Sta	tistics and GLM	1	Marc	h 07 20

```
hr11
                          0.336852
                                     0.004720
                                               71.372
                                                       < 2e-16 ***
hr12
                          0.494121
                                     0.004392
                                              112.494
                                                       < 2e-16 ***
                                                       < 2e-16 ***
hr13
                          0.679642
                                     0.004069
                                              167.040
hr14
                          0.673565
                                     0.004089 164.722
                                                       < 2e-16 ***
hr15
                          0.624910
                                     0.004178
                                              149.570
                                                       < 2e-16 ***
hr16
                          0.653763
                                     0.004132
                                              158.205
                                                       < 2e-16 ***
hr17
                          0.874301
                                     0.003784
                                              231.040
                                                       < 2e-16 ***
hr18
                          1.294635
                                     0.003254
                                              397.848
                                                       < 2e-16 ***
                                                       < 2e-16 ***
hr19
                          1.212281
                                     0.003321
                                              365.084
hr20
                          0.914022
                                     0.003700
                                              247.065
                                                       < 2e-16 ***
                                              147.045 < 2e-16 ***
hr21
                          0.616201
                                     0.004191
                                                       < 2e-16 ***
hr22
                          0.364181
                                     0.004659
                                               78.173
hr23
                                     0.005225 22.488 < 2e-16 ***
                          0.117493
                                     0.001955 7.502 6.27e-14 ***
workingday
                          0.014665
                          0.785292
                                     0.011475 68.434 < 2e-16 ***
temp
weathersitcloudy/mistv
                         -0.075231
                                     0.002179
                                              -34.528 < 2e-16 ***
weathersitlight rain/snow -0.575800
                                     0.004058 -141.905 < 2e-16 ***
weathersitheavy rain/snow -0.926287
                                     0.166782
                                               -5.554 2.79e-08 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

(Dispersion parameter for poisson family taken to be 1)

Null deviance: 1052921 on 8644 degrees of freedom Residual deviance: 228041 on 8605 degrees of freedom

AIC: 281159

Number of Fisher Scoring iterations: 5

```
hr20
                                    3.9400 22.872 < 2e-16 ***
                         90.1138
hr21
                         29.4071
                                    3.9362 7.471 8.74e-14 ***
hr22
                         -8.5883
                                    3.9332 -2.184 0.02902 *
hr23
                        -37.0194
                                    3.9344 -9.409 < 2e-16 ***
                          1.2696
                                    1.7845 0.711 0.47681
workingday
temp
                        157.2094
                                   10.2612 15.321 < 2e-16 ***
weathersitcloudy/misty -12.8903
                                    1.9643 -6.562 5.60e-11 ***
weathersitlight rain/snow -66.4944 2.9652 -22.425 < 2e-16 ***
weathersitheavy rain/snow -109.7446
                                   76.6674 -1.431 0.15234
```

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 76.5 on 8605 degrees of freedom Multiple R-squared: 0.6745, Adjusted R-squared: 0.6731 F-statistic: 457.3 on 39 and 8605 DF, p-value: < 2.2e-16

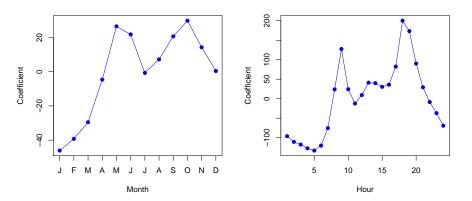
```
247.065 < 2e-16 ***
hr20
                    0.914022
                            0.003700
                                    147.045 < 2e-16 ***
hr21
                    0.616201
                            0.004191
                                    78.173 < 2e-16 ***
hr22
                    0.364181
                            0.004659
                    hr23
                            0.001955 7.502 6.27e-14 ***
workingday
                    0.014665
temp
                    0.785292
                            0.011475 68.434 < 2e-16 ***
weathersitcloudy/misty -0.075231 0.002179 -34.528 < 2e-16 ***
-5.554 2.79e-08 ***
weathersitheavy rain/snow -0.926287
                            0.166782
            0 '***, 0.001 '**, 0.01 '*, 0.05 '., 0.1 ', 1
Signif. codes:
```

(Dispersion parameter for poisson family taken to be 1)

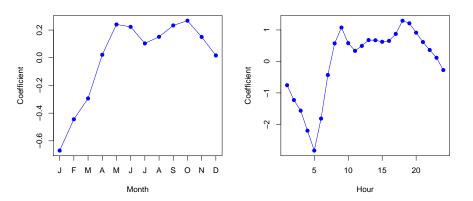
Null deviance: 1052921 on 8644 degrees of freedom Residual deviance: 228041 on 8605 degrees of freedom

AIC: 281159

Number of Fisher Scoring iterations: 5



A least squares linear regression model was fit to predict bikers in the Bikeshare data set. Left: The coefficients associated with the month of the year. Bike usage is highest in the spring and fall, and lowest in the winter. Right: The coefficients associated with the hour of the day. Bike usage is highest during peak commute times, and lowest overnight [James et al., 2021, Figure 4.13]



A Poisson regression model was fit to predict bikers in the Bikeshare data set. Left: The coefficients associated with the month of the year. Bike usage is highest in the spring and fall, and lowest in the winter. Right: The coefficients associated with the hour of the day. Bike usage is highest during peak commute times, and lowest overnight [James et al., 2021, Figure 4.15]

# Important distinction: Poisson and linear regression models

- Coefficient associated with workingday is statistically significant under the Poisson regression model, but not under the linear regression model. More realistic modeling!
- Mean-variance relationship: in Poisson regression, we implicitly assume that mean bike usage in a given hour equals the variance of bike usage during that hour. while a constant variance in linear regression model.
- Nonnegative fitted values: There are no negative predictions using the Poisson regression model.

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### Generalized linear models

- Recall that conditional on  $X_{[P]} \equiv (X_1, ..., X_P)$ , Y belongs to a certain family of distributions: Gaussian or normal distribution for linear regression, Bernoulli distribution for logistic regression and Poisson distribution for Poisson regression. What is the common thing?
- $\nearrow$   $Y \in \text{exponential family (including Gaussian, Bernoulli & Poisson).$
- Each approach models the mean of Y as a function of the predictors.
  - **1** Linear regression  $\mathbb{E}\left[Y|X_{[P]}\right] = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$ .
- $\red$  Using a link function  $\eta$  such that  $\eta(\mathbb{E}\left[Y|X_{[P]}\right]) = \beta_0 + \sum_{p=1}^P \beta_p X_p$ .

**HOW.** 
$$\eta(\mu) = \mu$$
,  $\eta(\mu) = \log(\mu/(1-\mu))$ ,  $\eta(\mu) = \log(\mu)$ .

### References



Bishop, C. M. (2006).

Pattern Recognition and Machine Learning.

Information Science and Statistics. New York: Springer, 1 edition.

(Cited on pages 13, 14, 18, 20, 21, 22, 23, 25, 26, 27, and 28.)



Giraud, C. (2021).

Introduction to High-Dimensional Statistics.

Chapman & Hall/CRC Monographs on Statistics & Applied Probability. Taylor & Francis.

(Cited on pages 29 and 30.)



James, G., Witten, D., Hastie, T., & Tibshirani, R. (2021). An Introduction to Statistical Learning: with Applications in R, volume 2 of Springer Texts in Statistics.

Springer.

(Cited on pages 40, 41, 54, and 55.)