

ECON3389 Machine Learning in Economics

Module 2 Classification

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Overview

Agenda:

- Qualitative outcomes and classification problem.
- LPM, logit and probit models.
- Estimation, interpretation and accuracy measures.
- Poisson Regression on count data

Readings:

- ISLR sections 4.1, 4.2, 4.3

Qualitative Outcomes

- So far our outcome variable Y has always been assumed to be quantitative, e.g. price, quantity, SAT score, etc.
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 - Online banking service assesses whether a transaction being performed is fraudulent based on user's IP address, past transaction history, transaction amount, etc.
 - A researchers performs an analysis of socio-economic factors that affect whether a student graduates from college or drops out.

Basic Classification Problem

- Consider a qualitative variable Y that for every observation i takes a single value from a finite set of possible unordered values $\mathcal{C} = \{y_1, y_2, \dots, y_C\}$.
 - $Y = \text{eye color}$, $\mathcal{C} = \{\text{brown, blue, green}\}$
 - $Y = \text{medical diagnosis}$, $\mathcal{C} = \{\text{stroke, drug overdose, epileptic seizure}\}$
 - $Y = \text{transaction status}$, $\mathcal{C} = \{\text{fraudulent, non-fraudulent}\}$

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- Given a feature vector X and a qualitative response Y , the classification task is to build a function $C(X)$ that takes as input the feature vector X and predicts its value for Y , i.e. $C(X) \in \mathcal{C}$.
- In most cases we are interested in estimating the probabilities that Y belongs to a category in $\mathcal{C}$ given X , i.e.

$$\Pr(Y = y_c | X) \quad \forall y_c \in \mathcal{C}$$

Linear Probability Model: Problems

- Suppose for our medical condition classification we code

$$Y = \begin{cases} 1, & \text{if Stroke} \\ 2, & \text{if Drug Overdose} \\ 3, & \text{if Epileptic Seizure} \end{cases}$$

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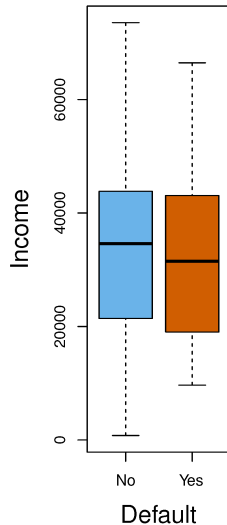
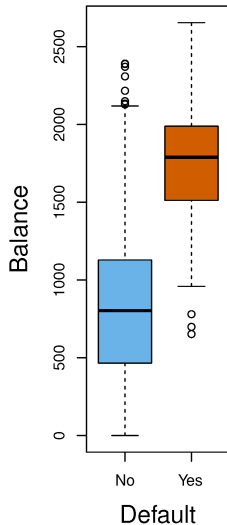
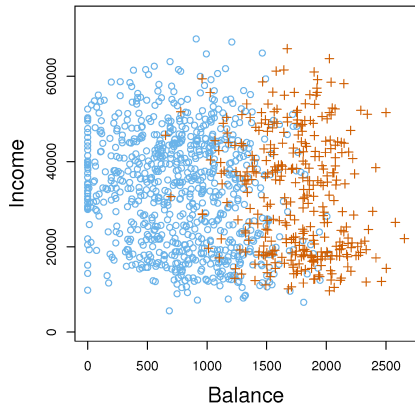
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- In most cases, it is not possible for us to create a natural ordering in quantitative data
- A different coding

$$Y = \begin{cases} 1, & \text{if Drug Overdose} \\ 2, & \text{if Stroke} \\ 3, & \text{if Epileptic Seizure} \end{cases}$$

Will generate a different model and different predictions

Example: Credit Card Defaults



Linear Probability Model

- Suppose for our credit card default classification we code

$$Y = \begin{cases} 0, & \text{if No} \\ 1, & \text{if Yes} \end{cases}$$

Can we use our standard regression model to estimate a regression of Y on X and classify outcome as **Yes** if $\hat{Y} > 0.5$?

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$$\mathbb{E}(Y|X) = ?$$

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- Given that Y is binary, we have

$$\mathbb{E}(Y|X) = 1 \cdot \Pr(Y = 1|X) + 0 \cdot \Pr(Y = 0|X) = \Pr(Y = 1|X)$$

which means that in this case standard linear regression will estimate the probability of outcome $Y = 1$, hence the name *linear probability model* or *LPM*.

Linear Probability Model

- LPM retains all properties of linear regression, but the interpretation of the results is slightly different:

$$\Pr(Y = 1|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

$$\beta_j = \frac{\partial \mathbb{E}[\Pr(Y = 1|X)]}{\partial X_j} = \frac{\mathbb{E}[\Delta \Pr(Y = 1|X)]}{\Delta X_j}$$

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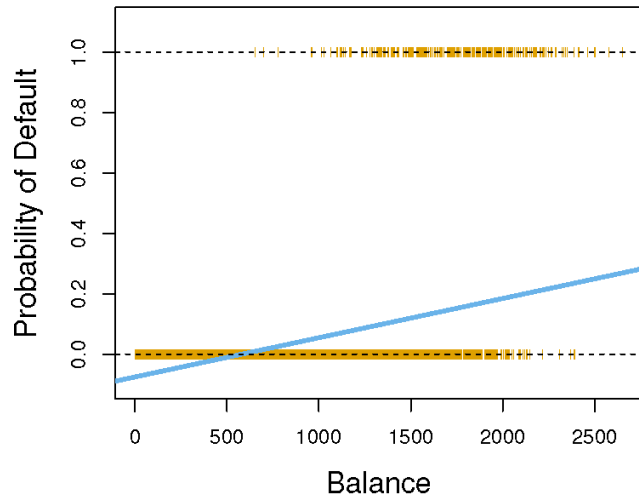
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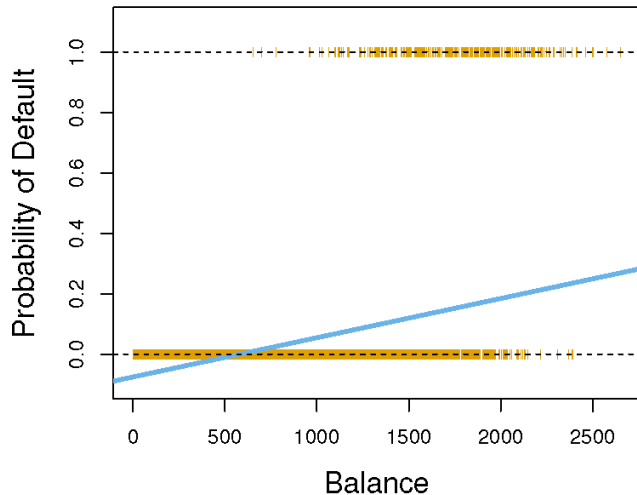
- LPM works very well in binary classification, especially if sample size is moderate to large.
- But it also has some inherent disadvantages

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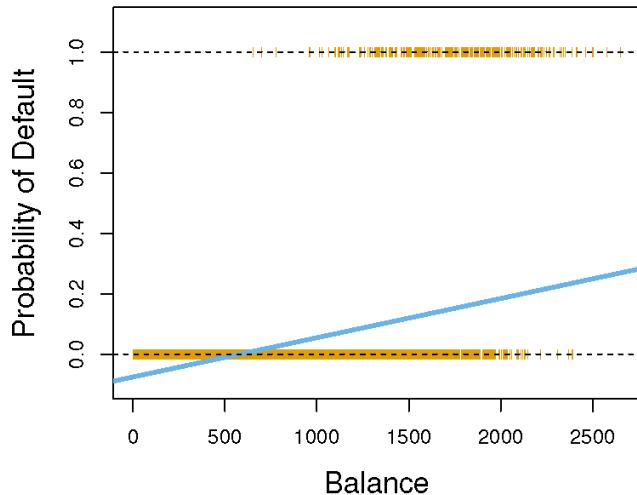
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- Blue line is estimated linear regression, which produces negative predictions for $\Pr(Y = 1|X)$ when **Balance** is less than 500.
- One way is to simply ignore the problem and bound any predictions from above and from below.
- But can we do better?

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- For any random variable Z its cdf $F_Z(\cdot)$ is by definition:

$$F_Z(a) = \Pr(Z \leq a)$$

- In classical statistical learning the two most common choice for $F(\cdot)$ are standard normal and logistic cdf.

Probit and Logit Models

- For simplicity, let's use the matrix notation:

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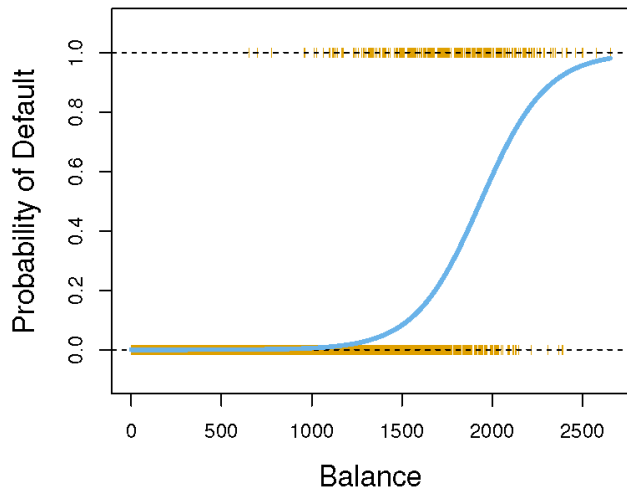
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- In *logit* model $F(\cdot)$ is assumed to be the cdf of a logistic distribution:

$$F(\mathbf{X}\boldsymbol{\beta}) = \Lambda(\mathbf{X}\boldsymbol{\beta}) = \int_{-\infty}^{\mathbf{X}\boldsymbol{\beta}} \frac{\exp(-z)}{(1 + \exp(-z))^2} dz = \frac{\exp^{\mathbf{X}\boldsymbol{\beta}}}{1 + \exp^{\mathbf{X}\boldsymbol{\beta}}}$$

Probit and Logit Models



With either normal or logistic cdf as our $F(\cdot)$ function the estimated probability will, by definition, always lie in $[0, 1]$ interval.

Generalized Linear Models

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- The link function is the key to GLMs: since the distribution of the *response variable* Y is non-normal (in our simple example it is binomial), it's what lets us connect the structural component $\mathbf{X}\beta$ to the response Y — it 'links' them (hence the name).

Generalized Linear Models

- Because our outcome Y is binary, we have $\mathbb{E}(Y|\mathbf{X}) = \Pr(Y = 1|\mathbf{X})$, and thus our inverse link function g^{-1} is simply the function that defines conditional probability of $Y = 1$ given $\mathbf{X}$.
- For probit and logit models the corresponding cumulative distribution functions act as inverse link functions:

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- Note: standard MLR is also a special case of GLM with $g(\mu) = \mu = \mathbf{X}\beta$.
- The two key differences of probit/logit models and usual MLR are estimation method and marginal effects calculation/interpretation.

Maximum Likelihood Estimation: Idea

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- In other words, it will find the parameter value that maximize the likelihood of the observed data being drawn from $f(x|\theta)$
- Suppose $x_1, x_2, \dots, x_n$ form a random sample from a normal distribution for which the mean μ is unknown and variance σ^2 is known
- The likelihood function of μ is

$$L(\mu) = f_n(\mathbf{x}|\mu) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \quad (2)$$

Maximum Likelihood Estimation: Example 1

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- **Model:** $L(p) = L(p; n, x) = \binom{n}{x} p^x (1 - p)^{n-x} = \binom{100}{56} p^{56} (1 - p)^{44}$
- $L(0.5) = 0.038$
- $L(0.52) = 0.058$
- $L(0.54) = 0.073$
- $L(0.56) = 0.081$
- $L(0.58) = 0.073$

Maximum Likelihood Estimation: Method

- **Method 1**

In the previous example, it is easy for us to write a simple equation that describes the likelihood surface that can be differentiated to find the MLE estimate

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$$\ln L = \ln \binom{100}{56} + \ln(p^{56}(1-p)^{44}) \quad (3)$$

$$\ln L = 56 \ln(p) + 44 \ln(1-p) \quad (4)$$

(5)

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- Step 2: Differentiate the log likelihood to find the optimal parameter

$$\frac{56}{p} - \frac{44}{(1-p)} = 0 \quad (6)$$

$$56(1-p) - 44p = 0 \quad (7)$$

$$p = \frac{56}{100} \quad (8)$$

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- In such cases we need to construct the overall likelihood surface using the individual likelihoods
- Each individual coin toss follows a Bernoulli distribution. Suppose $X = 1$ when heads and 0 otherwise

$$L(p; x) = p^x(1 - p)^{1-x}$$

Maximum Likelihood Estimation: Method

- **Method 2:** Remember the data is given to us

Observation	Outcome (x)	Likelihood of outcome
1	1	p
2	0	$1-p$
3	1	p
...		
99	0	$1-p$
100	1	p
Total	56	?

- What is the overall/joint likelihood of entries in the second column?

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...		
99	0	1-p
100	1	p
Total	56	?

- What is the overall/joint likelihood of entries in the second column?
- Each coin toss is independent

$$L(p) = p.p.p.p..(1-p)(1-p)...(1-p) \quad (9)$$

$$L(p) = p^{56}(1-p)^{44} \quad (10)$$

$$\ln L(p) = \ln(p^{56}(1-p)^{44}) \quad (11)$$

OLS as a special case of MLE

- Main assumption: The errors follow a normal distribution with mean 0 and variance σ^2

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

$$\epsilon_i = Y_i - \beta_0 - \beta_1 X_i$$

OLS as a special case of MLE

- Main assumption: The errors follow a normal distribution with mean 0 and variance σ^2

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- The likelihood function of (β) is

$$L(\beta) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp^{-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}}$$

$$\ln(L(\beta)) = \sum_{i=1}^n \ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \sum_{i=1}^n \frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}$$

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- The first term does not depend on (β) and the second term has a constant σ^2 that we can bring outside the summation

$$\ln(L(\beta)) = -\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

Maximum Likelihood Estimation

- Because we no longer have a direct connection between Y and our structural component $\mathbf{X}\beta$, we need to specify our loss function in a different way. Using our link function, we can for every observation i write down the probability of observing a certain value of Y_i given values of $\mathbf{X}_i$

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- For example, for a logit model we have:

$$\Pr(Y = Y_i | \mathbf{X}_i) = \left(\frac{\exp^{X_i \beta}}{1 + \exp^{X_i \beta}} \right)^{Y_i} \left(1 - \frac{\exp^{X_i \beta}}{1 + \exp^{X_i \beta}} \right)^{1 - Y_i}$$

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- With the default assumption of i.i.d. observations we can write down the joint probability or *likelihood function* of seeing our sample:

$$\ell(\beta) = \prod_{i=1}^n \Pr(Y = Y_i | \mathbf{X}_i)$$

Maximum Likelihood Estimation

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- Under some general conditions $\hat{\beta}_{ML}$ is efficient, consistent and asymptotically normal, just like $\hat{\beta}_{OLS}$

	Coefficient	Std. error	z-statistic	p-value
Intercept	-10.6513	0.3612	-29.5	<0.0001
balance	0.0055	0.0002	24.9	<0.0001

- But unlike OLS, ML is a more general estimation procedure and allows one to recover structural parameters such as β in models that are far more flexible than standard MLR.

Logistic Regression

- A key difference of logit/probit models from LPM is the fact that marginal effects are now calculated and interpreted in a different way:

$$\Pr(Y = 1|\mathbf{X}) = p(\mathbf{X}) = \frac{\exp^{X\beta}}{1 + \exp^{X\beta}}$$

$$\frac{p(\mathbf{X})}{1 - p(\mathbf{X})} = \exp^{X\beta}$$

$$\ln \frac{p(\mathbf{X})}{1 - p(\mathbf{X})} = X\beta$$

- The quantity on the left is called *log-odds* or *logit*
- The logistic regression model has a logit that is linear in X
- In a logistic regression model, increasing X by one unit changes the log odds by its corresponding β

Marginal Effects in Probit/Logit

- The other key difference of logit/probit models from LPM is the fact that marginal effects are now calculated and interpreted in a different way:

$$\text{Probit : } \frac{\partial p(\mathbf{X})}{\partial X_j} = \frac{\partial \Phi(\mathbf{X}\beta)}{\partial X_j} \beta_j \neq \beta_j \quad \text{Logit : } \frac{\partial p(\mathbf{X})}{\partial X_j} = \frac{\partial \Lambda(\mathbf{X}\beta)}{\partial X_j} \beta_j \neq \beta_j$$

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- The marginal effects now depend on values of all variables in $\mathbf{X}$, so we need to either estimate the marginal effects at a specific value of all our predictors (typically means or medians) or calculate their average over all values of $\mathbf{X}$ in our sample.

Multinomial Logistic Regression

- It is possible to extend the two-class logistic regression approach to the setting of $K > 2$ classes
- Suppose we have K classes. First we need to define a base class (K^{th} one)

$$\Pr(Y = k|\mathbf{X}) = \frac{\exp^{X\beta_k}}{1 + \sum_{l=1}^{K-1} \exp^{X\beta_l}}$$
$$\Pr(Y = K|\mathbf{X}) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp^{X\beta_l}}$$

- It can be shown that the above model implies

$$\frac{\Pr(Y = k|\mathbf{X})}{\Pr(Y = K|\mathbf{X})} = \exp^{X\beta_k}$$
$$\ln \frac{\Pr(Y = k|\mathbf{X})}{\Pr(Y = K|\mathbf{X})} = X\beta_k$$

- The interpretation of the β_k is with respect to the base category K

Goodness-of-fit Measures

- While LPM can use the standard R^2 as a well-defined goodness-of-fit measure, it is not an option for logit/probit models due to the different loss function.
- In standard MLR an single R^2 value of 0.95 is an evidence of an excellent fit, but in classification problems we are often more interested in *class-specific* performance, especially in areas such as medicine or biology.

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- Consider the case where $Y = 1$ means a positive test result. Then our model's predictions fall into one of the 4 possible cases:

	$Y = 0$	$Y = 1$
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- For city administration FPs in traffic cameras and speeding tickets are more important.
- In judicial system both FP and FN are equally important.

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- Consider the following *confusion matrix*, depicting the prediction results for the **Default** dataset, using 50% as a threshold for probability of default:

		True default status		
		No	Yes	Total
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	Yes	23	81	104
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 - However, out of 333 true defaults we managed to miss $252/333 = 75.67\%$, which could be an unacceptably high error rate for this class.

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- This why in classification problems it is important to evaluate class-specific precision via the following four measures:

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- As one can easily see, all four measures are related to each other. In particular, the following two identities must always hold:

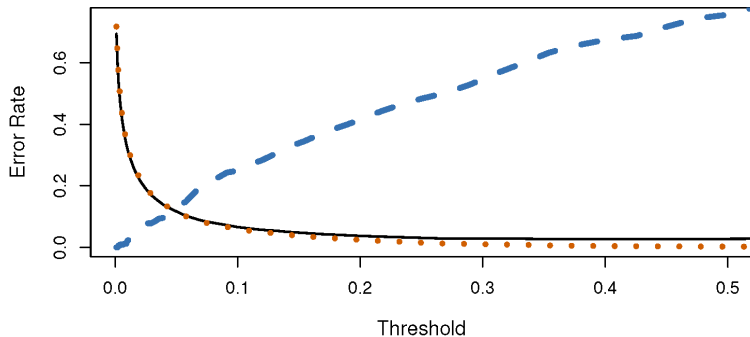
$$TNR + FPR = 100\% \quad \text{and} \quad TPR + FNR = 100\%$$

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The table on the previous slide was constructed using the rule $\hat{Y} = 1$ if $\hat{\Pr}(Y = 1|\mathbf{X}) > 0.5$, because 0.5 is the most common probability threshold used for classification predictions. However, the values of all 4 goodness-of-fit metrics will change if we change this threshold.

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Black line: total error rate

Blue dashes: FNR

Orange dots: FPR

Based on this chart, we might want to set our threshold to 0.05 to achieve better error rate composition.

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$$\ln \left(\frac{p(\mathbf{X})}{1 - p(\mathbf{X})} \right) = \mathbf{X}\beta \quad \Rightarrow \quad \beta_j = \frac{\partial \ln \left(\frac{p(\mathbf{X})}{1 - p(\mathbf{X})} \right)}{\partial X_j}$$

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- **Generalized choice models and information theory** (Matejka, F. and McKay, A. (2015)).