Classification models

Filipe Rodrigues

Francisco Pereira

DTU Management Engineering
Department of Management Engineering

Outline

- Case study: Modeling travel mode choices
- Logistic regression
- Generalized linear models (GLMs)
- Hierarchical models

Modeling travel mode choices

- Travel diary data
  - 394 survey observations from 80 individuals
  - 4 travel modes: plane, train, bus or car
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- Trip attributes (features):
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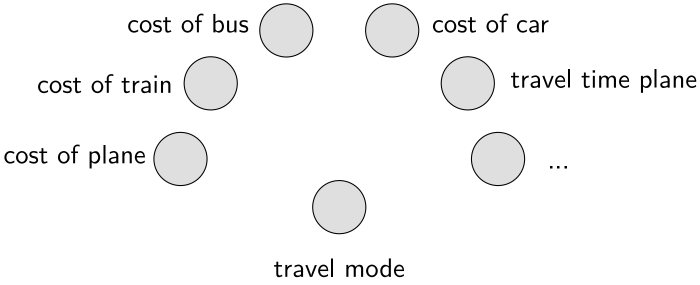
  - Household income
  - Traveling group size
- Some possible applications:
  - Understanding people's choices
  - Developing pricing policies
  - Incentivising mode change
  - Suggesting car pooling

Modeling travel mode choices (cont'd)

- Let's start thinking about the graphical model...



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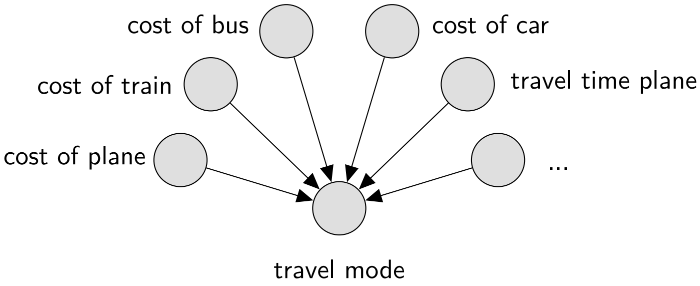

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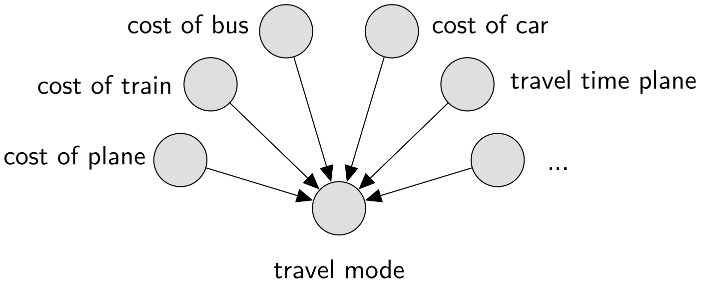
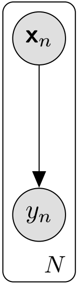


- What distribution should we assign to the "travel mode" variable?
  - Travel mode is a **discrete variable**!
  - We are now in a **classification** setting
- How should we model the dependency of the travel mode on the other variables?

Discrete output variables

- We can represent our model for the entire dataset compactly as:



N is the number of trips in the dataset
y_n is the travel mode of the n^{th} trip in the dataset
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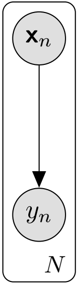

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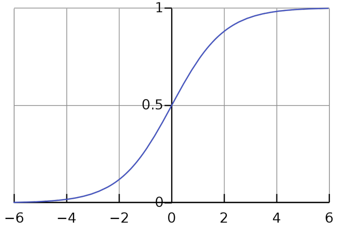
- Looks familiar?
- But how should we model the dependency of y_n on $\mathbf{x}_n$?
    - We can assume a parameterized linear relationship: $y_n = \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n$
    - But $y_n \notin \mathbb{R}$! Instead: $y_n \in \{$plane, train, bus, car$\}$

Binary logistic regression

- Consider the binary case: $y_n \in \{0, 1\}$
- We need a function that maps from $\mathbb{R}$ to $[0, 1]$
- A sigmoid (“S"-shaped) function does precisely that!
- E.g. logistic sigmoid:

$$\begin{aligned}\text{Sigmoid}(z) &= \frac{1}{1+e^{-z}} \\ &= \frac{e^z}{e^z+1}\end{aligned}$$



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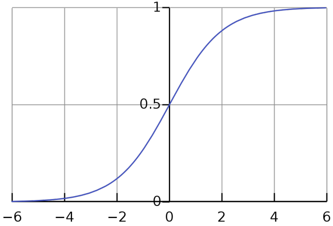

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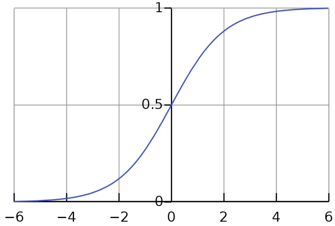

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- The probability of class “0" is simply: $p(y_n = 0) = 1 - \text{Sigmoid}(z_n)$

Binary logistic regression as a graphical model

- We have a dataset $\mathcal{D}$ consisting of N observations of the targets $y_n \in \{0, 1\}$ which depend on their corresponding explanatory variables $\mathbf{x}_n$

$$\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N}$$

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  (1) Draw coefficients $\beta \sim \mathcal{N}(\beta|\mathbf{0}, \lambda\mathbf{I})$
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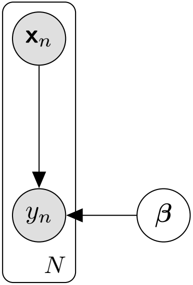

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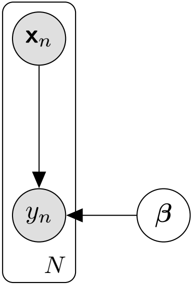

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- Joint probability distribution factorizes as

$$p(\mathbf{y}, \beta|\mathbf{X}, \lambda) = \underbrace{p(\beta|\lambda)}_{\text{prior}} \times \underbrace{\prod_{n=1}^{N} p(y_n|\beta, \mathbf{x}_n)}_{\text{likelihood}}$$

where $\mathbf{y} = \{y_n\}_{n=1}^N$, $\mathbf{X} = \{\mathbf{x}_n\}_{n=1}^N$ and β are the model parameters.

Multi-class logistic regression

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$$\text{Softmax}(\mathbf{x}_n, \boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_C)_c = \frac{\exp(\boldsymbol{\beta}_c^\mathsf{T} \mathbf{x}_n)}{\sum_{k=1}^C \exp(\boldsymbol{\beta}_k^\mathsf{T} \mathbf{x}_n)}, \quad \text{for } c \in \{1, \dots, C\}$$

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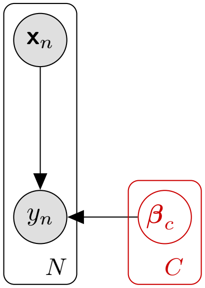
- The output of the softmax is then a vector $\boldsymbol{\eta} = [\eta_1, \dots, \eta_C]$ where $\eta_c = \text{Softmax}(\mathbf{x}_n, \boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_C)_c$
- The value of η_c can be interpreted as the probability of the n^{th} instance belonging to class c
- The softmax ensures that $\sum_{c=1}^{C} \eta_c = 1$

Multi-class logistic regression as a graphical model

- Updated graphical model



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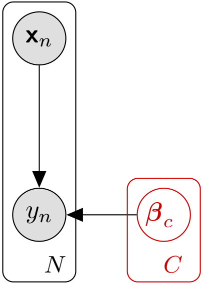

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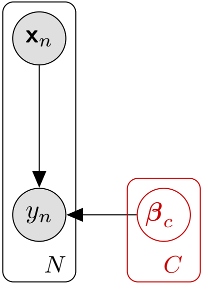

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Inference

- **Goal:** compute **posterior** distribution on $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_C$
- Following Bayes' theorem

$$\underbrace{p(\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_C | \mathbf{y}, \mathbf{X}, \lambda)}_{\text{posterior}} \propto \underbrace{\left(\prod_{c=1}^{C} \mathcal{N}(\boldsymbol{\beta}_c | \mathbf{0}, \lambda \mathbf{I}) \right)}_{\text{prior}}$$
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- Exact inference is intractable
- Must resort to **approximate inference** methods
- Not a problem for Stan :-)

Playtime!

- Ancestral sampling from multi-class logistic regression model
    - See "Logistic regression - Ancestral sampling.ipynb" notebook
    - Expected duration: 15 minutes
- Bayesian multi-class logistic regression model of travel mode choices
    - See "Travel mode choice - Logistic regression.ipynb" notebook
    - Expected duration: 1 hour

Generalized linear models (GLMs)

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  - Linear regression
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- In other words, we just changed the **form of the likelihood**!
- All belong to a general class of models called **generalized linear models**
  - The idea is to use a general exponential family for the response distribution
  - Can handle real, binary, categorical, positive real, positive integer and ordinal responses

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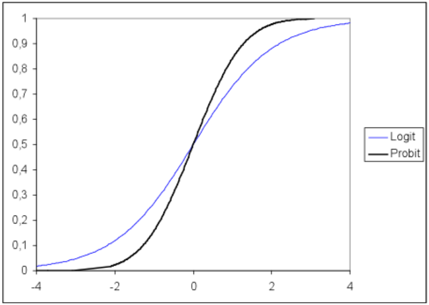

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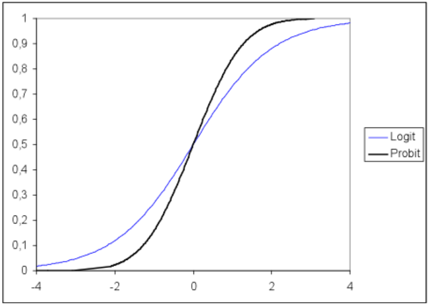

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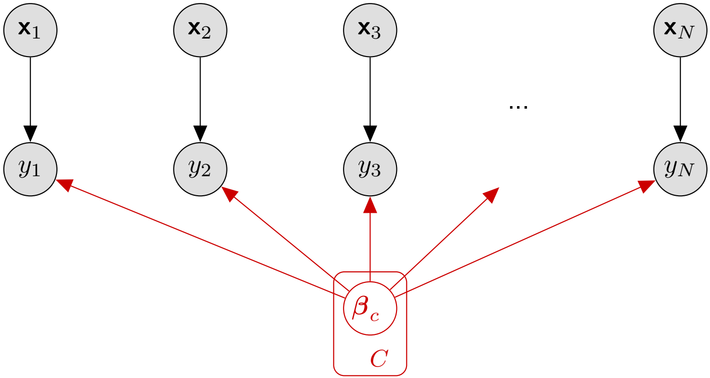
Playtime!

- Probit regression vs logistic regression model
- See "Travel mode choice - Probit regression.ipynb" notebook

Going back to our travel mode choice case study...

- Let's revise the **modeling assumptions** that we made



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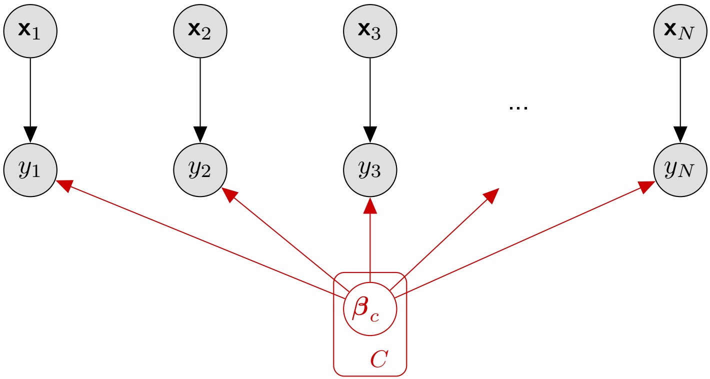

- Single set of parameters $\{\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_C\}$ for **all** the observations
  - This corresponds to saying that all individuals give the same importance (weight) to all the features (e.g. travel time) and have the same biases!

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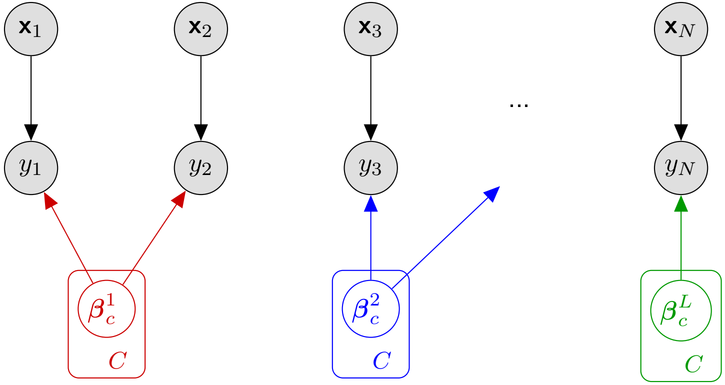
- Alternatively, we can assign each individual his/her own parameters



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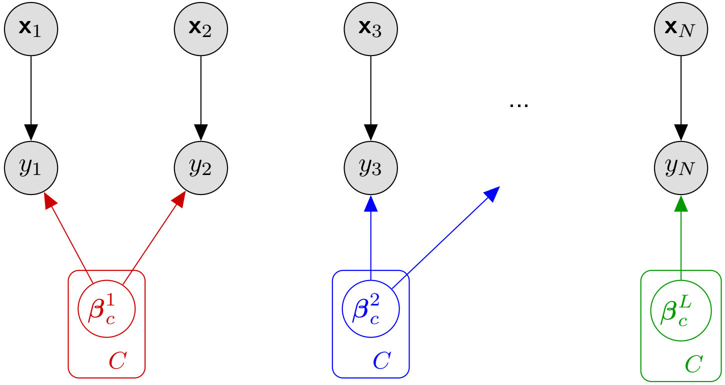
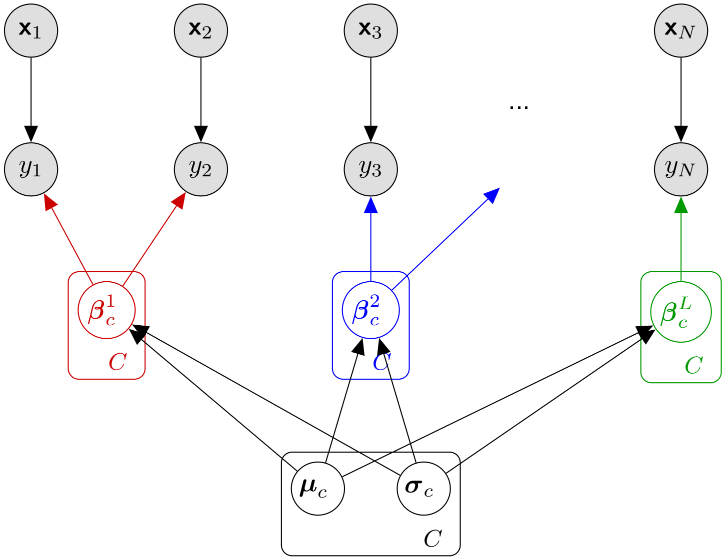


- Each individual $l \in \{1, \ldots, L\}$ gets his/her own set of parameters $\{\beta_1^l, \ldots, \beta_C^l\}$
  - Allows to capture personalized preferences and biases
  - But can lead to terrible overfitting! (more parameters than observations)

Going back to our travel mode choice case study...

- A compromise between the two: **hierarchical models**



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- A compromise between two extremes:
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Note

This concept can also be applied to other types of models! E.g. linear regression, poisson regression, etc.

Hierarchical logistic regression model

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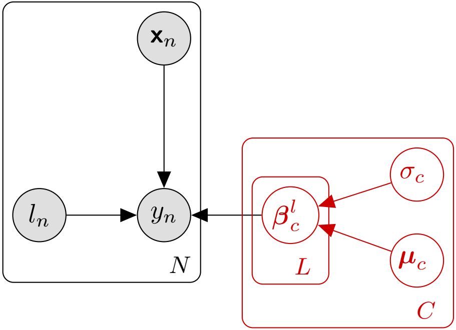

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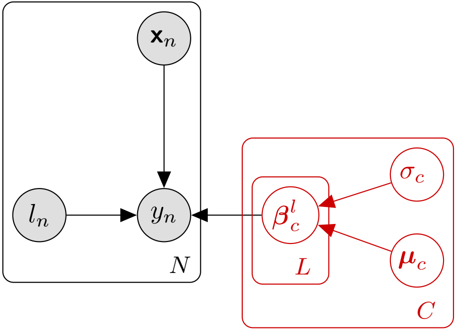

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- Joint probability distribution:

$$p(\mathbf{y}, \mathbf{B}^1, \dots, \mathbf{B}^L, \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_C, \sigma_1, \dots, \sigma_C | \mathbf{X}, \mathbf{l})$$

$$= \underbrace{\left(\prod_{c=1}^{C} p(\boldsymbol{\mu}_c)\, p(\sigma_c) \prod_{l=1}^{L} p(\boldsymbol{\beta}_c^l | \boldsymbol{\mu}_c, \sigma_c) \right)}_{\text{hierarchical prior}} \times \underbrace{\prod_{n=1}^{N} p(y_n | \mathbf{x}_n, l_n, \mathbf{B}^1, \dots, \mathbf{B}^L)}_{\text{likelihood}}$$

where we defined $\mathbf{B}^l = \{\beta_1^l, \dots, \beta_C^l\}$

Hierarchical logistic regression model

- Generative process

(1) For each class $c \in \{1, \ldots, C\}$

    (a) Draw global mean parameters $\boldsymbol{\mu}_c \sim \mathcal{N}(\boldsymbol{\mu}_c | \mathbf{0}, \lambda \mathbf{I})$
    (b) Draw global variance parameter $\sigma_c \sim \mathcal{N}(\sigma_c | 0, \tau)$
    (c) For each level $l \in \{1, \ldots, L\}$
        (a) Draw coefficients $\boldsymbol{\beta}_c^l \sim \mathcal{N}(\boldsymbol{\beta}_c^l | \boldsymbol{\mu}_c, e^{\sigma_c} \mathbf{I})$

(2) For each feature vector $\mathbf{x}_n$

    (a) Draw class $y_n \sim \text{Multinomial}(y_n | \text{Softmax}(\mathbf{x}_n, \boldsymbol{\beta}_1^{l_n}, \ldots, \boldsymbol{\beta}_C^{l_n}))$

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- There are many variants of this that we can consider
  - A vector of variances $\boldsymbol{\sigma}_c$ rather than a single variance σ_c for all the features
  - Different prior distributions on $\boldsymbol{\mu}_c$, σ_c and even $\boldsymbol{\beta}_c^l$
  - Hierarchical prior only on the biases (intercepts) rather than on all the $\boldsymbol{\beta}_c$
  - More levels, etc.

Playtime!

- Bayesian **hierarchical** multi-class logistic regression model of travel mode choices
- Each individual has his/her own bias towards certain travel modes
- See "Travel mode choice - Hierarchical models.ipynb" notebook
- Expected duration: 1 hour