

Handling missing values: model-based approaches (continued)



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MSc Data Science

Recap on missing values

Mathematical framework

Statistical models of incomplete data

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Example: heath records

	Center	Accident	Age	Sex	Weight	Height	BMI	BP	SBP
1	Beaujon	Fall	54	m	85	NR	NR	180	110
2	Lille	Other	33	m	80	1.8	24.69	130	62
3	Pitie Salpetriere	Gun	26	m	NR	NR	NR	131	62
4	Beaujon	AVP moto	63	m	80	1.8	24.69	145	89
6	Pitie Salpetriere	AVP bicycle	33	m	75	NR	NR	104	86
7	Pitie Salpetriere	AVP pedestrian	30	w	NR	NR	NR	107	66
9	HEGP	White weapon	16	m	98	1.92	26.58	118	54
10	Toulon	White weapon	20	m	NR	NR	NR	124	73

.....

	SpO2	Temperature	Lactates	Hb	Glasgow	Transfusion
1	97	35.6	<NA>	12.7	12	yes	
2	100	36.5	4.8	11.1	15	no	
3	100	36	3.9	11.4	3	no	
4	100	36.7	1.66	13	15	yes	
6	100	36	NM	14.4	15	no	
7	100	36.6	NM	14.3	15	yes	
9	100	37.5	13	15.9	15	yes	
10	100	36.9	NM	13.7	15	no	

Figure: Traumabase data set (figure from Julie Josse).

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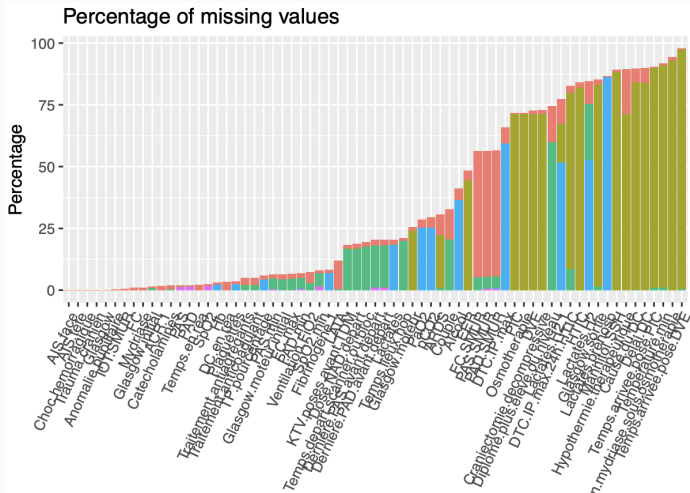


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The need for some assumptions

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Example 1 (bad thermometer): we have a thermometer that breaks when the temperature is above 39 degrees Celsius. Then, **it is impossible to learn the distribution of temperatures above 39 degrees, even given a very large data set!**

When learning with missing values, **we need to make strong assumptions on the missingness process.** We will see some of these assumptions today, in particular the ones called **missing completely at random (MCAR)** and **missing at random (MAR).**

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This explains why **model-based approaches are a natural way to deal with missing values.**

A mathematical framework for incomplete data

We assume that there exists a complete data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$. We do not observe \mathbf{X} , and only have access to an incomplete version $\mathbf{Z} \in \tilde{\mathbb{R}}^{n \times p}$ where some values have been replaced by NAs. The values of the observed data matrix \mathbf{Z} belong to $\tilde{\mathbb{R}} = \mathbb{R} \cup \{\text{NA}\}$.

We also define a binary matrix $\mathbf{M} \in \{0, 1\}^{n \times d}$ whose nonzero entries correspond to missing values.

$$\mathbf{X} = \begin{pmatrix} 1 & 3 & 9 \\ 2 & 7 & 0 \end{pmatrix}, \mathbf{M} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \mathbf{Z} = \begin{pmatrix} \text{NA} & 3 & \text{NA} \\ 2 & \text{NA} & \text{NA} \end{pmatrix}.$$

Keep in mind that \mathbf{X} is hidden: we only have access to \mathbf{M} and \mathbf{Z} , and we will need to build our models and algorithms accordingly.

Supervised vs unsupervised

To keep things simple, we are going to consider **unsupervised learning of continuous data** $\mathbf{X} \in \mathbb{R}^{n \times d}$.

If you want to look at the supervised case, pretty much everything we're going to see today is still valid if you replace \mathbf{X} by (\mathbf{X}, \mathbf{Y}) . Of course, a few things will need to be adapted.

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All the data we have access to are in \mathbf{Z} , so a first idea would be to directly model \mathbf{Z} . The issue with this is that **the entries of \mathbf{Z} live in $\tilde{\mathbb{R}} = \mathbb{R} \cup \{\text{NA}\}$, which is not a well-behaved mathematical set.**

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- **(\mathbf{X}, \mathbf{M}) lives in the easier-to-deal-with space $\mathbb{R}^{n \times d} \times \{0, 1\}^{n \times p}$** , and in the rest of the course, we learned how to create statistical models for data that lives in this kind of space,

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- a joint model $p(\mathbf{X}, \mathbf{M})$ will imply a model $p(\mathbf{Z})$, so **we are still indirectly modelling \mathbf{Z} .**

Building a joint model $p(\mathbf{X}, \mathbf{M})$

We will call $p(\mathbf{X}, \mathbf{M})$ a joint model, because it jointly models the features \mathbf{X} and the missingness pattern \mathbf{M} . Part of the features are not observed so this will be a latent-variable model (the latent variables being the missing values).

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Today, we will focus on models where the ordering of the observations does not matter, so we will assume that $(\mathbf{x}_1, \mathbf{m}_1), \dots, (\mathbf{x}_n, \mathbf{m}_n)$ (the rows of \mathbf{X} and \mathbf{M}), are independent and identically distributed samples from a distribution $p(\mathbf{x}, \mathbf{m})$. This means that the model can be written

$$p(\mathbf{X}, \mathbf{M}) = \prod_{i=1}^n p(\mathbf{x}_i, \mathbf{m}_i).$$

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In that context, what we "just" need to specify is $p(\mathbf{x}, \mathbf{m})$, a distribution over $\mathbb{R}^d \times \{0, 1\}^d$. Now, we will look at the assumptions we mentioned in the beginning of the lecture.

Building a joint model $p(\mathbf{x}, \mathbf{m})$

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Now, what's left is to specify $p(\mathbf{m}|\mathbf{x})$. In general, this is very hard, and we usually need to have strong knowledge about the problem at hand. Indeed, let us go back to the election example: we would need to know which voters are more likely not to respond to model $p(\mathbf{m}|\mathbf{x})$ properly (and knowing this is hard!). Surprisingly, under some suitable assumptions, it is actually possible to not model $p(\mathbf{m}|\mathbf{x})$ at all, similarly to when we did not model $p(\mathbf{x})$ in logistic regression.

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A convenient thing is to split a complete feature vector \mathbf{x} into **observed features \mathbf{x}^{obs}** and **missing ones \mathbf{x}^{miss}** , such that $\mathbf{x} = (\mathbf{x}^{obs}, \mathbf{x}^{miss})$. Using this in the equation gives

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The likelihood of an incomplete data point is the marginal distribution of what we observe **$p(\mathbf{x}^{obs}, \mathbf{m})$** . This can be written

$$p(\mathbf{x}^{obs}, \mathbf{m}) = \int p(\mathbf{m}|\mathbf{x}^{obs}, \mathbf{x}^{miss})p(\mathbf{x}^{obs}, \mathbf{x}^{miss})d\mathbf{x}^{miss}.$$

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We want to simplify

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A first way to do this is to assume that \mathbf{m} and \mathbf{x} are actually independent. This is called the missing completely at random (MCAR) assumption. In that case,

$$p(\mathbf{m}|\mathbf{x}^{obs}, \mathbf{x}^{miss}) = p(\mathbf{m}),$$

and we can write

$$p(\mathbf{x}^{obs}, \mathbf{m}) = p(\mathbf{m}) \int p(\mathbf{x}^{obs}, \mathbf{x}^{miss})d\mathbf{x}^{miss} = p(\mathbf{m})p(\mathbf{x}^{obs}).$$

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Let's assume that we have chose a parametric model $p_\theta(\mathbf{x})$ for the features. Under the MCAR assumption, the likelihood of the data is

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^n \log p_\theta(\mathbf{x}_i^{obs}, \mathbf{m}_i) = \sum_{i=1}^n \log p(\mathbf{m}_i) p_\theta(\mathbf{x}_i^{obs}) \\ &= \sum_{i=1}^n \log p(\mathbf{m}_i) + \sum_{i=1}^n \log p_\theta(\mathbf{x}_i^{obs});\end{aligned}$$

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and since the **red** term does not depend on θ , **maximising $\ell(\theta)$ is equivalent to maximising**

$$\sum_{i=1}^n \log p_\theta(\mathbf{x}_i^{obs}),$$

which is the likelihood of the observed features only.

Going beyond MCAR

Under the quite strong MCAR assumption, we just have to maximise

$$\sum_{i=1}^n \log p_{\theta}(\mathbf{x}_i^{obs}),$$

to find a good value for θ . What happens when the MCAR assumption is violated? Kinda surprisingly, nothing changes under a much weaker assumption called missing at random (MAR).

Building a MAR joint model $p(\mathbf{x}, \mathbf{m}) = p(\mathbf{m}|\mathbf{x})p(\mathbf{x})$

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Missing at random (MAR) assume that

$$p(\mathbf{m}|\mathbf{x}^{obs}, \mathbf{x}^{miss}) = p(\mathbf{m}|\mathbf{x}^{obs}),$$

which means that \mathbf{m} and \mathbf{x}^{miss} are independent given the observed data \mathbf{x}^{obs} .

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What happens under MAR with $p(\mathbf{m}|\mathbf{x}^{obs}, \mathbf{x}^{miss}) = p(\mathbf{m}|\mathbf{x}^{obs})$?

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How to compute $p_{\theta}(\mathbf{x}_i^{obs})$ for a Gaussian?

Partitioned Gaussians

Given a joint Gaussian distribution $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}$ and

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix}, \quad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}$$
$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}, \quad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}.$$

Conditional distribution:

$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Lambda}_{aa}^{-1})$$
$$\boldsymbol{\mu}_{a|b} = \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b).$$

Marginal distribution:

$$p(\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa}).$$