Missing Data

and how to deal with them...

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Machine Learning development from Model-Centric to Data-Centric

Andrew Ng:

> When a system isn't performing well, many teams instinctually try to improve the code.
> But for many practical applications, it's more effective instead to focus on improving the data,

https://www.deeplearning.ai/the-batch/issue-84/

Model-Centric view

- Collect what data you can
- Develop a model good enough to deal with the noise in the data
- Hold the data fixed and iteratively improve the code/model

Data-Centric view

- The consistency of the data is paramount
- Use tools to improve the data quality
- Hold the model fixed and iteratively improve the data

https://www.deeplearning.ai/the-batch/issue-84/

From big data to good data

MLOps' most important task:

> ensure consistently high-quality data in all phases of the ML project lifecycle

Good data is

- Defined consistently
- Cover of important cases
- Has timely feedback from production data
- Sized appropriately

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Good data without missing data

- Getting high-quality data also includes tackling noise data
- Data can become noise caused of missings

Missing data

Can arise for many reasons:

- Non-Response e.g. in surveys
- Lost data due to machine or human mistakes
- Bug issues in non-mandatory fields
- join, merge
- Different variable per source
- Different number of categories per source
- …

The problem

```
x <- c(10, NA, 20, 30, 40, 20)

mean(x)
```

```
[1] NA
```

```
randomForest(Ozone ~ . , data=airquality)
```

```
Error in na.fail.default(structure(list(Ozone = c(41L, 36L, 12L, 18
```

The problem

- Many AI/ML/Data science methods are developed for complete data
- Using only the complete cases for the analysis can lead to dramatic information loss
- Inappropriate approach imposes noise or bias on data
- Can lead to incorrect conclusions due to absense of relevant information
- The quality of statistical analysis can be only as good as the quality of the data

Terminology

- **Full / complete data** $Z = (Z^{\text{obs}}, Z^{\text{mis}})$
- **Observed data** Z^{obs}
- **Unobserved / missing data** Z^{mis}
- **Complete cases** subset of rows without missing values
- Given $n \times p$ data matrix Z, which can contain missing data
- $Z = (Y, X)$, i.e. Y matrix dependent and X matrix independent variables
- Indicator matrix R build from Z as

$$R_{ij} = \begin{cases} 1 & \text{if } Z_{ij} \text{ obs} \\ 0 & \text{if } Z_{ij} \text{ mis} \end{cases} \quad \text{for } i = 1, \ldots, n \text{ and } j = 1, \ldots, p.$$

Types of missingness

Missing completely at random (MCAR)

Probability of missingness is completely independent from observed and unobserved/missing values:

$$P(r_i \mid z_i) = P(r_i \mid z_i^{\text{obs}}, z_i^{\text{mis}}) = P(r_i), \quad \text{for } i = 1, \ldots, n,$$

z_i^{obs} observed, z_i^{mis} missing values from the i-th row z_i of the data matrix Z

- No particular reason that the data is missing
- Often an unrealistic assumption
- **Example:** Weighing scale that ran out of batteries

Missing at random (MAR)

Probability of missingness of values is only dependent of the observed values z_i^{obs}

$$P(r_i \mid z_i) = P(r_i \mid z_i^{\text{obs}}, z_i^{\text{mis}}) = P(r_i \mid z_i^{\text{obs}}), \quad \text{for } i = 1, \ldots, n.$$

- More realistic than MCAR
- Modern missing data methods generally start from the MAR assumption
- **Example:** Weighing scale may produce more missing data when placed on a soft surface and type of surface is known

Missing not at random (MNAR)

Probability of missingness of values is dependent of the observed z_i^{obs} and unobserved values z_i^{mis}

$$P(r_i \mid z_i) = P(r_i \mid z_i^{\text{obs}}, z_i^{\text{mis}}), \quad \text{for } i = 1, \ldots, n.$$

- Cause of missingness it not known
- We cannot draw any conclusion from observed data
- **Example:** Weighing scale mechanism may wear out over time, but time is not part of the dataset

How to deal with missingness

Strategies to deal with missing data

- Prevention - impossible for ex-post analyses
- Dropping missing values
- Imputation techniques
  - Single imputation
  - Multiple imputation

Look at the data

Airquality Dataset

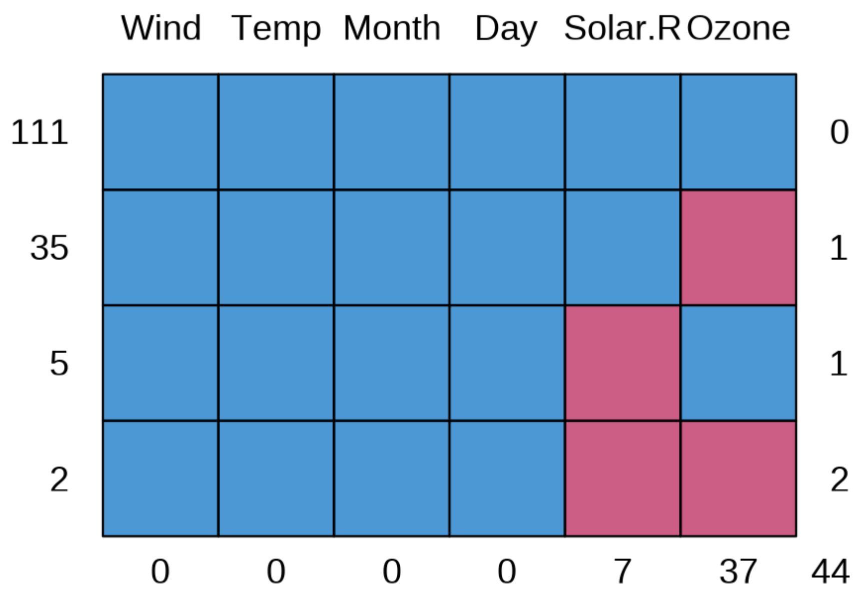
- Daily air quality measurements in New York, May to September 1973.
- Daily readings of the following air quality values for May 1, 1973 (a Tuesday) to September 30, 1973.
    - **Ozone:** Mean ozone in parts per billion from 1300 to 1500 hours at Roosevelt Island
    - **Solar.R:** Solar radiation in Langleys in the frequency band 4000–7700 Angstroms from 0800 to 1200 hours at Central Park
    - **Wind:** Average wind speed in miles per hour at 0700 and 1000 hours at LaGuardia Airport
    - **Temp:** Maximum daily temperature in degrees Fahrenheit at La Guardia Airport.

Source: The data were obtained from the New York State Department of Conservation (ozone data) and the National Weather Service (meteorological data).

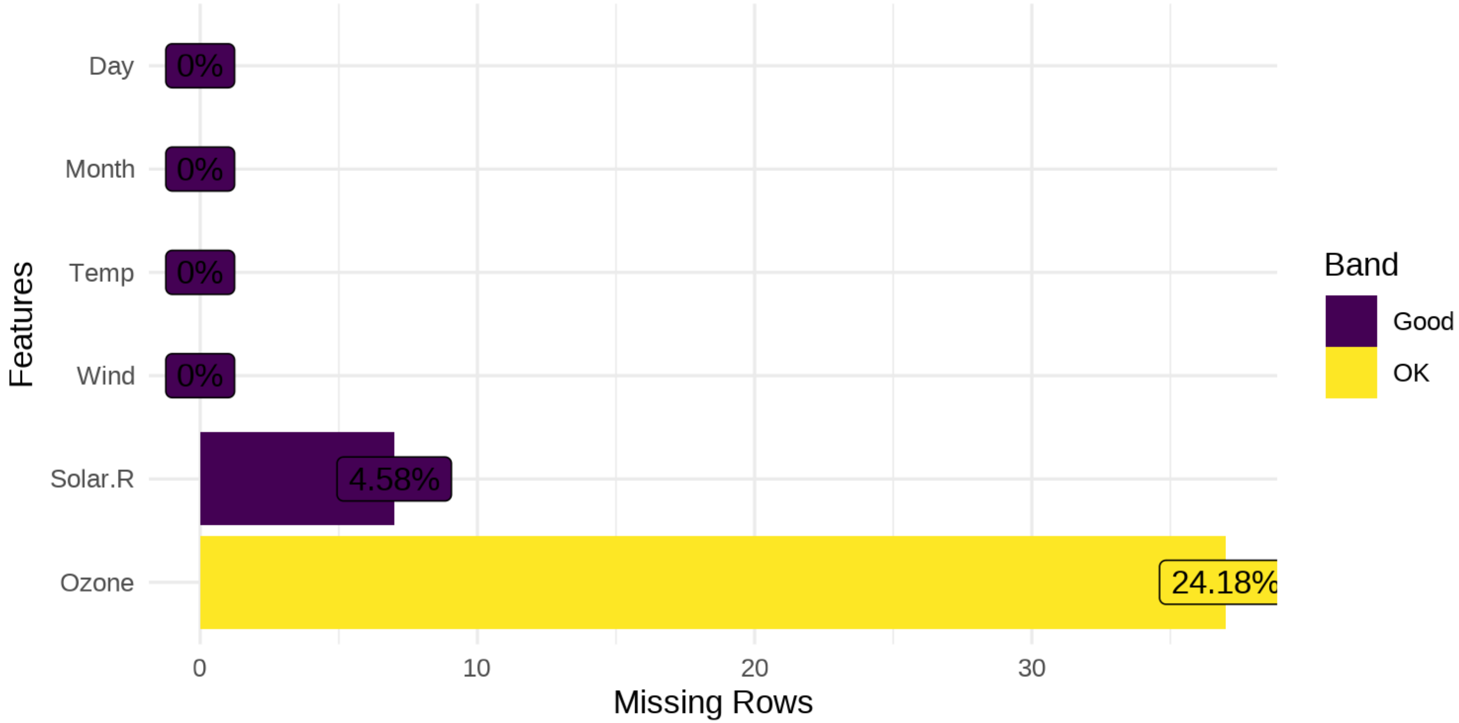
Airquality Dataset

Ozone	Solar.R	Wind	Temp	Month	Day
41	190	7.4	67	5	1
36	118	8.0	72	5	2
12	149	12.6	74	5	3
18	313	11.5	62	5	4
NA	NA	14.3	56	5	5
28	NA	14.9	66	5	6
23	299	8.6	65	5	7
19	99	13.8	59	5	8
8	19	20.1	61	5	9
NA	194	8.6	69	5	10

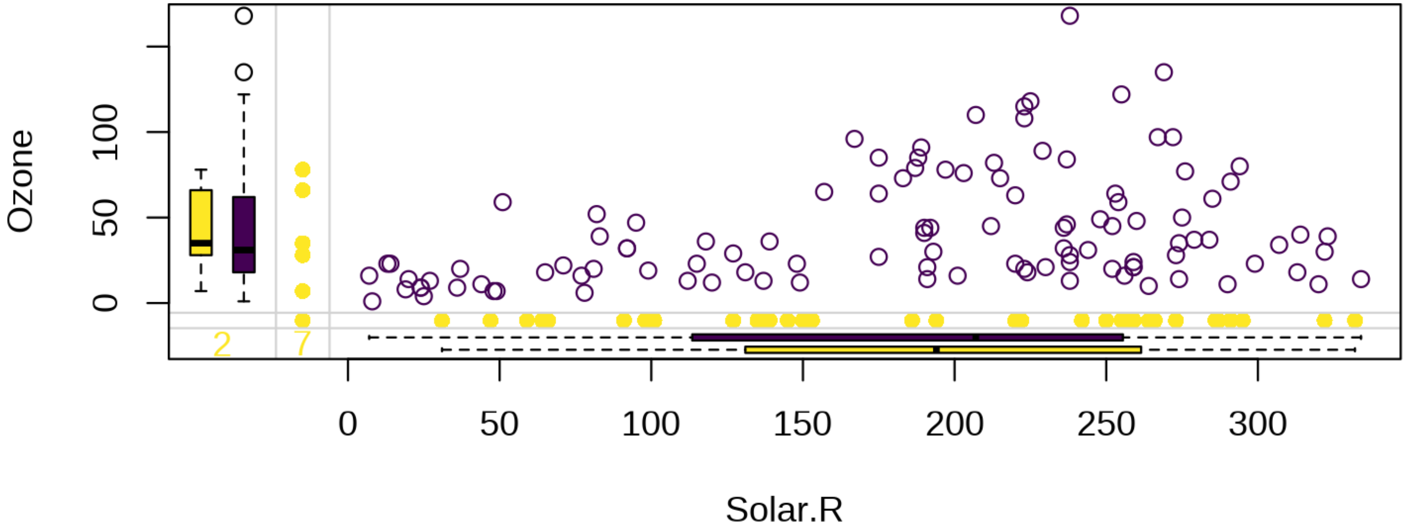
Missing data pattern



Missing value frequency



Marginplot



Dropping (ignoring) missing values

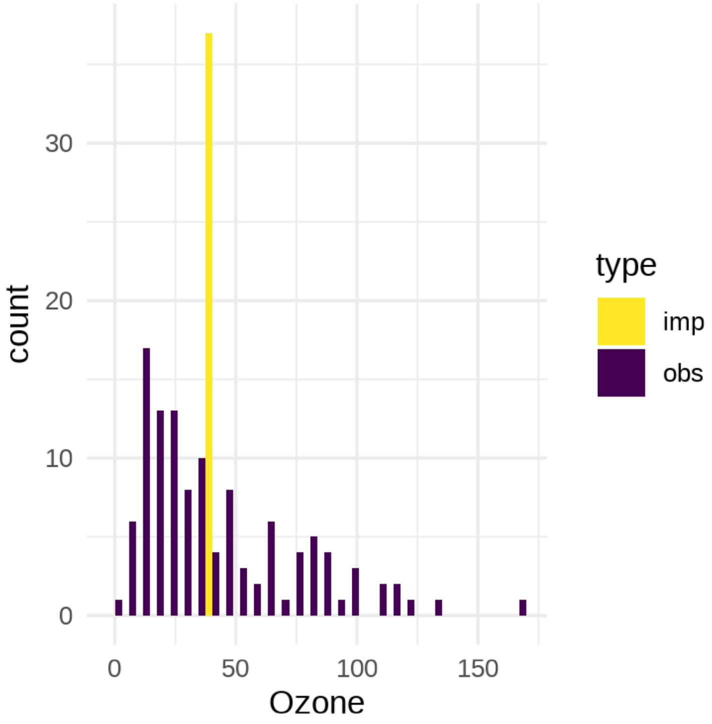
Listwise deletion

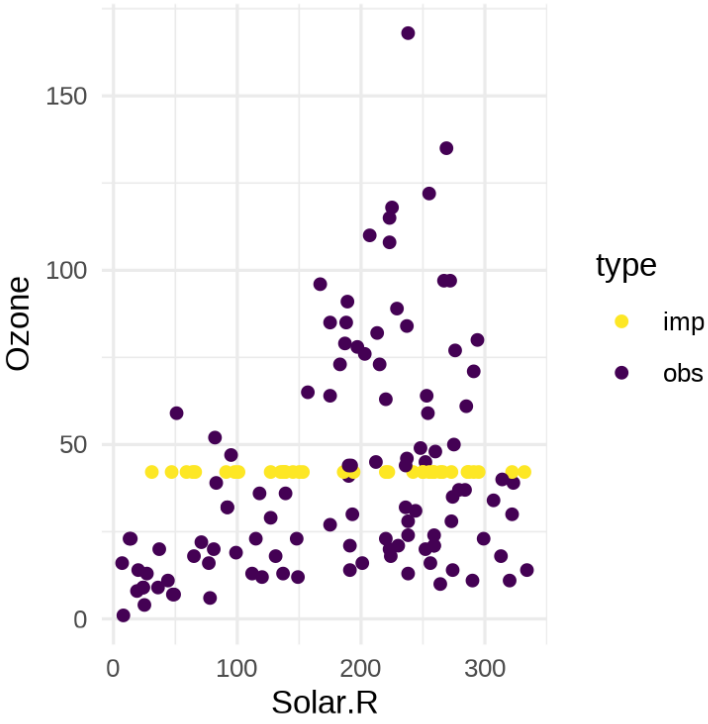
- Only the complete cases are analyzed
- Advantages:
  - Simple - Often the default way of handling incomplete data
  - Under MCAR: unbiased estimates of means, variances and regression weights
  - Schafer and Graham (2002): *If a missing data problem can be resolved by discarding only a small part of the sample, then the method can be quite effective.*
- Disadvantages:
  - Loss of information dependent on the fraction of missing data
  - Larger standard errors
  - Under MAR: biased, even for simple statistics like the mean

Mean/Median imputation

- Missing values are replaced by
  - The mean value for quantitative variables
  - The most frequently occurring category for qualitative variables
- Imputed value is an estimate, thus there is uncertainty about its true value
- Uncertainty is measued by its standard error
- Too small standard errors

Mean/Median imputation



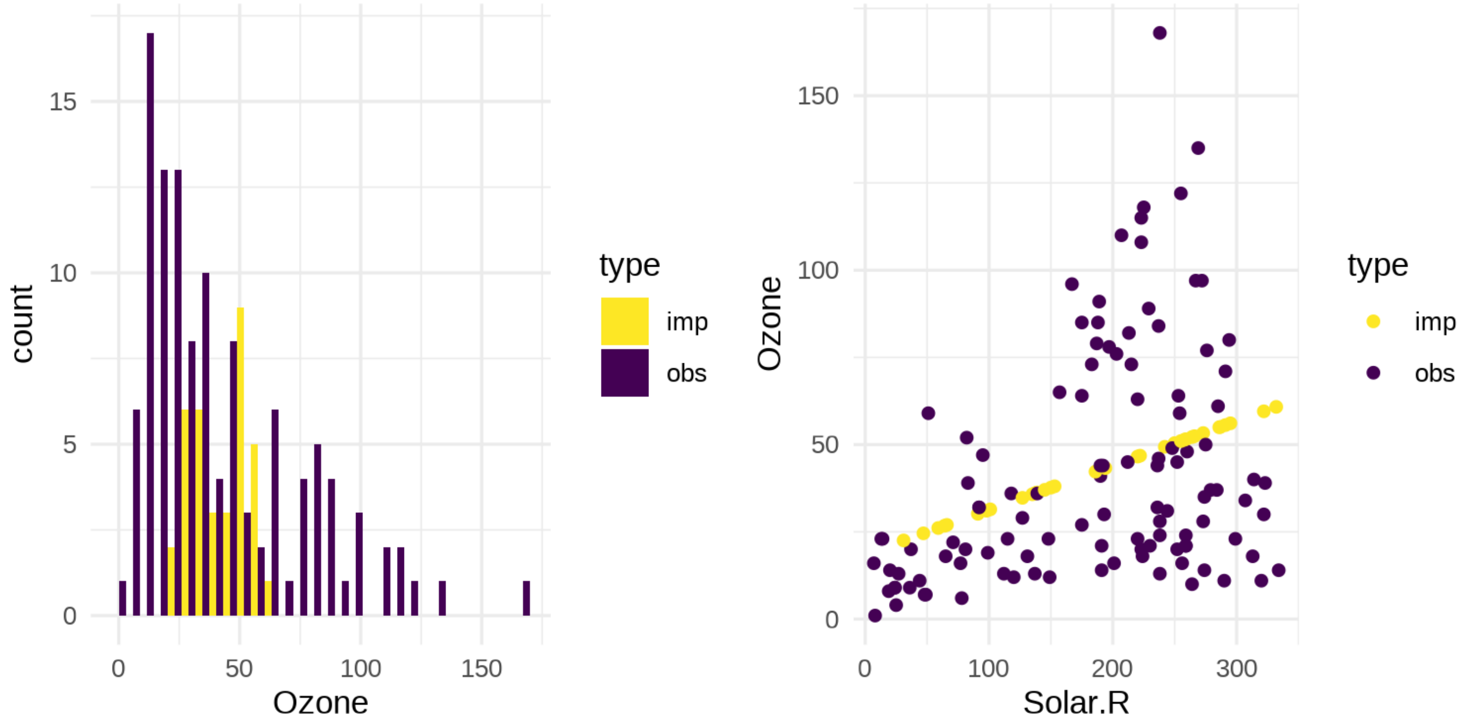


Regression Imputation

- Regression imputation incorporates knowledge of other variables
- The first step involves building a model from the observed data
- Calculate predictions for the incomplete cases under the fitted model

$$\text{Ozone} = \alpha + \beta_1(\text{Solar. R}) + \epsilon$$

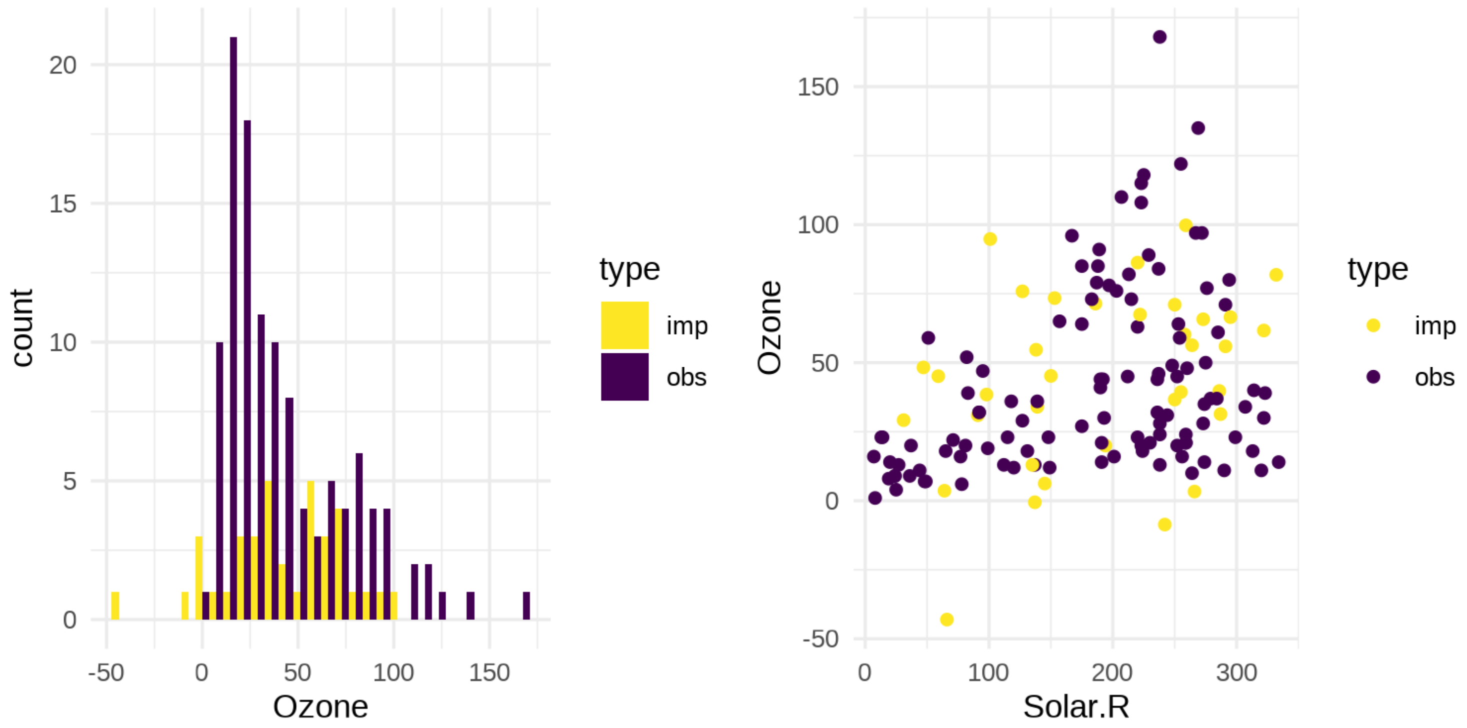
Regression Imputation



Stochastic Regression Imputation

- Regression imputation disadvantage:
  - Fitted model is used without error terms
  - Imputed results are too close to the regression line
  - Biased correlations, reduced the variance of the data
- Stochastic regression adds an error term when imputing the values

Stochastic Regression Imputation



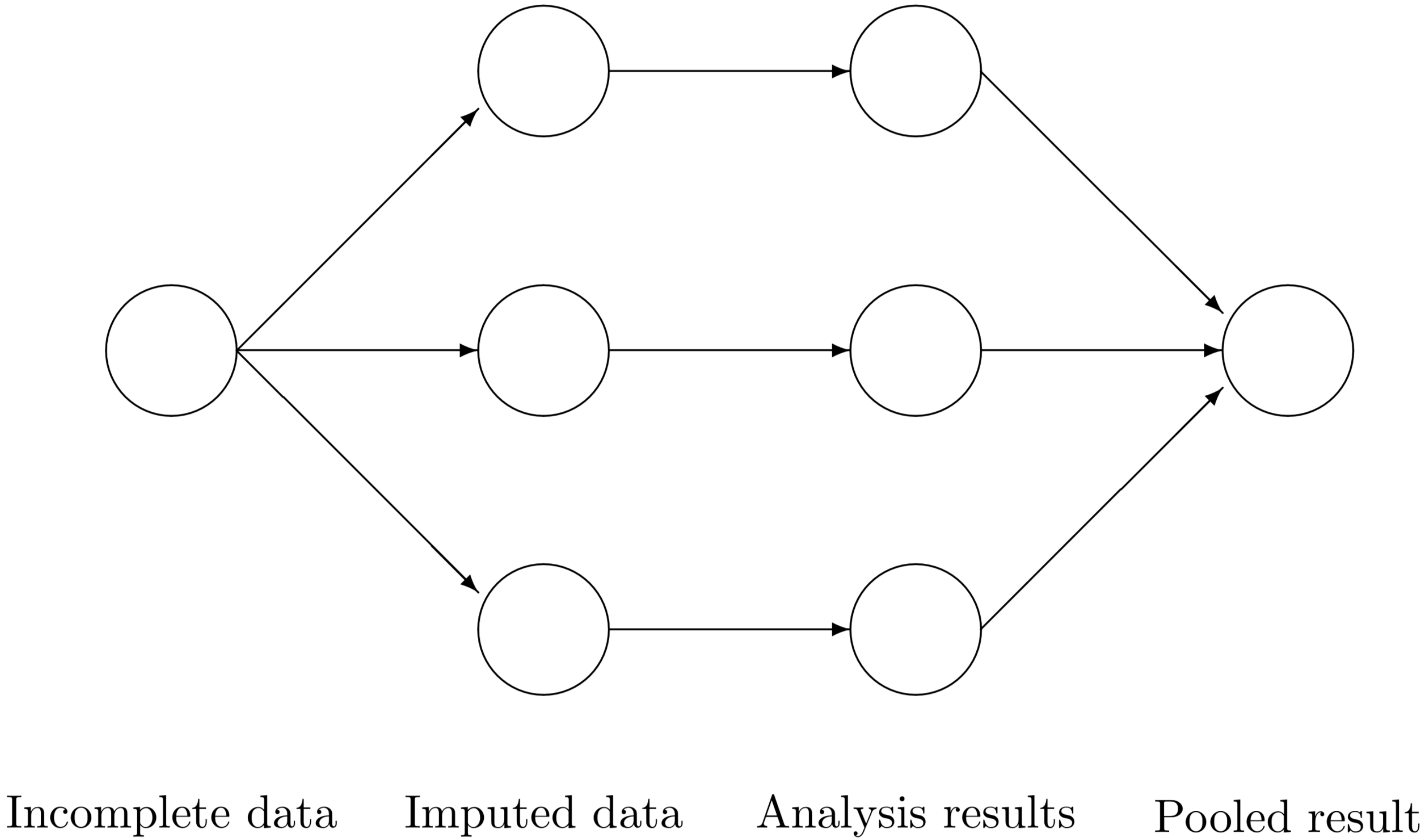
Multiple imputation

- Missing values are replaced by chained regression, where m complete datasets are generated (Raghunathan, Lepkowski, Van Hoewyk, and Solenberger (2001))
- Accounts for uncertainty by creating multiple imputed version of data
- Bootstrapping (subselection of the data, do the imputation, …)
- Generative models (draw samples from the estimated distribution)
- MICE (multivariate imputation by chained equations)

Multiple imputation (vanBuuren (2018))

1. Specify an imputation model $P(Y_j^{\text{mis}}|Y_j^{\text{obs}}, Y_{-j}, R)$ for variable Y_j with $j = 1, \ldots, p$.
2. For each j, fill in starting imputations $\dot{Y}_j^0$ by random draws from Y_j^{obs}.
3. Repeat for $t = 1, \ldots, m$.
4. Repeat for $j = 1, \ldots, p$.
5. Define $\dot{Y}_{-j}^t = (\dot{Y}_1^t, \ldots, \dot{Y}_{j-1}^t, \dot{Y}_{j+1}^{t-1}, \ldots, \dot{Y}_p^{t-1})$ as the currently complete data except Y_j.
6. Draw $\dot{\phi}_j^t \sim P(\phi_j^t|Y_j^{\text{obs}}, \dot{Y}_{-j}^t, R)$.
7. Draw imputations $\dot{Y}_j^t \sim P(Y_j^{\text{mis}}|Y_j^{\text{obs}}, \dot{Y}_{-j}^t, R, \dot{\phi}_j^t)$.
8. End repeat j.
9. End repeat t.

Multiple imputation



Source: https://stefvanbuuren.name/fimd/sec-nutshell.html

Multiple imputation

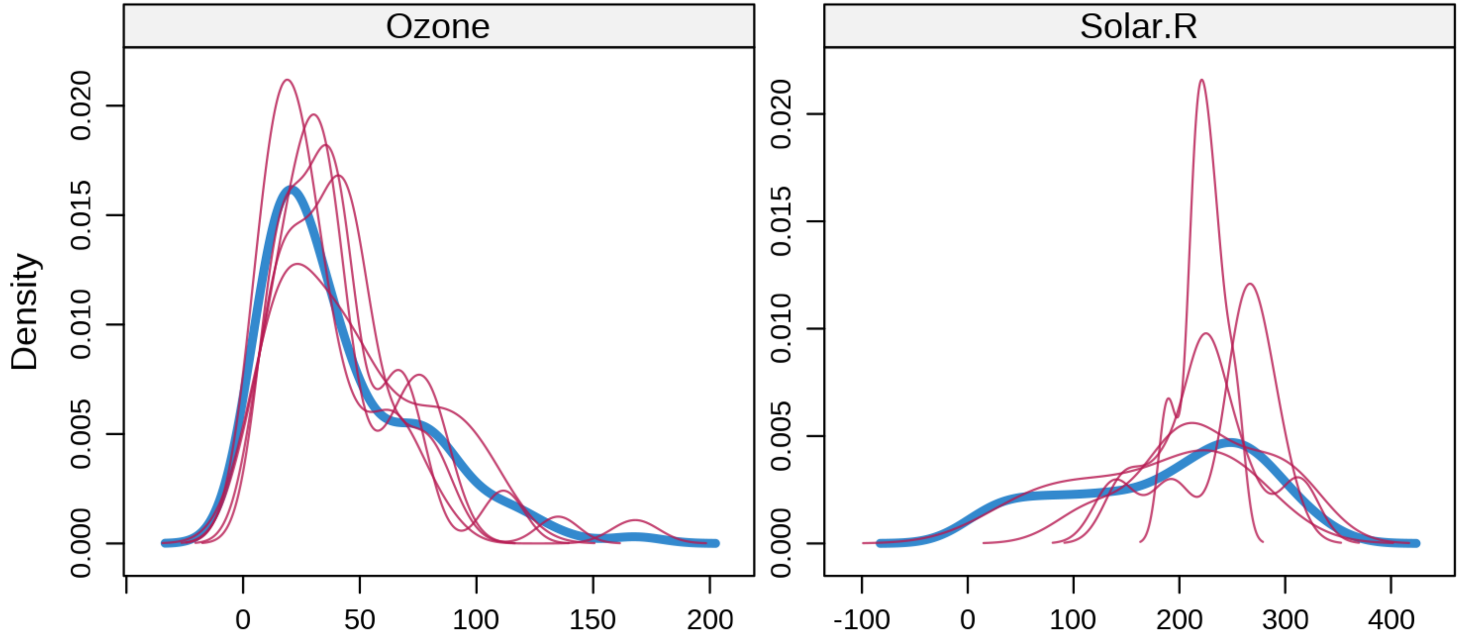
How large should m be (vanBuuren (2018))?

Classic advice: $m = 3, 5, 10$. More recently: set m higher: 20 to 100.

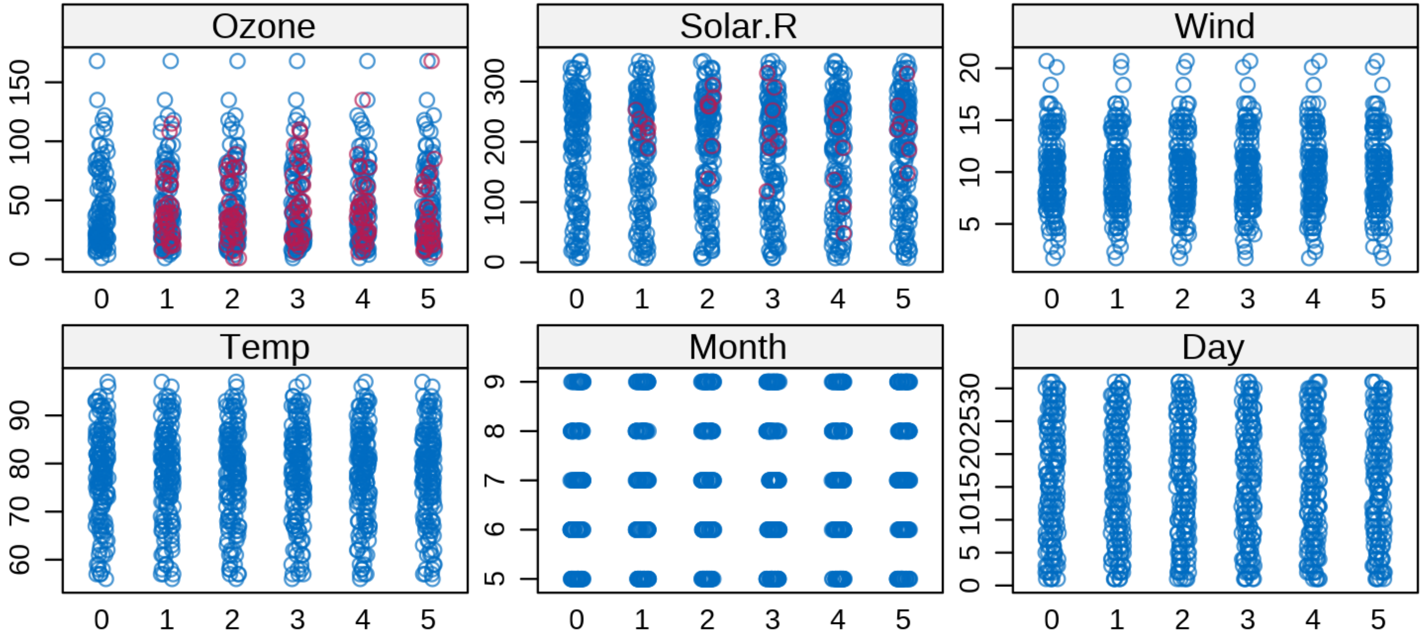
Some advice:

- Use $m = 5$ or $m = 10$ if the fraction of missing information is low
- Develop your model with $m = 5$. Do final run with m equal to percentage of incomplete cases

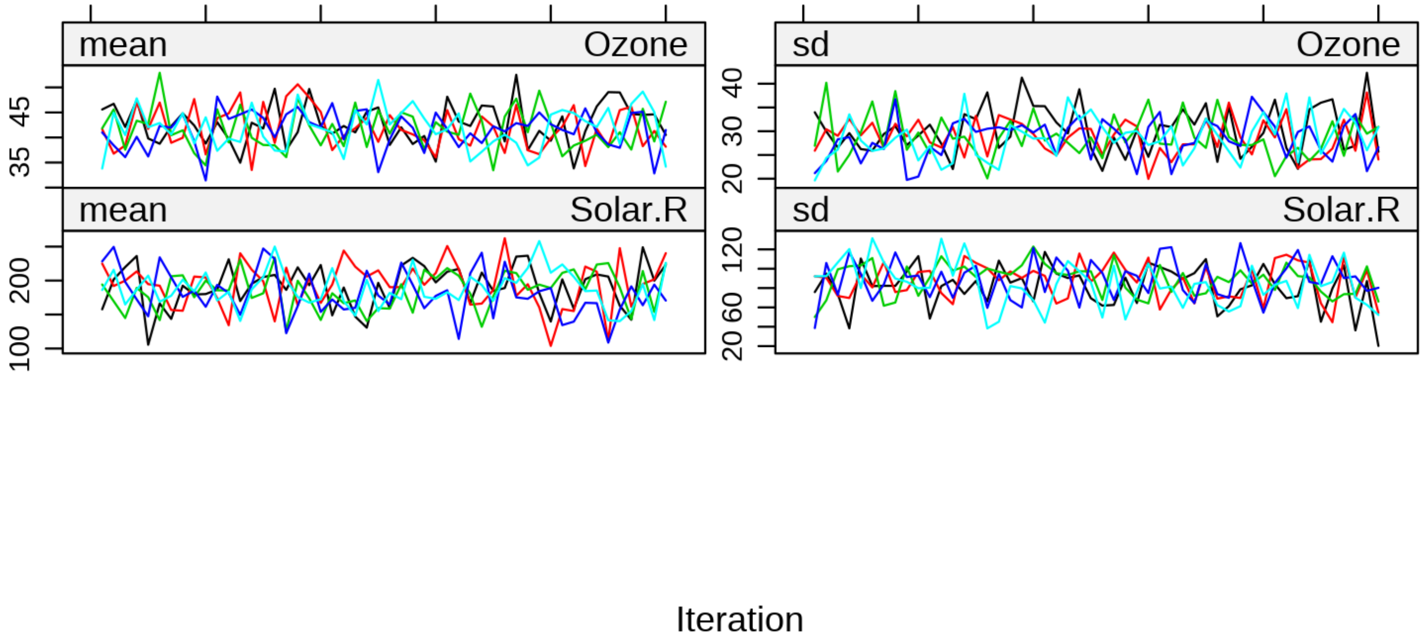
Multiple imputation



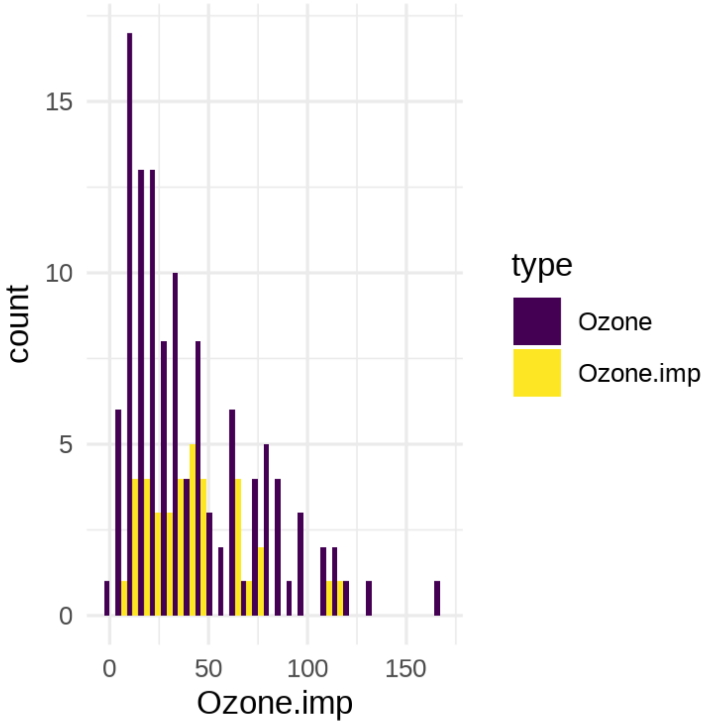
Multiple imputation

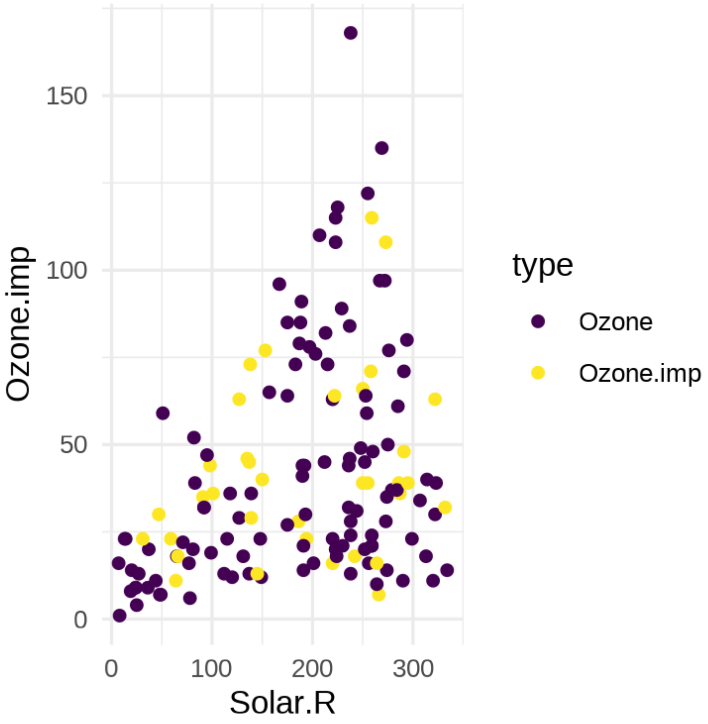


Multiple imputation



Multiple imputation





Multiple imputation in detail...

1. Start

Ozone	Solar.R	Wind	Temp	Month	Day
NA	194	8.6	69	5	10
7	NA	6.9	74	5	11
16	256	9.7	69	5	12

2. Mean Imputation

Ozone	Solar.R	Wind	Temp	Month	Day
11.5	194	8.6	69	5	10
7.0	225	6.9	74	5	11
16.0	256	9.7	69	5	12

Multiple imputation in detail...

3. Set Ozone to NA's / Regression on complete cases

Ozone	Solar.R	Wind	Temp	Month	Day
NA	194	8.6	69	5	10
7	225	6.9	74	5	11
16	256	9.7	69	5	12

4. Predict Ozone

Ozone	Solar.R	Wind	Temp	Month	Day
12.51	194	8.6	69	5	10
7.00	225	6.9	74	5	11
16.00	256	9.7	69	5	12

Multiple imputation in detail...

5. Set Solar.R to NA's / Regression on complete cases

Ozone	Solar.R	Wind	Temp	Month	Day
12.51	194	8.6	69	5	10
7.00	NA	6.9	74	5	11
16.00	256	9.7	69	5	12

6. Predict Solar.R

Ozone	Solar.R	Wind	Temp	Month	Day
12.51	194.00	8.6	69	5	10
7.00	201.41	6.9	74	5	11
16.00	256.00	9.7	69	5	12

Multiple imputation in detail...

7. Set Ozone to NA's / Regression on complete cases

Ozone	Solar.R	Wind	Temp	Month	Day
NA	194.00	8.6	69	5	10
7	201.41	6.9	74	5	11
16	256.00	9.7	69	5	12

Repeat until convergence

Software (R)

mice

Multiple imputation using Fully Conditional Specification (FCS) implemented by the MICE algorithm as described in Van Buuren and Groothuis-Oudshoorn (2011)

VIM

New tools for the visualization of missing and/or imputed values are introduced, which can be used for exploring the data and the structure of the missing and/or imputed values.

Amelia

Implements Bootstrap multiple imputation using EM to estimate the parameters, for quantitative data it imputes assuming a Multivariate Gaussian distribution.

Software (Python)

sklearn.impute

- SimpleImputer: Imputation transformer for completing missing values.
- IterativeImputer: Multivariate imputer that estimates each feature from all the others.
- KNNImputer: Imputation for completing missing values using k-Nearest Neighbors.

missingno

Small toolset of flexible and easy-to-use missing data visualizations and utilities that allows you to get a quick visual summary of the completeness (or lack thereof) of your dataset.

fancyimpute

A variety of matrix completion and imputation algorithms (including MICE) implemented in Python 3.6.

Best practices (vanBuuren (2018))

- Distinguishing the type of missingness is not easy, sometimes it's impossible
- The size and balance of data must be considered before distinguising the type
- Under MCAR, one can analyze the observed observation and ignore discard any missing observations
- **Rule of thumb:** Assume MAR unless there is a good reason not to!

Takeaways

- Understand the missing type and data before anything (tips: missing rate, balance, correlation, data size, …)
- There is no single magical method to deal with missingness, the right choice depends on your data
- Benefit from multiple imputation to account for uncertainty
- Be vigilant in using open source packages
- Check literature for new methodologies

Thank you! Questions?

Slides: https://github.com/wittmaan/missing-data

Literature

Raghunathan, T. E., J. M. Lepkowski, J. Van Hoewyk, et al. (2001). "A Multivariate Technique for Multiply Imputing Missing Values Using a Sequence of Regression Models". In: *Survey Methodology* 27, pp. 85-96.

Schafer, J. L. and J. W. Graham (2002). "Missing Data: Our View of the State of the Art". In: *Psychol Methods* 7, pp. 147-177.

vanBuuren, S. (2018). *Flexible Imputation of Missing Data*. second. Accessed: 2021-05-02. CRC Press.

vanBuuren, S. and K. Groothuis-Oudshoorn (2011). "mice: Multivariate Imputation by Chained Equations in R". In: *Journal of Statistical Software* 45, pp. 1-67.

Links

- https://www.deeplearning.ai/the-batch/issue-84/
- https://stefvanbuuren.name/publication/vanbuuren-2018/
- http://pol346.com/2021/week10_02.html#1
- https://htmlpreview.github.io/?https://raw.githubusercontent.com/ehsanx/spph504-007/master/Lab6/lab6part1.html
- https://rstudio-pubs-static.s3.amazonaws.com/445649_5f323f9cc6aa4333b404882e67e9c344.html
- https://s3.amazonaws.com/assets.datacamp.com/production/course_17404/slides/ch