# 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

  $\rightarrow$ *This will allow multiple models to do well*
- 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 (definition of labels y is unambiguous)
- Cover of important cases (good coverage of inputs x)
- Has timely feedback from production data (distribution covers data drift and concept drift)
- Sized appropriately

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

# Good data without missing data

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

# Missing data

**Missing data is everwhere** sooner or later anyone who does statistics will encounter 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 / incomplete data** $Z^{\text{obs}}$
- **Unobserved / missing data** $Z^{\text{mis}}$
- **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

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

# Types of missingness

# Missing completely at random (MCAR)

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

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

$z_i^{\text{obs}}$ observed, $z_i^{\text{mis}}$ 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 for missingness of values is only dependent of the observed values $z_i^{\text{obs}}$

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

- 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 for missingness of values is dependent of the observed $z_i^{\text{obs}}$ and unobserved values $z_i^{\text{mis}}$

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

- 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

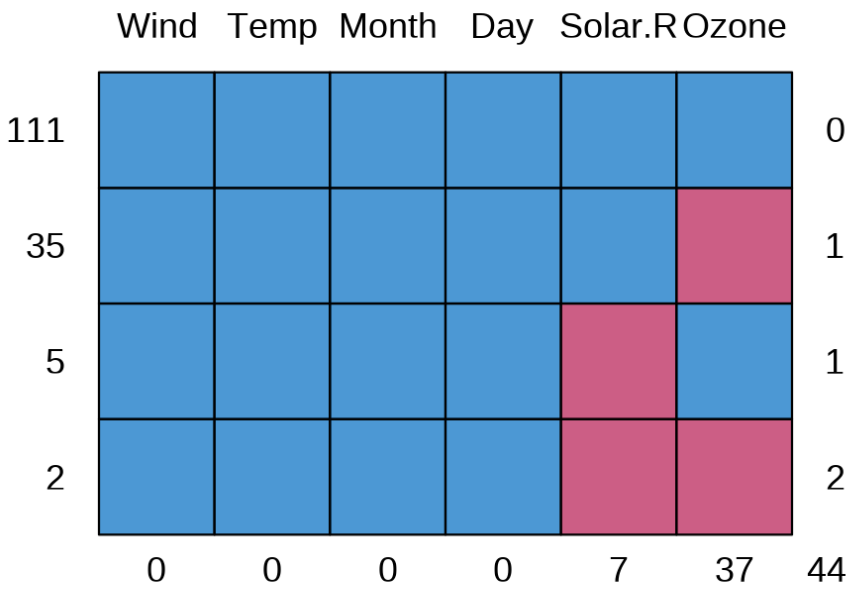
- Daily air quality measurements in New York, May to September 1973.
- Daily readings of the following air quality values for May 1, 1973 (a Tuesday) to September 30, 1973.
    - **Ozone:** Mean ozone in parts per billion from 1300 to 1500 hours at Roosevelt Island
    - **Solar.R:** Solar radiation 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).

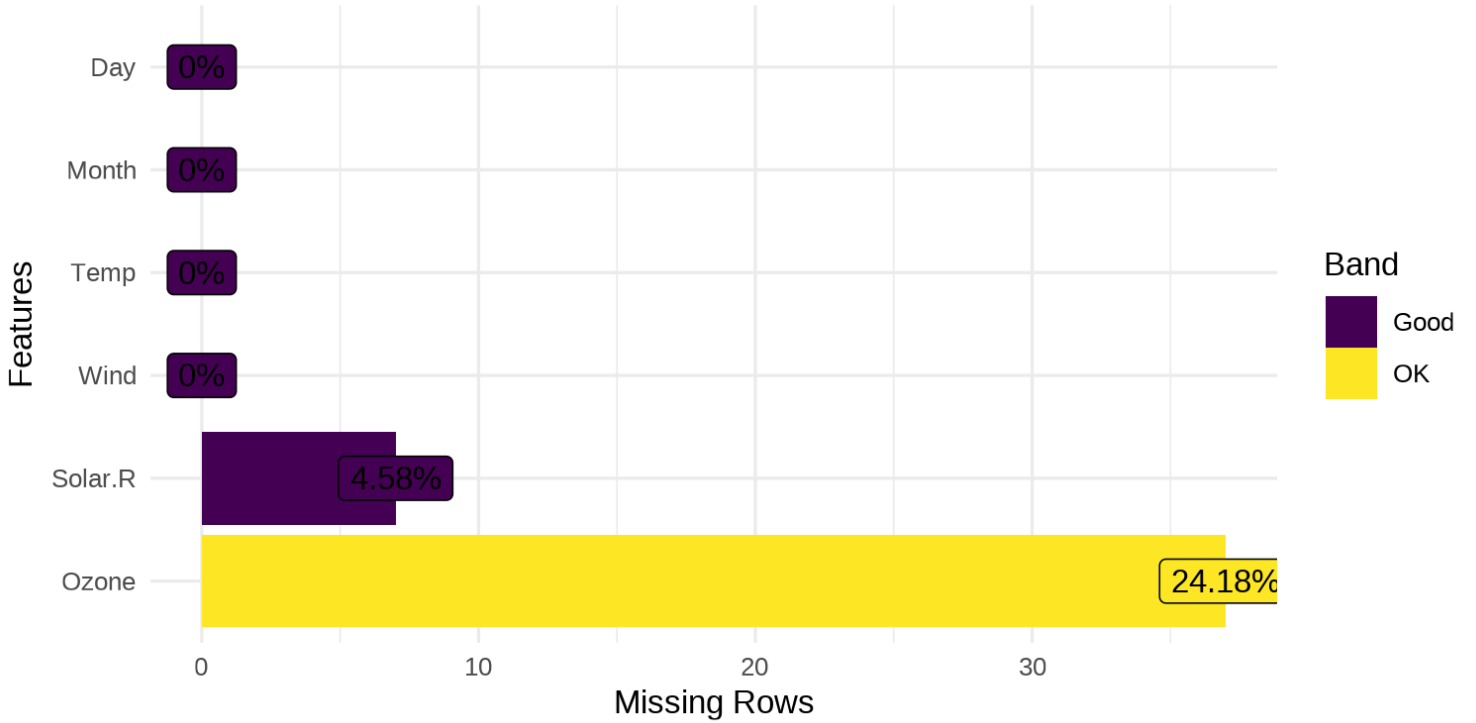
# Airquality Dataset

| 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 |

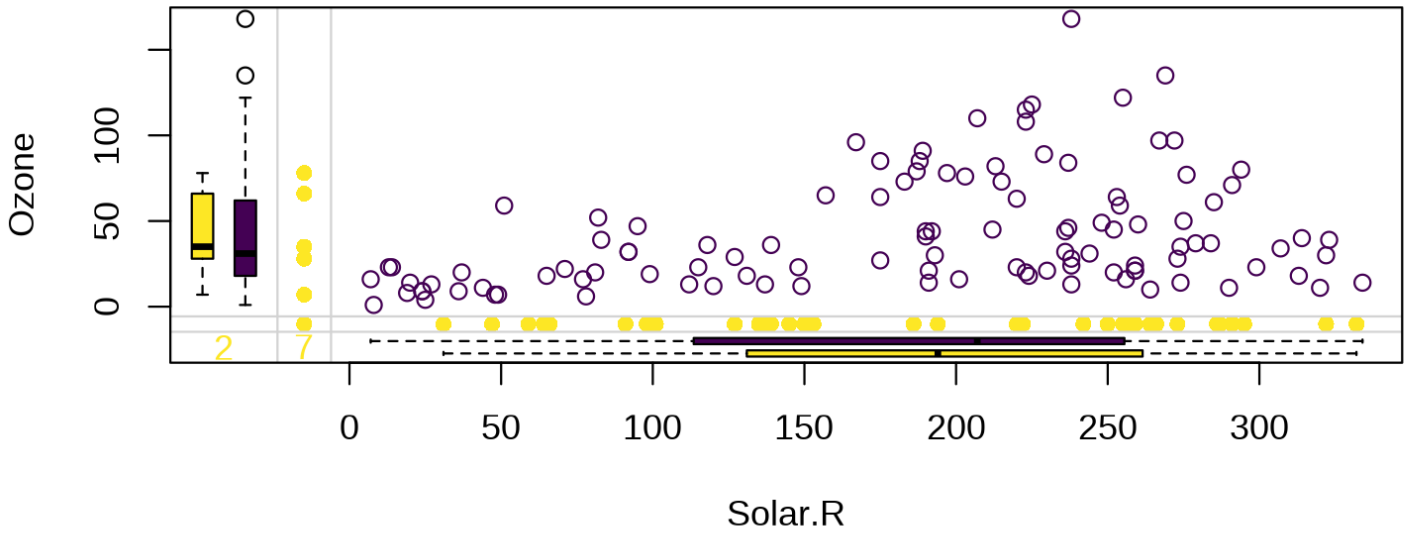
# Missing data pattern



# Missing value frequency



# Marginplot



# Dropping (ignoring) missing values

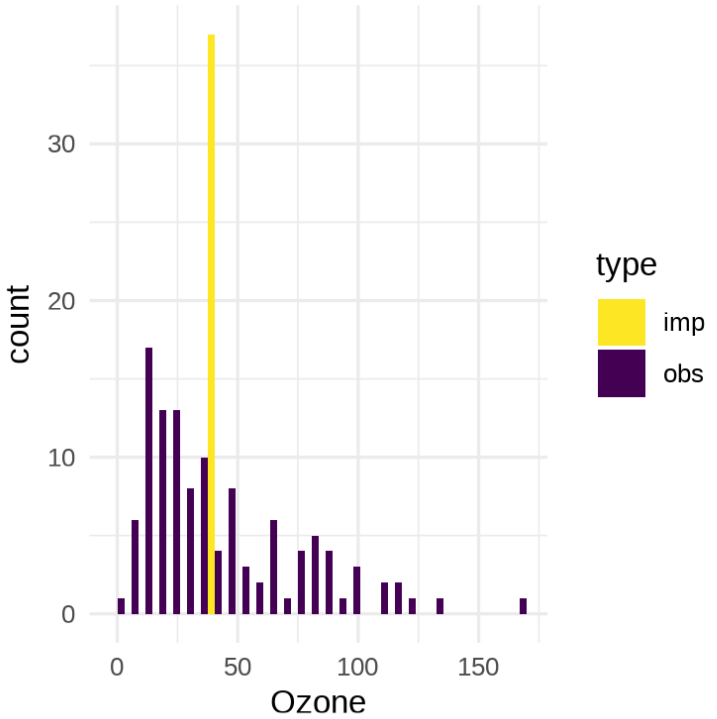
## Listwise deletion

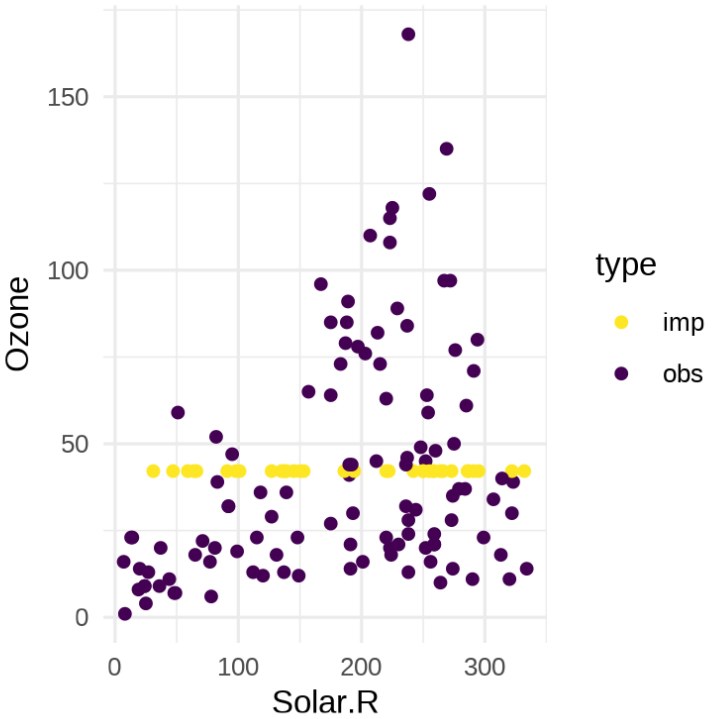
- Only the complete cases are analyzed
- Advantages:
  - Simple - Often the default way of handling incomplete data
  - Under MCAR: unbiased estimates of means, variances and regression weights
  - Schafer and Graham (2002): *If a missing data problem can be resolved by discarding only a small part of 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



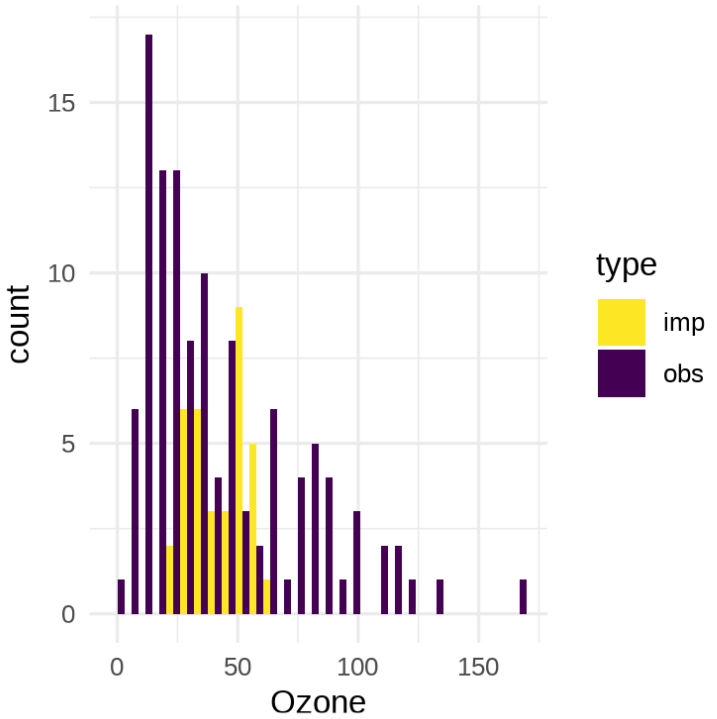



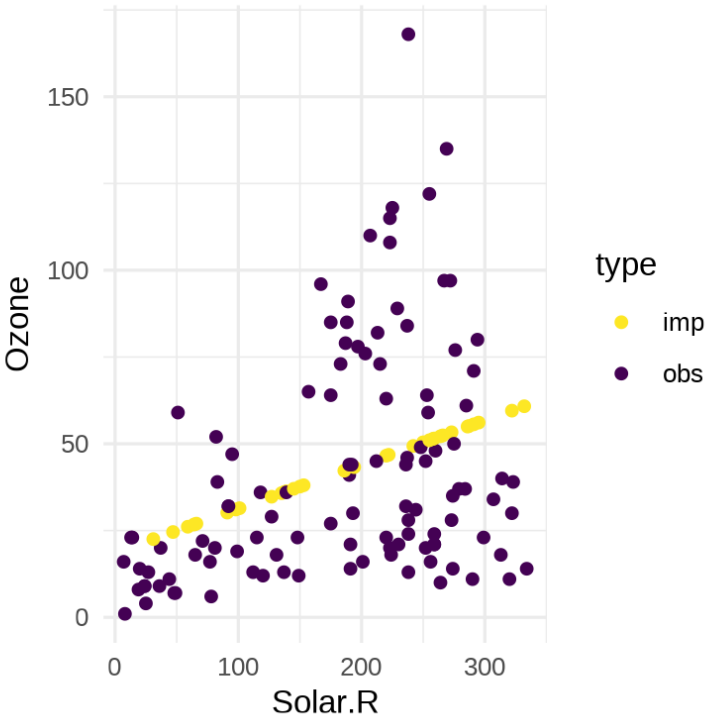
# Regression Imputation

- 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



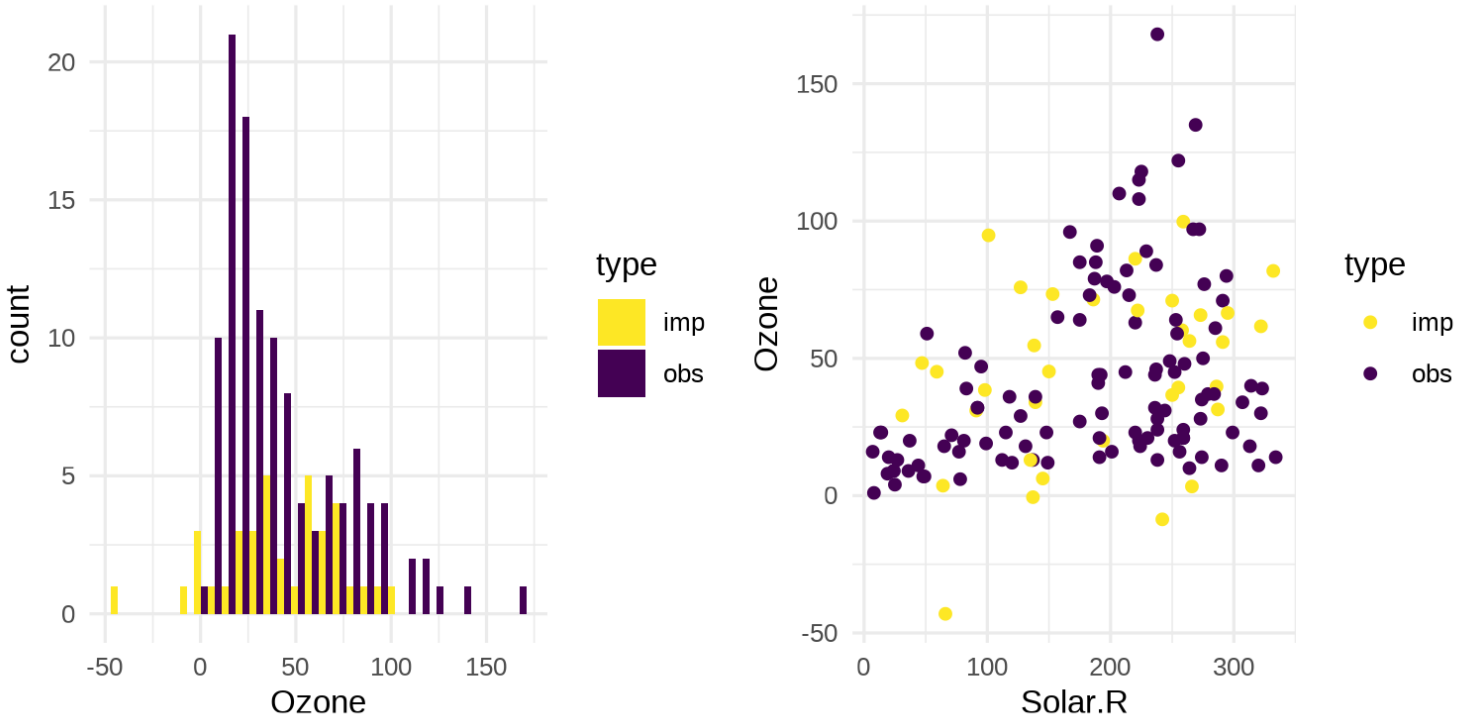



# Stochastic Regression Imputation

- 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

  $\rightarrow$ *Potentially better reflects the correlations between variables*

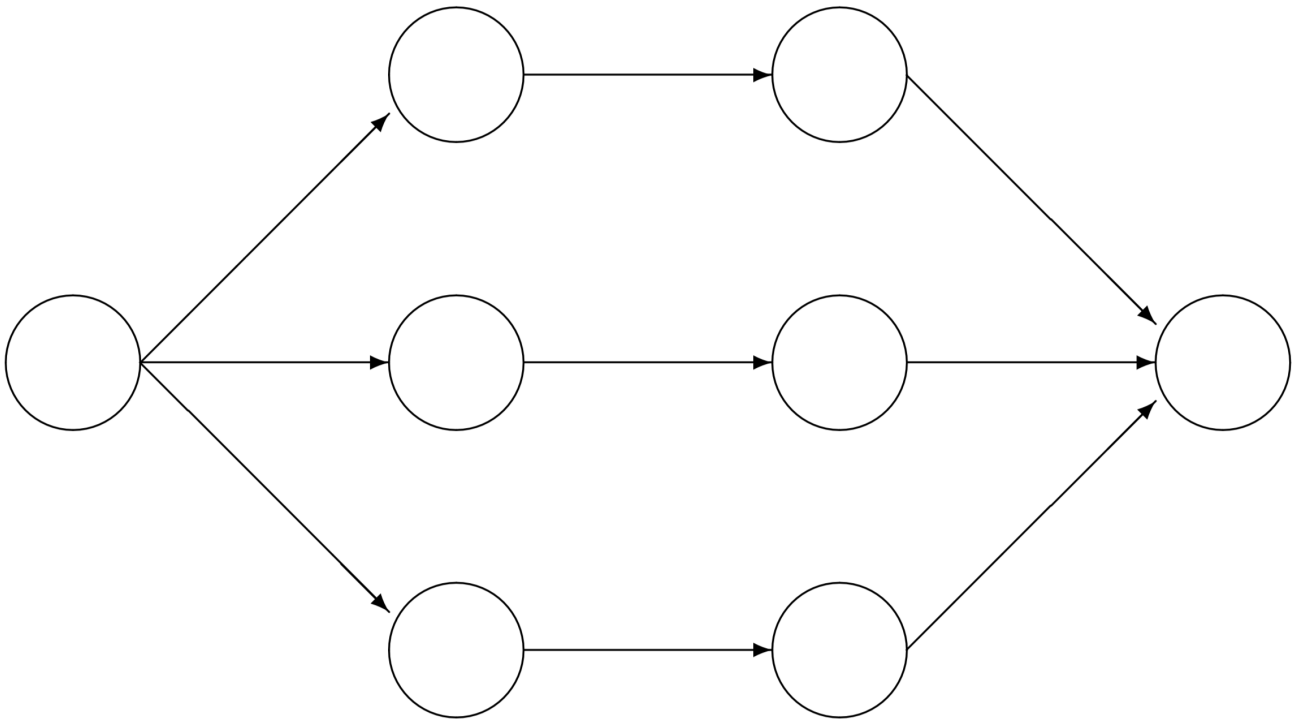
# Stochastic Regression Imputation



# Multiple imputation

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

# Multiple imputation




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

# 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 $Y_j^{\text{obs}}$.
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

1. Create $m$ complete versions of the data by replacing missing values by plausible ones with a random component (steps 1 to 3)

2. The $m$ imputed datasets are

    - identical for the observed data entries
    - differ in the imputed values

    *The magnitude of these difference reflects uncertainty about what value to impute*

3. Analyze each of the $m$ complete datasets. Each set of parameter estimates differs slightly because of the random component

4. Pool the $m$ parameter estimates into one estimate. Variance combines

    - the conventional sampling variance (within-imputation variance)
    - extra variance caused by the missing data (between-imputation variance).

# Multiple imputation

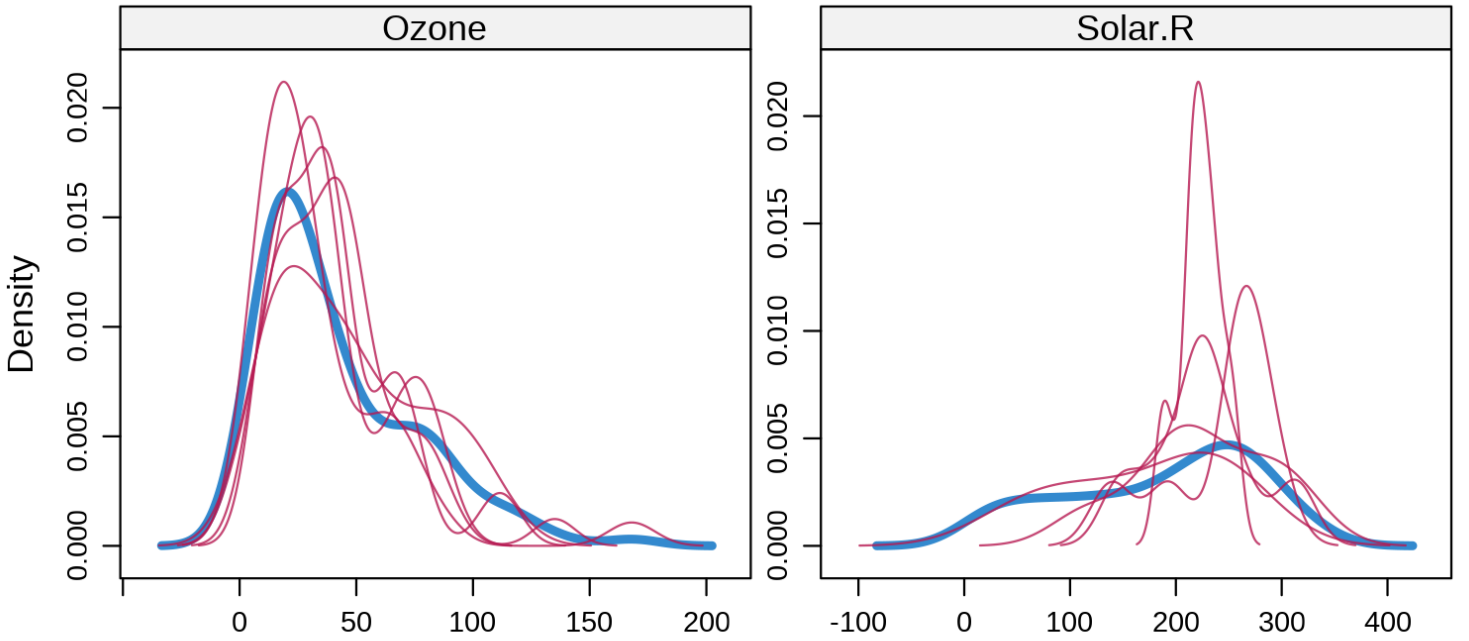
## How large should $m$ be (vanBuuren (2018))?

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

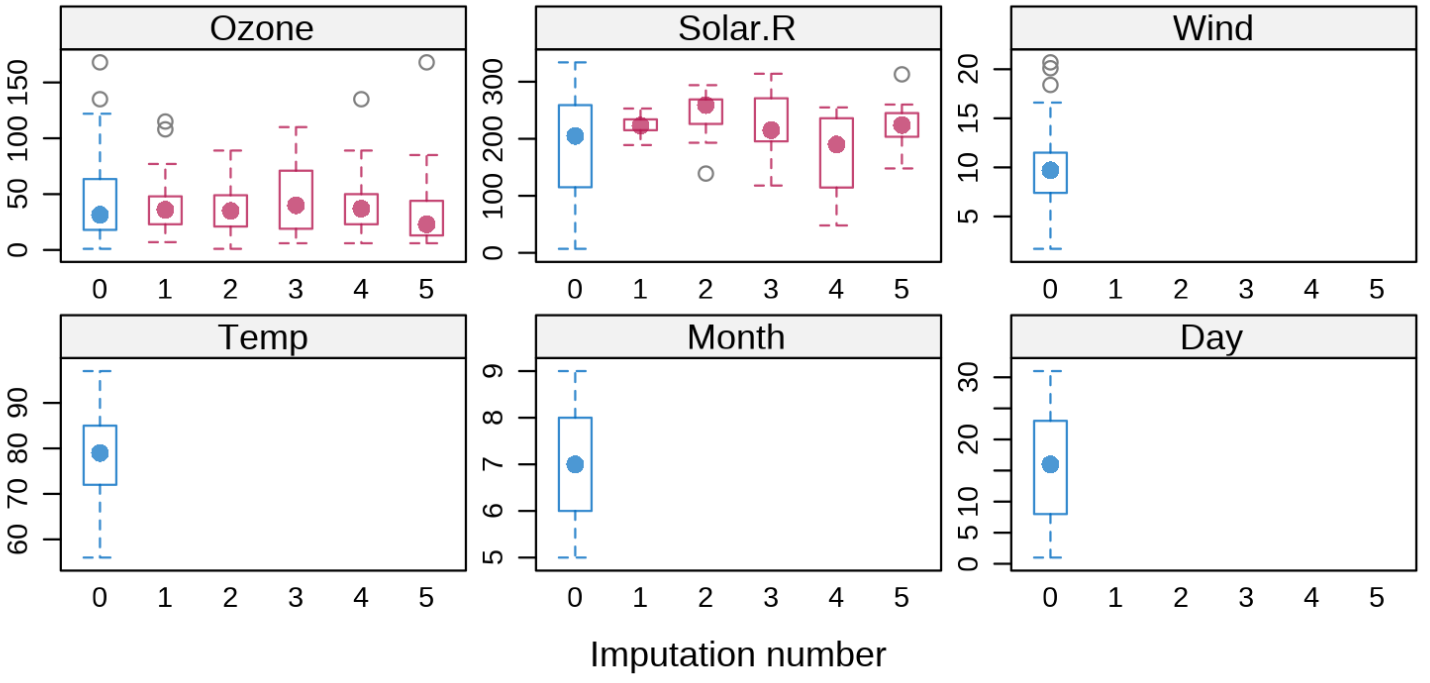
Some advice:

- 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

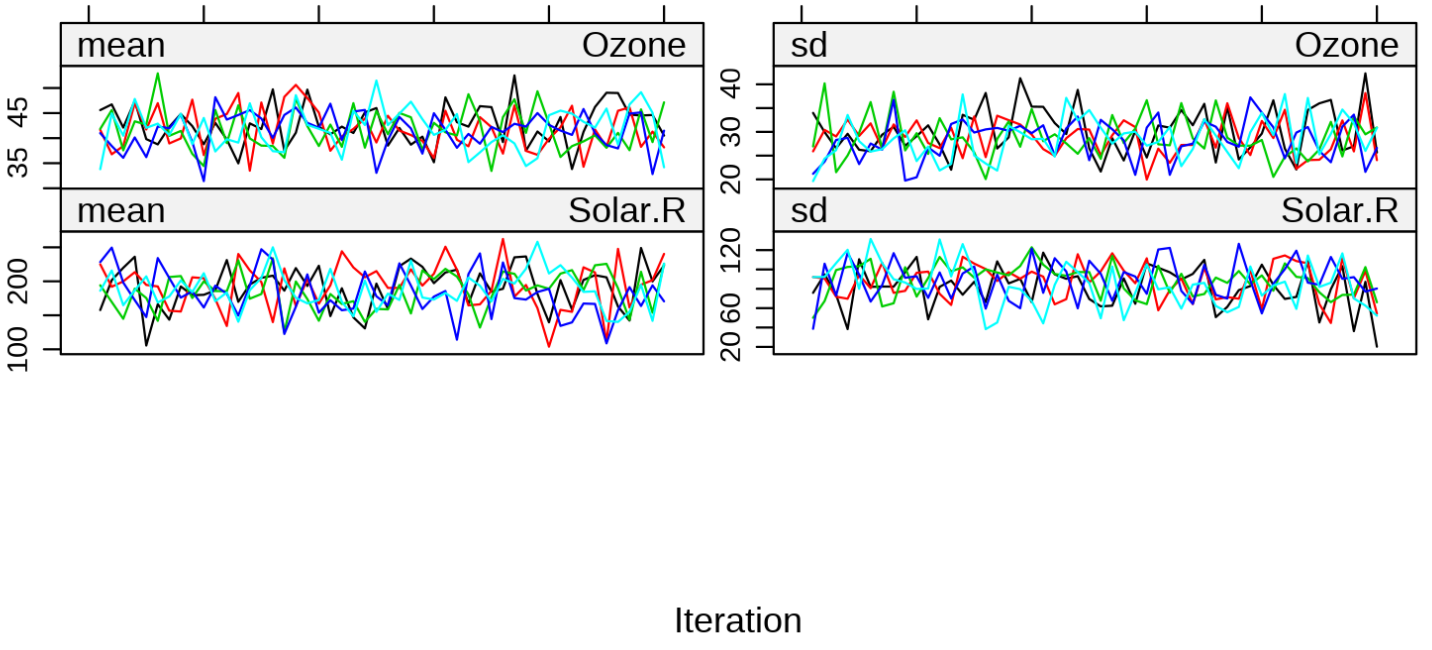
# Multiple imputation



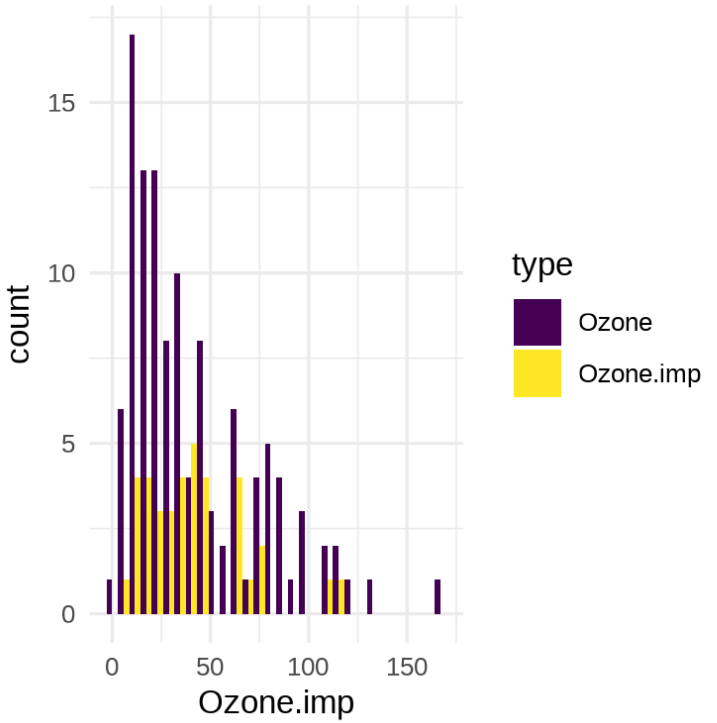
# Multiple imputation

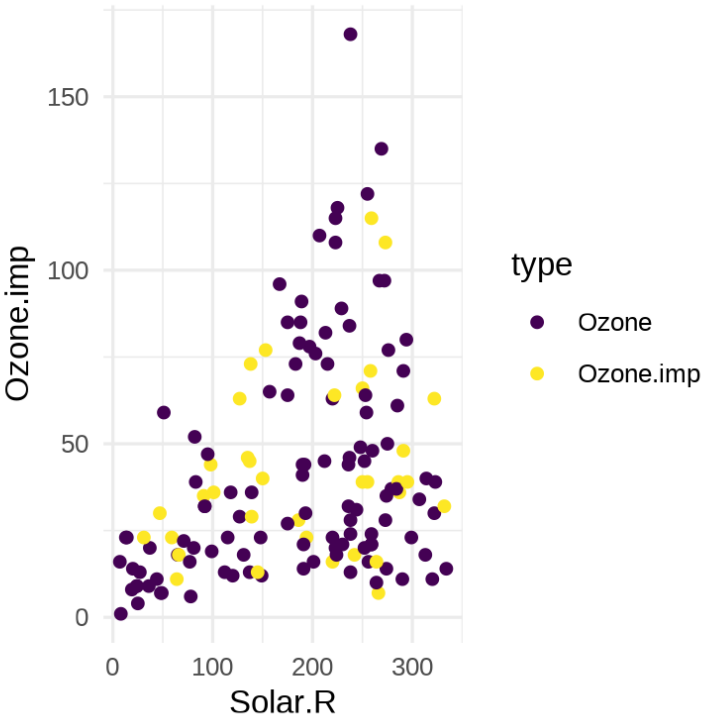


# Multiple imputation



# 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