data cleaning principles

Karl Broman

Biostatistics & Medical Informatics, UW-Madison

kbroman.org github.com/kbroman @kbroman@fosstodon.org bit.ly/datacleaning2023



Tidy data are all alike, but every messy dataset is messy in its own way.

Hadley Wickham

If I clean up [Medicare] data ...
does any of the knowledge I gain ...
apply to the processing of RNA-seq data?

Roger Peng

Data Mishaps Night

Join us for the first inaugural Data Mishaps Night! We will feature a lineup of data mistake stories with a focus on the human aspect of data work and lessons learned the hard way.



Caitlin Hudon & Laura Ellis dataMishapsNight.com

Data cleaning

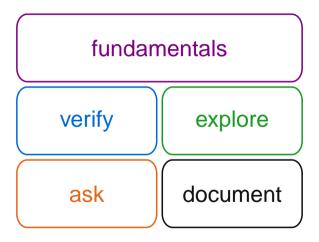
- ▶ tedious
- embarrassing
- needs context
- ► doesn't feel like progress

Data cleaning

- tedious
- embarrassing
- needs context
- ▶ doesn't feel like progress

- requires creativity
- ▶ requires coding prowess
- source of many problems

Data cleaning principles



1. Don't clean data when you're tired or hungry.

(paraphrasing Ghazal Gulati)

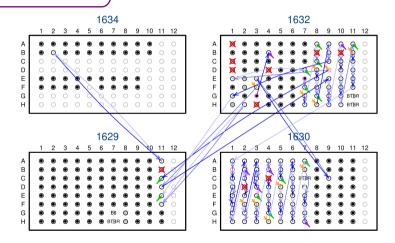
2. Don't trust anyone (even yourself)

2. Don't trust anyone (even yourself)

"my motto is 'trust no one' ...except maybe @kwbroman?"

Jenny Bryan

3. Think about what might have gone wrong and how it might be revealed



4. Use care in merging

| | A | В | С | D | Е | F | G | | |
|----|--------|------------|------------|------------|------------|------------|-----------|------------|------------|
| 1 | id | glucose.0 | glucose.5 | glucose.15 | glucose.30 | insulin.0 | insulin.5 | | |
| 2 | DO-221 | 145.742786 | 206.452638 | 216.640608 | 299.55501 | 0.74455 | 2.0264 | | |
| 3 | DO-222 | | Α | В | C | D | E | F | G |
| 4 | DO-223 | | | | | | | - | |
| | | 1 | id | glucose.0 | insulin.0 | glucose.5 | insulin.5 | glucose.15 | insulin.15 |
| 5 | DO-224 | 2 | DO-321 | 66.839405 | 0.04 | 246.685995 | 0.04 | 305.26214 | 0.04 |
| 6 | DO-225 | 3 | DO-322 | 98.12509 | 0.51185 | 246.25574 | 1.4062 | 301.8201 | 2.828 |
| 7 | DO-226 | 4 | DO-323 | 94.68305 | 1,7812 | 448.1068 | 1.0248 | 521.61894 | 1.02725 |
| 8 | DO-227 | 5 | DO-324 | 121.051535 | 0.0882 | 407.355505 | 0.63475 | 470.541525 | 0.8195 |
| 9 | DO-228 | 6 | DO-325 | 122.95695 | 0.19155 | 298.193665 | 0.6467 | 323.148455 | 0.40515 |
| 10 | DO-229 | б | DO-325 | 122.95695 | 0.19155 | 298.193665 | 0.6467 | 323.148455 | 0.40515 |
| | | 7 | DO-326 | 201.447755 | 0.7454 | 386.51887 | 0.6081 | 654.99799 | 1.07225 |
| 11 | DO-230 | 8 | DO-327 | 130.025425 | 0.0509 | 477.302675 | 0.166 | 610.49733 | 0.4842 |
| | | 9 | DO-328 | 143.60919 | 0.23435 | 438.88705 | 0.70505 | 406.249135 | 0.2498 |
| | | 10 | DO-329 | 125.29262 | 0.04 | 543.74634 | 1.7366 | 520.205245 | 0.8498 |
| | | 11 | DO-330 | 135.61874 | 0.91275 | 393.03416 | 3.73095 | 454.62209 | 1.7325 |

5. Dates & categories suck

Principle:

a fundamental truth that guides our thinking

5. Dates & categories suck

6. Check that distinct things are distinct

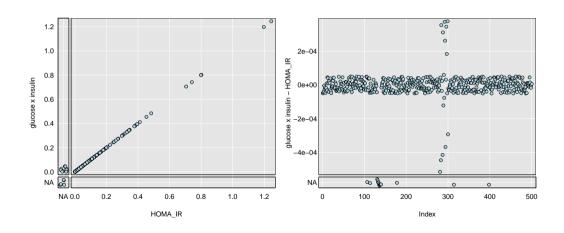
| | А | В | С | D | Е | F | G |
|----|---------------|------|--------|--------|----------|----------|--------|
| 1 | WiscID | ID | NEOID | Fem_CA | Fem_Imax | Fem_Imin | Fem_J |
| 2 | F2.C1W.F.1248 | 1248 | NEO183 | 0.7524 | 0.1427 | 0.1006 | 0.2433 |
| 3 | F2.C1W.M.1250 | 1250 | NEO184 | 0.7669 | 0.1556 | 0.09652 | 0.2521 |
| 4 | F2.C1W.F.1251 | 1251 | NEO185 | 0.7613 | 0.1549 | 0.09659 | 0.2515 |
| 5 | F2.C1W.F.1254 | 1254 | NEO186 | 0.7475 | 0.1503 | 0.08603 | 0.2363 |
| 6 | F2.C1W.M.1257 | 1257 | NEO187 | 0.8197 | 0.1849 | 0.1056 | 0.2905 |
| 7 | F2F.715 | 715 | NEO764 | 0.6017 | 0.09662 | 0.05969 | 0.1563 |
| 8 | F2F.751 | 751 | NEO765 | 0.7273 | 0.1304 | 0.08735 | 0.2178 |
| 9 | F2F.1251 | 1251 | NEO766 | 0.6675 | 0.1157 | 0.07814 | 0.1938 |
| 10 | F2M.1340 | 1340 | NEO768 | 0.6656 | 0.1387 | 0.08122 | 0.2199 |
| 11 | F2.C1W.M.739 | 739 | NEO779 | 0.9336 | 0.2828 | 0.1628 | 0.4456 |

7. Check that matching things match

| | А | В | С | D |
|----|---------------|-----|-------|----------|
| 1 | id | sex | n_gen | age_days |
| 2 | F20.25 | М | 20 | 75 |
| 3 | F21.30 | М | 21 | 75 |
| 4 | F21.68 | М | 21 | 71 |
| 5 | F22.52 | М | 22 | 73 |
| 6 | F21.71 | F | 22 | 63 |
| 7 | F22.116 | F | 22 | 57 |
| 8 | F21.F20.9.M5 | М | 20 | 82 |
| 9 | F21.F20.18.M5 | М | 20 | 77 |
| 10 | F20.26 | М | 20 | 75 |
| 11 | F21.62 | М | 21 | 72 |

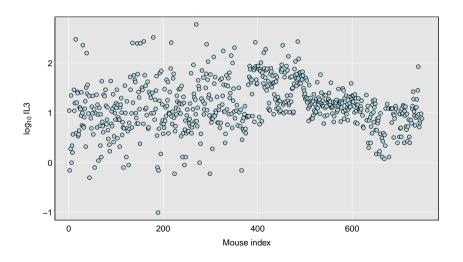
| | А | В | С | D |
|----|---------|-----|---------------|-------|
| 1 | id | sex | age_at_dosing | n_gen |
| 2 | F22.69 | F | 67 | 22 |
| 3 | F22.106 | F | 69 | 22 |
| 4 | F22.70 | F | 67 | 22 |
| 5 | F22.107 | F | 69 | 22 |
| 6 | F21.71 | F | 65 | 21 |
| 7 | F22.116 | F | 62 | 22 |
| 8 | F22.73 | F | 65 | 22 |
| 9 | F22.117 | F | 62 | 22 |
| 10 | F21.108 | F | 62 | 21 |
| 11 | F22.118 | F | 59 | 22 |

8. Check calculations

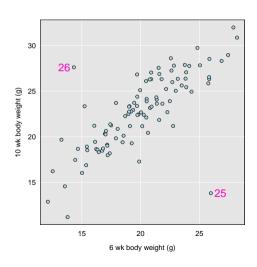


9. Look for other instances of a problem

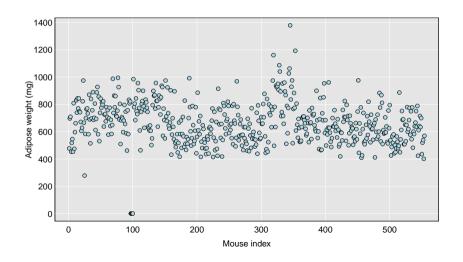
10. Make lots of plots



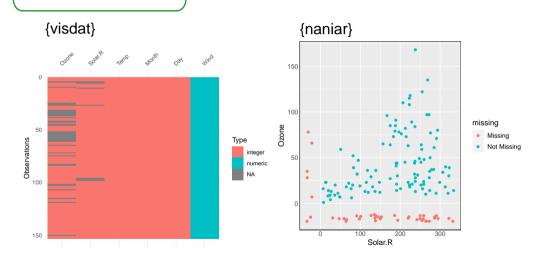
10. Make lots of plots



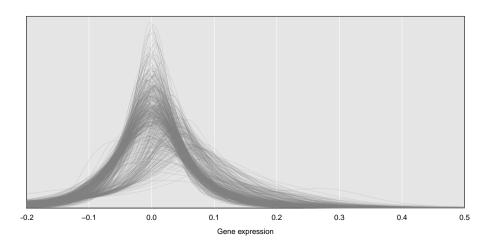
10. Make lots of plots



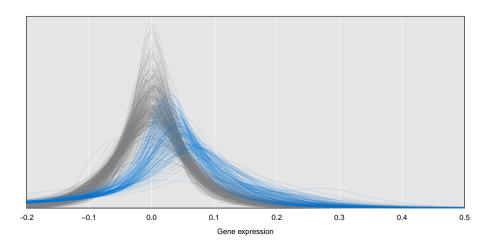
11. Look at missing value patterns



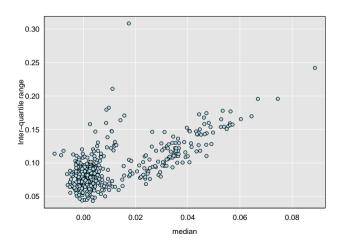
12. With massive data, make more plots not fewer



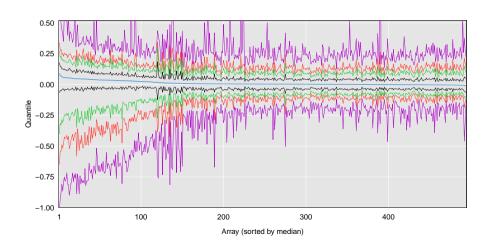
12. With massive data, make more plots not fewer



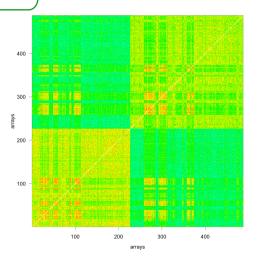
12. With massive data, make more plots not fewer



With massive data, make more plots not fewer



13. Follow up all artifacts



14. Ask questions

When were the data gathered?

How, and by whom?

Was the data gathered in batches?

How were the data files created?

Was any calibration or normalization done?

15. Ask for the primary data

| | А | В | С | D | E | F | G | Н |
|----|-----------|-----------|------------|--------|---------|---------|--------|-------|
| 1 | MouseNum | Wean Date | Assay Date | Weight | Glucose | Insulin | Trigly | НОМА |
| 2 | Mouse3001 | 6/22/2005 | 8/18/2005 | 47.3 | 617 | 11.7 | 175.1 | 321.9 |
| 3 | Mouse3002 | 6/22/2005 | 8/18/2005 | 51 | 256.5 | 50.6 | 97.6 | 576.6 |
| 4 | Mouse3003 | 6/22/2005 | 8/18/2005 | 50.6 | 274.9 | 52.5 | 160.5 | 641.3 |
| 5 | Mouse3004 | 6/22/2005 | 8/18/2005 | 46 | 615.1 | 9 | 238.7 | 246 |
| 6 | Mouse3005 | 6/30/2005 | b | 42.4 | NA | NA | 102.3 | 587.1 |
| 7 | Mouse3006 | 6/30/2005 | b | 39.7 | NA | NA | 209.4 | 338.7 |
| 8 | Mouse3007 | 6/30/2005 | b | 36.9 | NA | NA | 69.8 | 140.6 |
| 9 | Mouse3008 | 6/30/2005 | b | 50 | 195.5 | 45.3 | 142.1 | 393.4 |
| 10 | Mouse3009 | 6/30/2005 | b | 40.1 | 569.4 | 12.4 | 411 | 312.9 |
| 11 | Mouse3010 | 6/30/2005 | b | 40.7 | 593.8 | 15.6 | 333.6 | 411.8 |

16. Ask for metadata

"What the heck is 'FAD_NAD SI 8.3_3.3G'?"

16. Ask for metadata

| | А | В | С | D |
|---|-------------------|-------------------|-------------|--|
| 1 | name | plot_name | group | description |
| 2 | mouse | Mouse | demographic | Animal identifier |
| 3 | sex | Sex | demographic | Male (M) or Female (F) |
| 4 | sac_date | Date of sac | demographic | Date mouse was sacrificed |
| 5 | partial_inflation | Partial inflation | clinical | Indicates if mouse showed partial pancreatic inflation |
| 6 | coat_color | Coat color | demographic | Coat color, by visual inspection |
| 7 | crumblers | Crumblers | clinical | Indicates if mouse stored food in their bedding |
| 8 | diet_days | Days on diet | clinical | Number of days on high-fat diet |

17. Ask why data are missing

Assay failed?

Below detection limit?

Viewed as outliers?

Subjects dropped out?

document

18. Create checklists & pipelines

- ☐ Percent missing genotypes
- ☐ Sample duplicates
- ☐ Sex and X/Y genotypes
- ☐ Heterozygosity
- ☐ Genotype frequencies
- □ Crossover counts
- ☐ Genotyping error rates

document

19. Document not just what but why

Gough project diagnostics

Karl Broman, 3 March 2014

Combine genotypes and phenotypes

I've combined the initial genotypes (using the re-clustered genotypes for plates 14-16) with the well-behaved portion of the re-run genotypes. I'm focusing on 36813 markers that are informative (though, as we'll see, there are still a lot of badly behaved and basically non-informative markers that need to be removed). I've combined data on replicate samples, to give one set of genotype calls for each sample.

There are 1497 genotyped mice and 1464 phenotyped mice. All of the mice in the phenotype data have genotypes, but there are 33 genotyped mice with no phenotypes, including 3 Gough mice and 30 F2 progeny.

document

20. Expect to recheck

Data cleaning principles

fundamentals

- 1. Don't clean data when tired or hungry
- 2. Don't trust anyone (even yourself)
- 3. Think about what might have gone wrong
- 4. Use care in merging
- 5. Dates & categories suck

verify

- 6. Verify that distinct things are distinct
- 7. Verify that matching things match
- 8. Check calculations
- 9. Look for other instances of problems

explore

- 10. Make lots of plots
- 11. Look at missing value patterns
- 12. With big data make more plots
- 13. Follow up all artifacts

ask

- 14. Ask questions
- 15. Ask for the primary data
- 16. Ask for metadata
- 17. Ask why data are missing

document

- 18. Create checklists & pipelines
- 19. Document not just what but why
- 20. Expect to recheck

I will let the data speak for itself when it cleans itself.

Allison Reichel

Slides: bit.ly/datacleaning2023



kbroman.org
github.com/kbroman
@kbroman@fosstodon.org

fundamentals

- 1. Don't clean data when tired or hungry
- 2. Don't trust anyone (even yourself)
- 3. Think about what might have gone wrong
- 4. Use care in merging
- 5. Dates & categories suck

verify

- 6. Verify that distinct things are distinct
- 7. Verify that matching things match
- 8. Check calculations
- 9. Look for other instances of problems

explore

- 10. Make lots of plots
- 11. Look at missing value patterns
- 12. With big data make more plots
- 13. Follow up all artifacts

ask

- 14. Ask questions
- 15. Ask for the primary data
- 16. Ask for metadata
- 17. Ask why data are missing

document

- 18. Create checklists & pipelines
- 19. Document not just what but why
- 20. Expect to recheck