

VERSIONING, PROVENANCE, AND REPRODUCABILITY

Christian Kaestner

Required reading: Halevy, Alon, Flip Korn, Natalya F. Noy, Christopher Olston, Neoklis Polyzotis, Sudip Roy, and Steven Euijong Whang. [Goods: Organizing google's datasets](#). In Proceedings of the 2016 International Conference

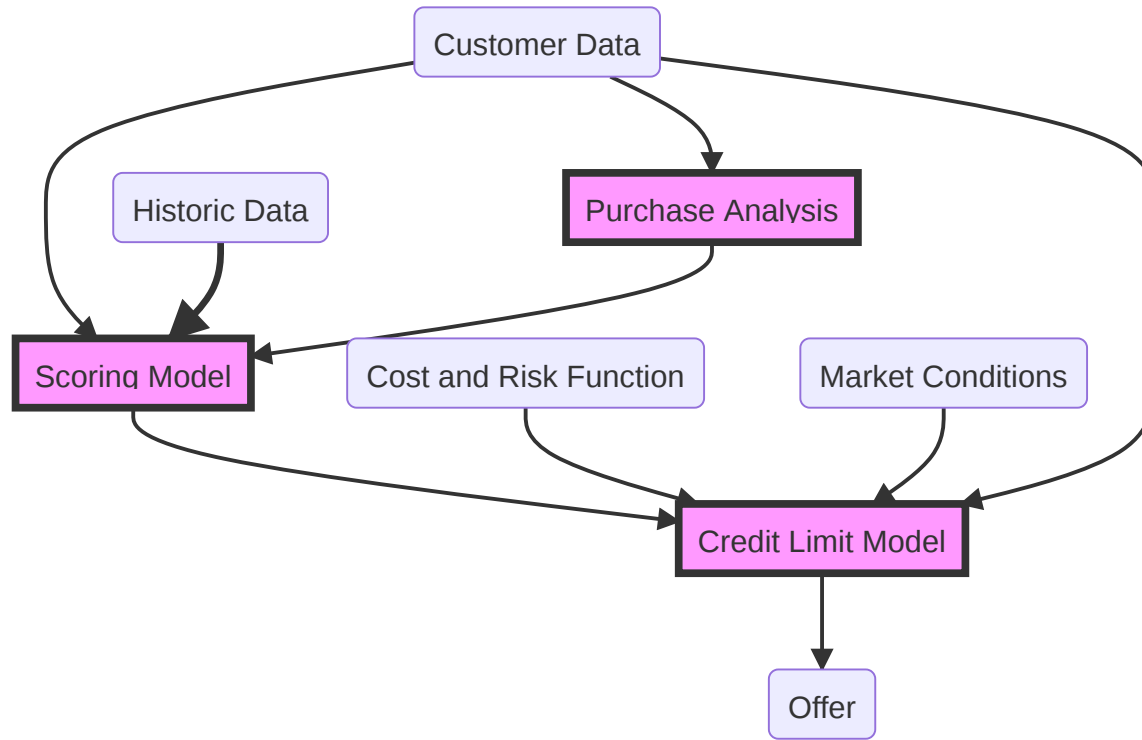
LEARNING GOALS

- Judge the importance of data provenance, reproducibility and explainability for a given system
- Create documentation for data dependencies and provenance in a given system
- Propose versioning strategies for data and models
- Design and test systems for reproducibility

CASE STUDY: CREDIT SCORING

Tweet

Tweet



DEBUGGING?

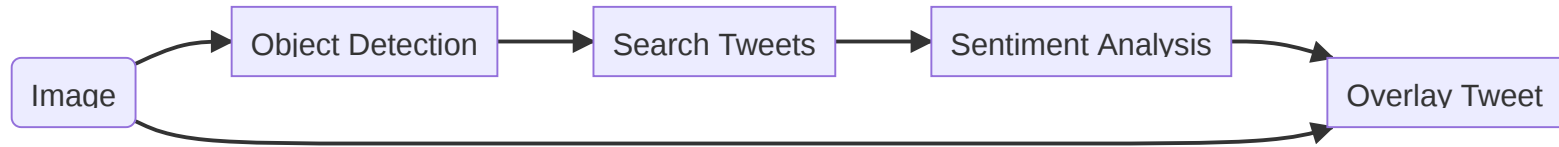
What went wrong? Where? How to fix?



DEBUGGING QUESTIONS BEYOND INTERPRETABILITY

- Can we reproduce the problem?
- What were the inputs to the model?
- Which exact model version was used?
- What data was the model trained with?
- What learning code (cleaning, feature extraction, ML algorithm) was the model trained with?
- Where does the data come from? How was it processed and extracted?
- Were other models involved? Which version? Based on which data?
- What parts of the input are responsible for the (wrong) answer? How can we fix the model?

MODEL CHAINING: AUTOMATIC MEME GENERATOR

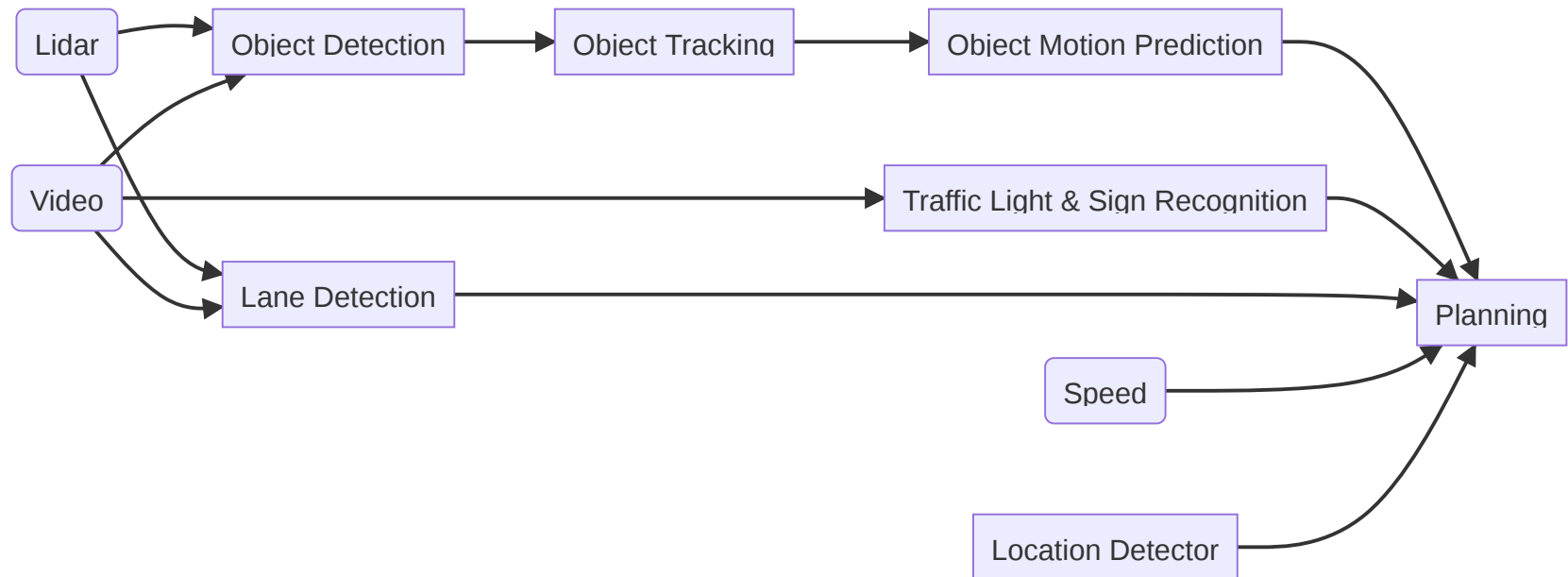


Version all models involved.

Example adapted from Jon Peck. [Chaining machine learning models in production with Algorithmia](#). Algorithmia blog, 2019

COMPLEX MODEL COMPOSITION: ML MODELS FOR FEATURE EXTRACTION

self driving car



Example: Zong, W., Zhang, C., Wang, Z., Zhu, J., & Chen, Q. (2018). [Architecture design and implementation of an autonomous vehicle](#). IEEE access, 6, 21956-21970.

BREAKOUT DISCUSSION: MOVIE PREDICTIONS

Assume you are receiving complains that a child gets mostly recommendations about R-rated movies

In a group, discuss how you could address this in your own system and post to #lecture

- How could you identify the problematic recommendation(s)?
- How could you identify the model that caused the prediction?
- How could you identify the training code and data that learned the model?
- How could you identify what training data or infrastructure code "caused" the recommendations?

K.G Orphanides. [Children's YouTube is still churning out blood, suicide and cannibalism](#). Wired UK, 2018

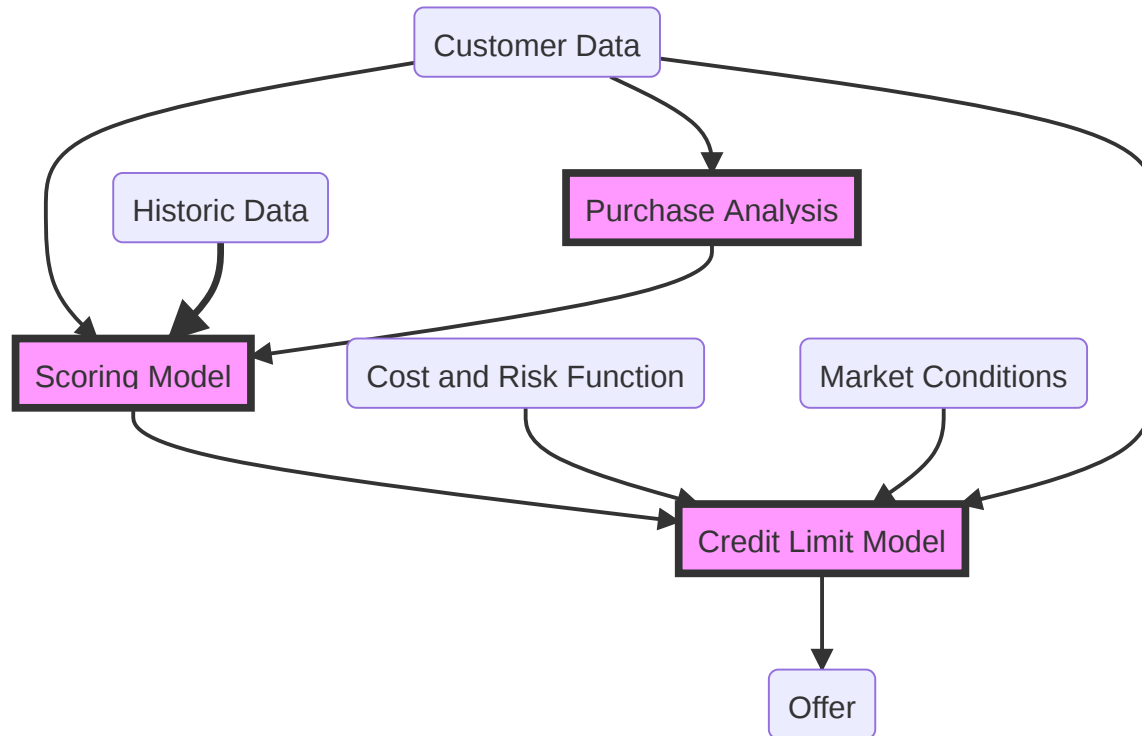
Kristie Bertucci. [16 NSFW Movies Streaming on Netflix](#). Gadget Reviews, 2020

PROVENANCE TRACKING

Historical record of data and its origin

DATA PROVENANCE

- Track origin of all data
 - Collected where?
 - Modified by whom, when, why?
 - Extracted from what other data or model or algorithm?
- ML models often based on data driven from many sources through many steps, including other models

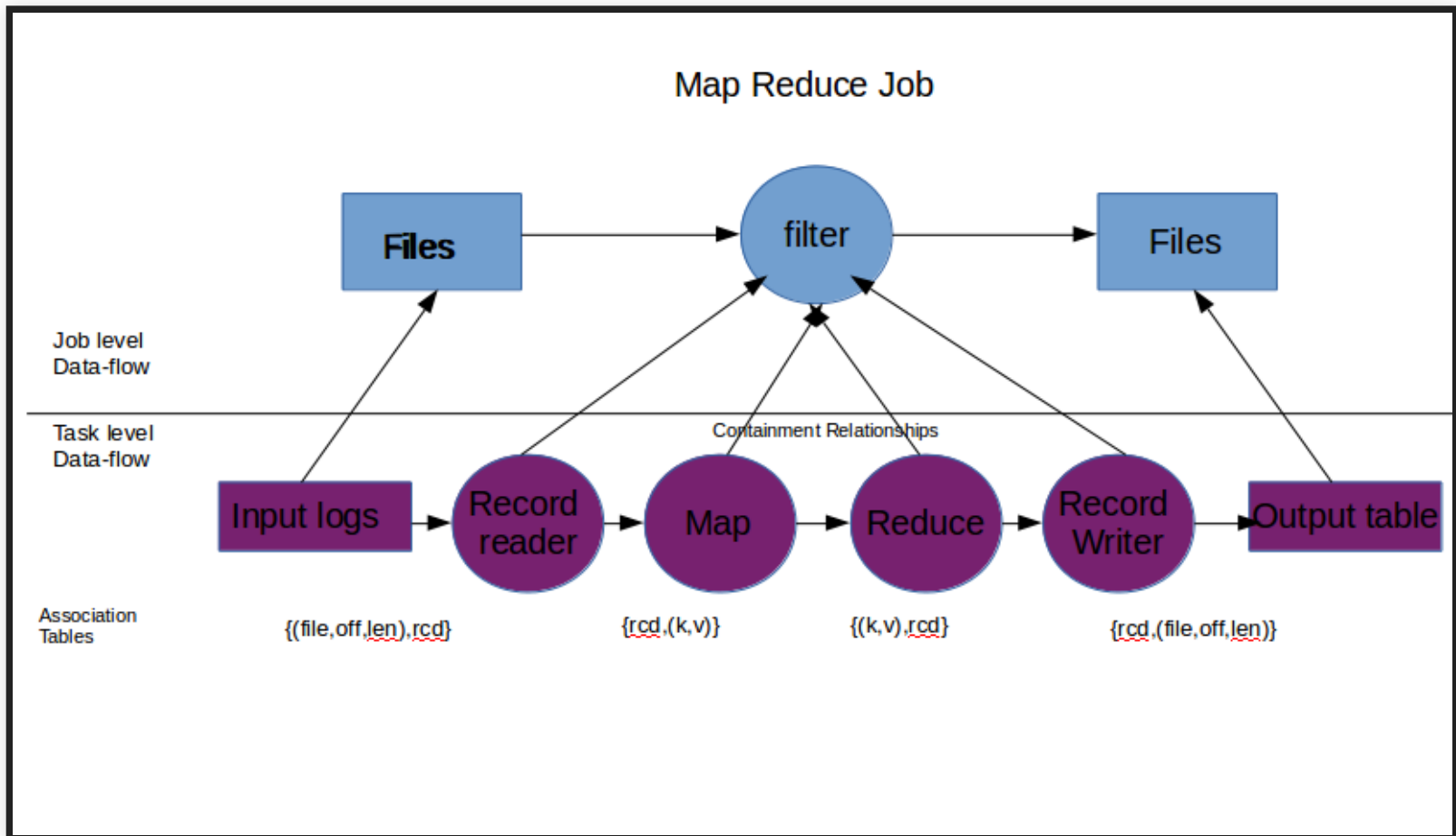


EXCURSION: PROVENANCE TRACKING IN DATABASES

- Whenever value is changed, record:
 - who changed it
 - time of change
 - history of previous values
 - possibly also justification of why
- Embedded as feature in some databases, can also be added in business logic
- Immutable data storage keeps history
- Possibly using cryptographic methods (e.g., signing documents and changes)

TRACKING DATA LINEAGE

- Document all data sources
 - Model dependencies and flows
 - Ideally model all data and processing code
 - Avoid "visibility debt"
-
- Advanced: Use infrastructure to automatically capture/infer dependencies and flows (e.g., [Goods](#) paper)



(CC BY-SA 4.0, [Skamisetty](#))

FEATURE PROVENANCE

- How are features extracted from raw data
 - during training
 - during inference
- Has feature extraction changed since the model was trained?

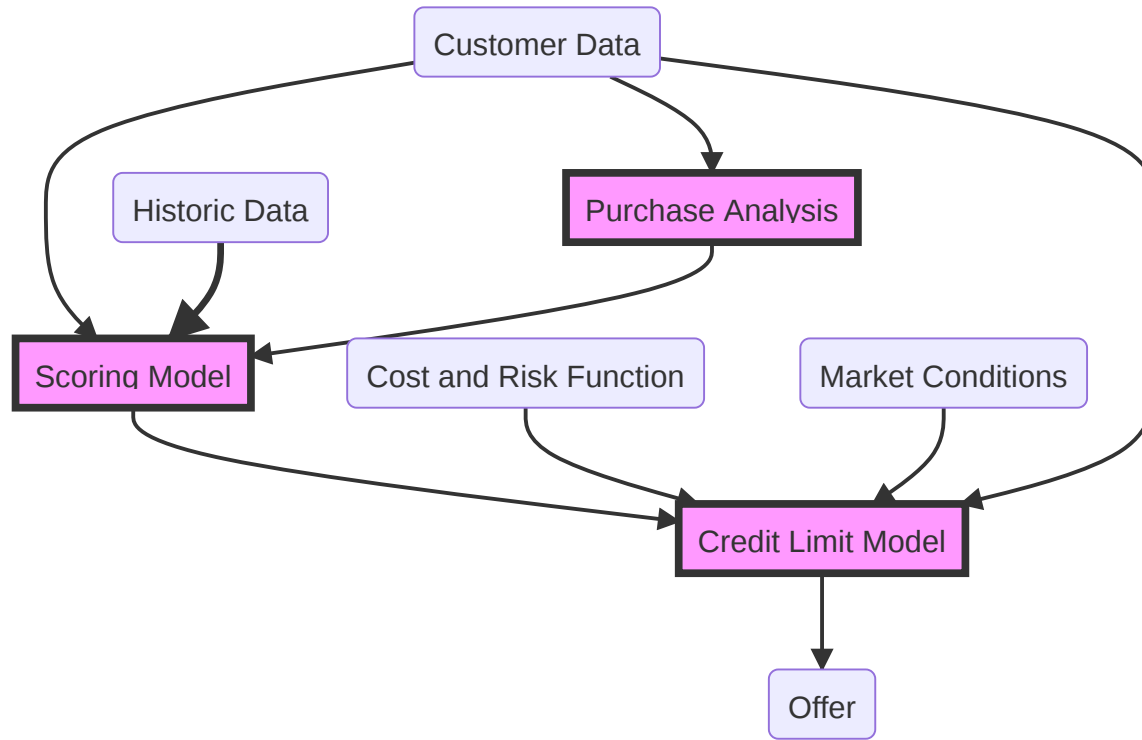
Example?

GOOD PRACTICE: FEATURE STORE

- Encapsulate feature extraction as functions
- Store centrally for reuse
- Use version control
- Use same feature code in training and inference code
- Advanced: Immutable features -- never change existing features, just add new ones (e.g., creditscore, creditscore2, creditscore3)

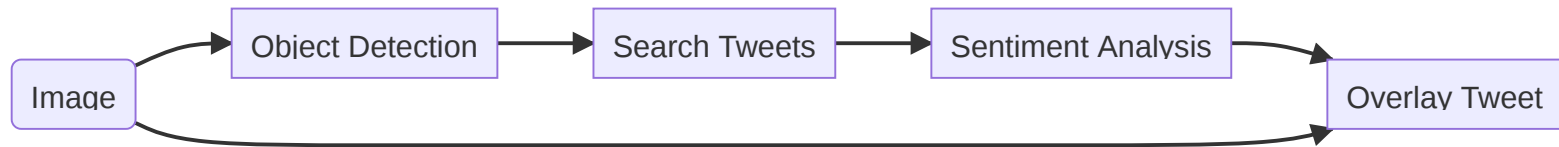
MODEL PROVENANCE

- How was the model trained?
- What data? What library? What hyperparameter? What code?
- Ensemble of multiple models?



IN REAL SYSTEMS: TRACKING PROVENANCE ACROSS MULTIPLE MODELS

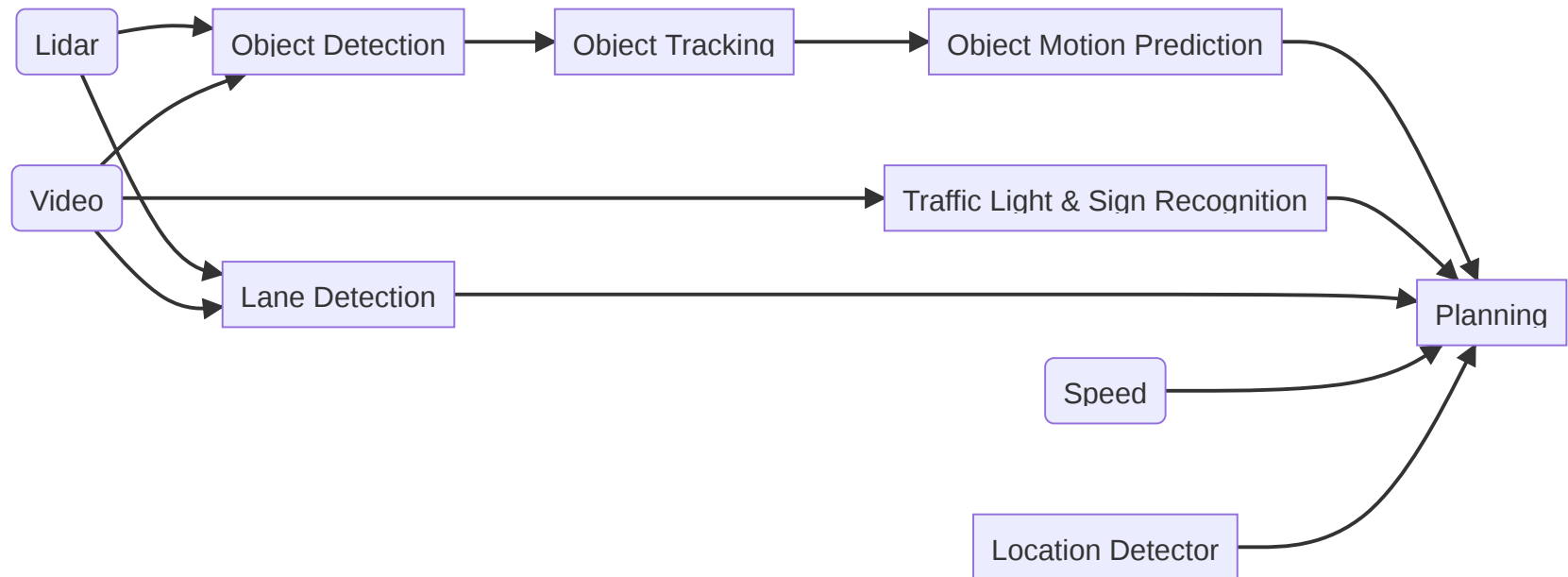
automated meme generator



Example adapted from Jon Peck. [Chaining machine learning models in production with Algorithmia](#). Algorithmia blog, 2019

COMPLEX MODEL COMPOSITION: ML MODELS FOR FEATURE EXTRACTION

self driving car



Example: Zong, W., Zhang, C., Wang, Z., Zhu, J., & Chen, Q. (2018). [Architecture design and implementation of an autonomous vehicle](#). IEEE access, 6, 21956-21970.

SUMMARY: PROVENANCE

- Data provenance
- Feature provenance
- Model provenance

PRACTICAL DATA AND MODEL VERSIONING

HOW TO VERSION LARGE DATASETS?



(movie ratings, movie metadata, user data?)

RECALL: EVENT SOURCING

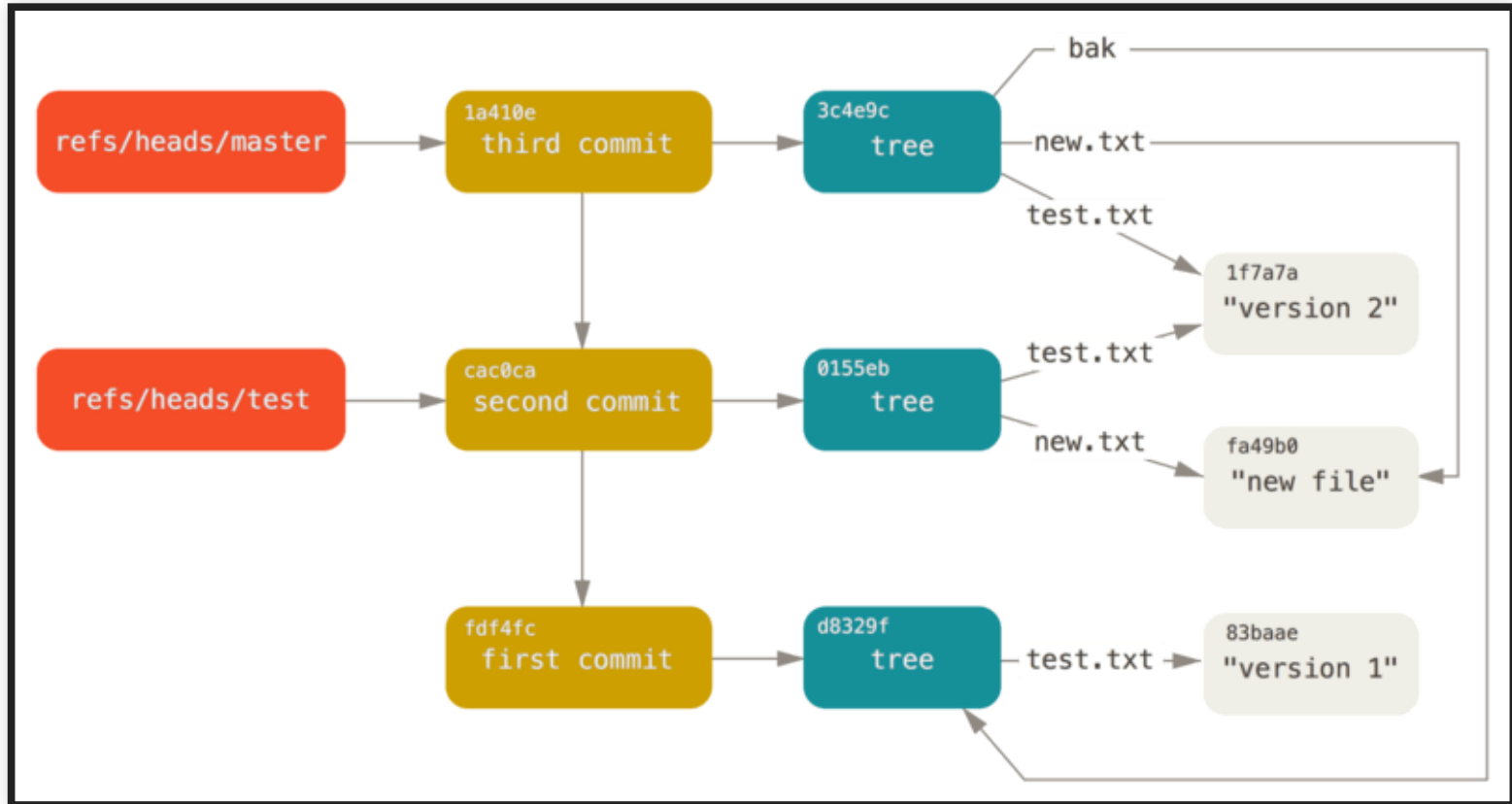
- Append only databases
- Record edit events, never mutate data
- Compute current state from all past events, can reconstruct old state
- For efficiency, take state snapshots
- Similar to traditional database logs

```
createUser(id=5, name="Christian", dpt="SCS")  
updateUser(id=5, dpt="ISR")  
deleteUser(id=5)
```

VERSIONING DATASETS

- Store copies of entire datasets (like Git)
- Store deltas between datasets (like Mercurial)
- Offsets in append-only database (like Kafka offset)
- History of individual database records (e.g. S3 bucket versions)
 - some databases specifically track provenance (who has changed what entry when and how)
 - specialized data science tools eg [Hangar](#) for tensor data
- Version pipeline to recreate derived datasets ("views", different formats)
 - e.g. version data before or after cleaning?
- Often in cloud storage, distributed
- Checksums often used to uniquely identify versions
- Version also metadata

ASIDE: GIT INTERNALS



Scott Chacon and Ben Straub. [Pro Git](#). 2014

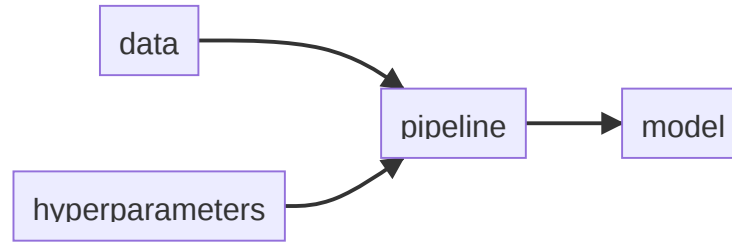
VERSIONING MODELS



VERSIONING MODELS

- Usually no meaningful delta, versioning as binary objects
- Any system to track versions of blobs

VERSIONING PIPELINES



VERSIONING DEPENDENCIES

- Pipelines depend on many frameworks and libraries
- Ensure reproducible builds
 - Declare versioned dependencies from stable repository (e.g. requirements.txt + pip)
 - Optionally: commit all dependencies to repository ("vendoring")
- Optionally: Version entire environment (e.g. Docker container)
- Avoid floating versions
- Test build/pipeline on independent machine (container, CI server, ...)

ML VERSIONING TOOLS (SEE MLOPS)

- Tracking data, pipeline, and model versions
- Modeling pipelines: inputs and outputs and their versions
 - explicitly tracks how data is used and transformed
- Often tracking also metadata about versions
 - Accuracy
 - Training time
 - ...

EXAMPLE: DVC

```
dvc add images  
dvc run -d images -o model.p cnn.py  
dvc remote add myrepo s3://mybucket  
dvc push
```

- Tracks models and datasets, built on Git
- Splits learning into steps, incrementalization
- Orchestrates learning in cloud resources

<https://dvc.org/>

DVC EXAMPLE

```
stages:
  features:
    cmd: jupyter nbconvert --execute featurize.ipynb
    deps:
      - data/clean
    params:
      - levels.no
    outs:
      - features
    metrics:
      - performance.json
  training:
    desc: Train model with Python
    cmd:
      - pip install -r requirements.txt
```

MLFLOW, MODELDB, NEPTUNE, TENSORBOARD, WEIGHTS & BIASES, COMET.ML

- Instrument pipeline with *logging* statements
- Track individual runs, hyperparameters used, evaluation results, and model files

Listing Price Prediction

Experiment ID: 0

Artifact Location: /Users/matei/mlflow/demo/mlruns/0

Search Runs:

metrics.R2 > 0.24

Search

Filter Params:

alpha, lr


Filter Metrics:

rmse, r2

Clear

4 matching runs

Compare Selected

Download CSV 

| | | | | | Parameters | | Metrics | | |
|--------------------------|-------|-------|-----------|---------|------------|----------|---------|-------|-------|
| | Time | User | Source | Version | alpha | l1_ratio | MAE | R2 | RMSE |
| <input type="checkbox"/> | 17:37 | matei | linear.py | 3a1995 | 0.5 | 0.2 | 84.27 | 0.277 | 158.1 |
| <input type="checkbox"/> | 17:37 | matei | linear.py | 3a1995 | 0.2 | 0.5 | 84.08 | 0.264 | 159.6 |
| <input type="checkbox"/> | 17:37 | matei | linear.py | 3a1995 | 0.5 | 0.5 | 84.12 | 0.272 | 158.6 |
| <input type="checkbox"/> | 17:37 | matei | linear.py | 3a1995 | 0 | 0 | 84.49 | 0.249 | 161.2 |

Matei Zaharia. [Introducing MLflow: an Open Source Machine Learning Platform](#), 2018

MODELDB EXAMPLE

```
from verta import Client
client = Client("http://localhost:3000")

proj = client.set_project("My first ModelDB project")
expt = client.set_experiment("Default Experiment")

# log the first run
run = client.set_experiment_run("First Run")
run.log_hyperparameters({"regularization" : 0.5})
run.log_dataset_version("training_and_testing_data", dataset_ver
model1 = # ... model training code goes here
run.log_metric('accuracy', accuracy(model1, validationData))
run.log_model(model1)

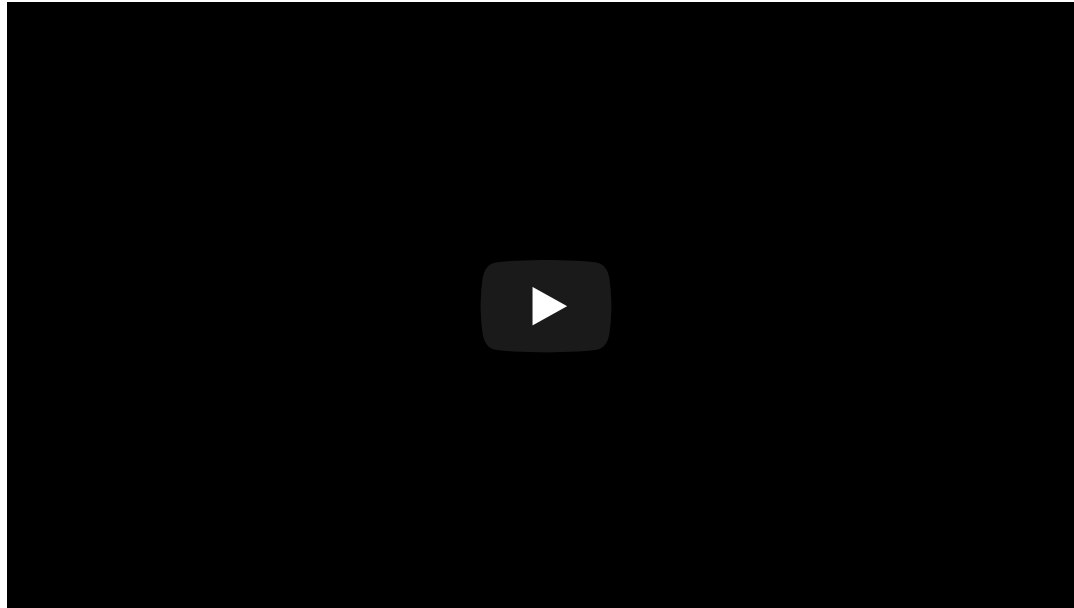
# log the second run
```

GOOGLE'S GOODS

- Automatically derive data dependencies from system log files
- Track metadata for each table
- No manual tracking/dependency declarations needed
- Requires homogeneous infrastructure
- Similar systems for tracking inside databases, MapReduce, Sparks, etc.

ASIDE: VERSIONING IN NOTEBOOKS WITH VERDANT

- Data scientists usually do not version notebooks frequently
- Exploratory workflow, copy paste, regular cleaning



Further reading: Kery, M. B., John, B. E., O'Flaherty, P., Horvath, A., & Myers, B. A. (2019, May). [Towards effective foraging by data scientists to find past analysis choices](#). In Proceedings of the 2019 CHI Conference on Human Factors in Computing Systems (pp. 1-13).

FROM MODEL VERSIONING TO DEPLOYMENT

- Decide which model version to run where
 - automated deployment and rollback (cf. canary releases)
 - Kubernetes, Cortex, BentoML, ...
- Track which prediction has been performed with which model version (logging)

LOGGING AND AUDIT TRACES

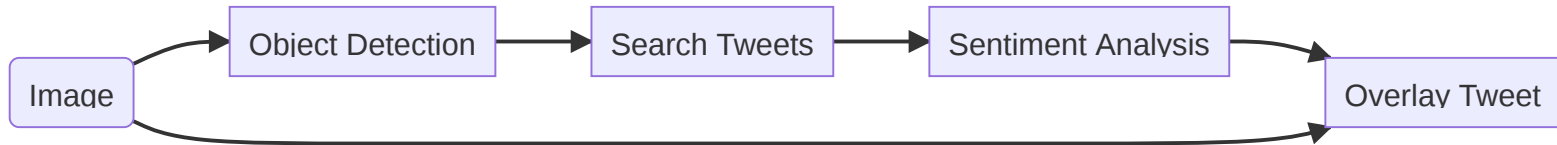
- Version everything
- Record every model evaluation with model version
- Append only, backed up

Key goal: If a customer complains about an interaction, can we reproduce the prediction with the right model? Can we debug the model's pipeline and data?

Can we reproduce the model?

```
<date>,<model>,<model version>,<feature inputs>,<output>  
<date>,<model>,<model version>,<feature inputs>,<output>  
<date>,<model>,<model version>,<feature inputs>,<output>
```

LOGGING FOR COMPOSED MODELS



Ensure all predictions are logged

BREAKOUT DISCUSSION: MOVIE PREDICTIONS (REVISITED)

Assume you are receiving complains that a child gets mostly recommendations about R-rated movies

Discuss again, updating the previous post in #1ecture:

- How would you identify the model that caused the prediction?
- How would you identify the code and dependencies that trained the model?
- How would you identify the training data used for that model?

K.G Orphanides. [Children's YouTube is still churning out blood, suicide and cannibalism](#). Wired UK, 2018

Kristie Bertucci. [16 NSFW Movies Streaming on Netflix](#). Gadget Reviews, 2020

REPRODUCABILITY

DEFINITIONS

- **Reproducibility:** the ability of an experiment to be repeated with minor differences from the original experiment, while achieving the same qualitative result
- **Replicability:** ability to reproduce results exactly, achieving the same quantitative result; requires determinism
- In science, reproducing results under different conditions are valuable to gain confidence
 - "conceptual replication": evaluate same hypothesis with different experimental procedure or population
 - many different forms distinguished "... replication" (e.g. close, direct, exact, independent, literal, nonexperimental, partial, retest, sequential, statistical, varied, virtual)

Juristo, Natalia, and Omar S. Gómez. "[Replication of software engineering experiments](#)." In Empirical software engineering and verification, pp. 60-88. Springer, Berlin, Heidelberg, 2010.

REPRODUCIBILITY OF NOTEBOOKS

- 2019 Study of 1.4M notebooks on GitHub:
 - 21% had unexecuted cells
 - 36% executed cells out of order
 - 14% declare dependencies
 - success rate for installing dependencies <40% (version issues, missing files)
 - notebook execution failed with exception in >40% (often ImportError, NameError, FileNotFoundError)
 - only 24% finished execution without problem, of those 75% produced different results
- 2020 Study of 936 executable notebooks:
 - 40% produce different results due to nondeterminism (randomness without seed)
 - 12% due to time and date
 - 51% due to plots (different library version, API misuse)
 - 2% external inputs (e.g. Weather API)
 - 27% execution environment (e.g., Python package versions)

Pimentel, João Felipe, Leonardo Murta, Vanessa Braganholo, and Juliana Freire. "A large-scale study about quality and reproducibility of jupyter notebooks." In 2019 IEEE/ACM 16th International Conference on Mining Software Repositories (MSR), pp. 507-517. IEEE, 2019.

Wang, Jiawei, K. U. O. Tzu-Yang, Li Li, and Andreas Zeller. "Assessing and restoring reproducibility of Jupyter notebooks." In 2020 35th IEEE/ACM international conference on automated software engineering (ASE), pp. 138-149. IEEE, 2020.

PRACTICAL REPRODUCABILITY

- Ability to generate the same research results or predictions
- Recreate model from data
- Requires versioning of data and pipeline (incl. hyperparameters and dependencies)

NONDETERMINISM

- Model inference almost always deterministic for a given model
- Some machine learning algorithms are nondeterministic
 - Nondeterminism in neural networks initialized from random initial weights
 - Nondeterminism from distributed learning
 - Nondeterminism in random forest algorithms
 - Determinism in linear regression and decision trees
- Many notebooks and pipelines contain nondeterminism
 - Depend on snapshot of online data (e.g., stream)
 - Depend on current time
 - Initialize random seed
 - Different memory addresses for figures
- Different library versions installed on the machine may affect results

RECOMMENDATIONS FOR REPRODUCIBILITY

- Version pipeline and data (see above)
- Document each step
 - document intention and assumptions of the process (not just results)
 - e.g., document why data is cleaned a certain way
 - e.g., document why certain parameters chosen
- Ensure determinism of pipeline steps (-> test)
- Modularize and test the pipeline
- Containerize infrastructure -- see MLOps

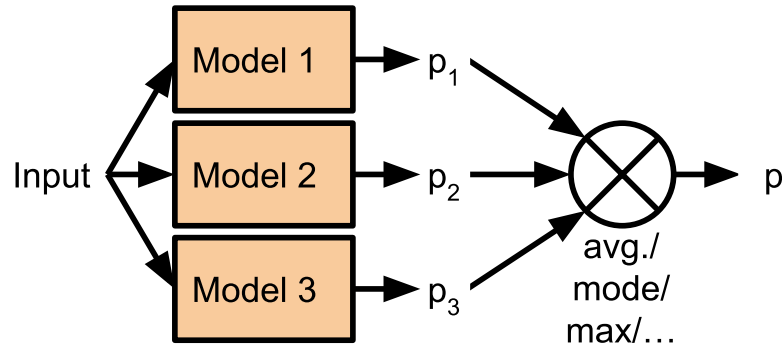
DEBUGGING AND FIXING MODELS

See also Hulten. Building Intelligent Systems. Chapter 21

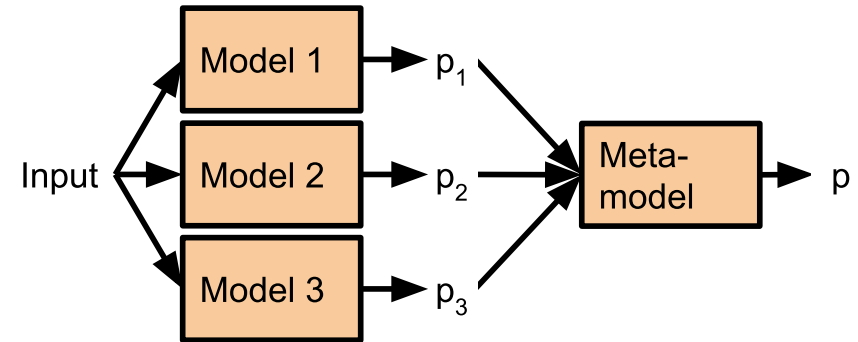
See also Nushi, Besmira, Ece Kamar, Eric Horvitz, and Donald Kossmann. "[On human intellect and machine failures: troubleshooting integrative machine learning systems.](#)" In *Proceedings of the Thirty-First AAAI Conference on Artificial Intelligence*, pp. 1017-1025. 2017.

RECALL: COMPOSING MODELS: ENSEMBLE AND METAMODELS

Ensemble

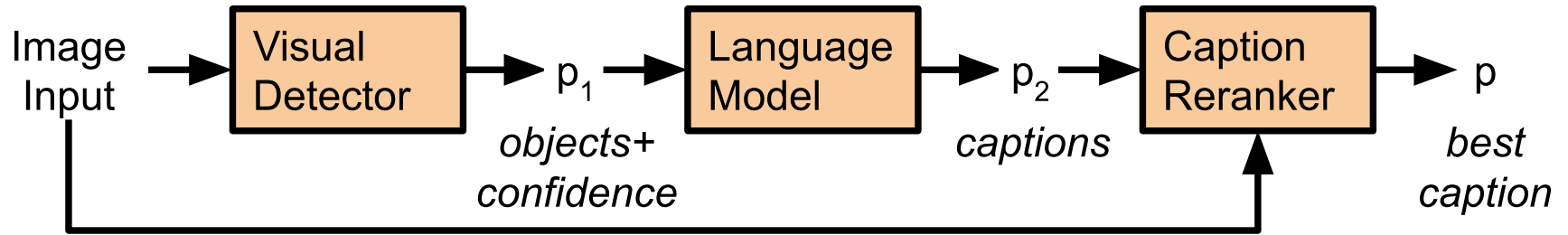


Metamodel / model stacking

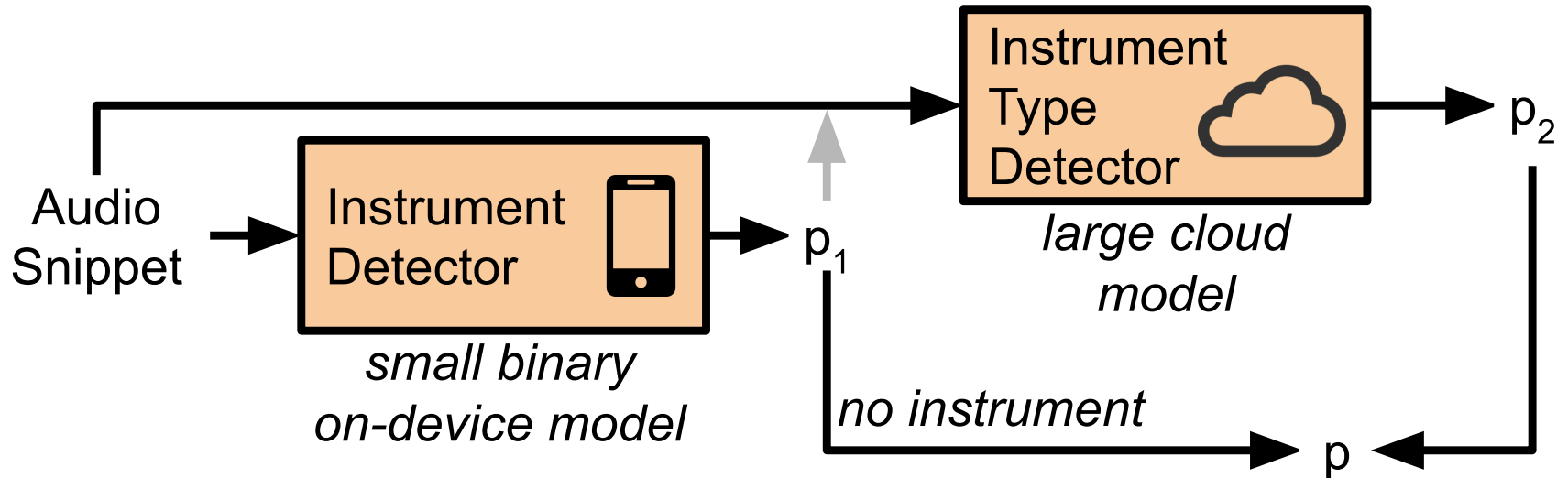


Legend:  machine-learned model,  non-ML aggregation function, p prediction

RECALL: COMPOSING MODELS: DECOMPOSING THE PROBLEM, SEQUENTIAL



RECALL: COMPOSING MODELS: CASCADE/TWO-PHASE PREDICTION



DECOMPOSING THE IMAGE CAPTIONING PROBLEM?



Speaker notes

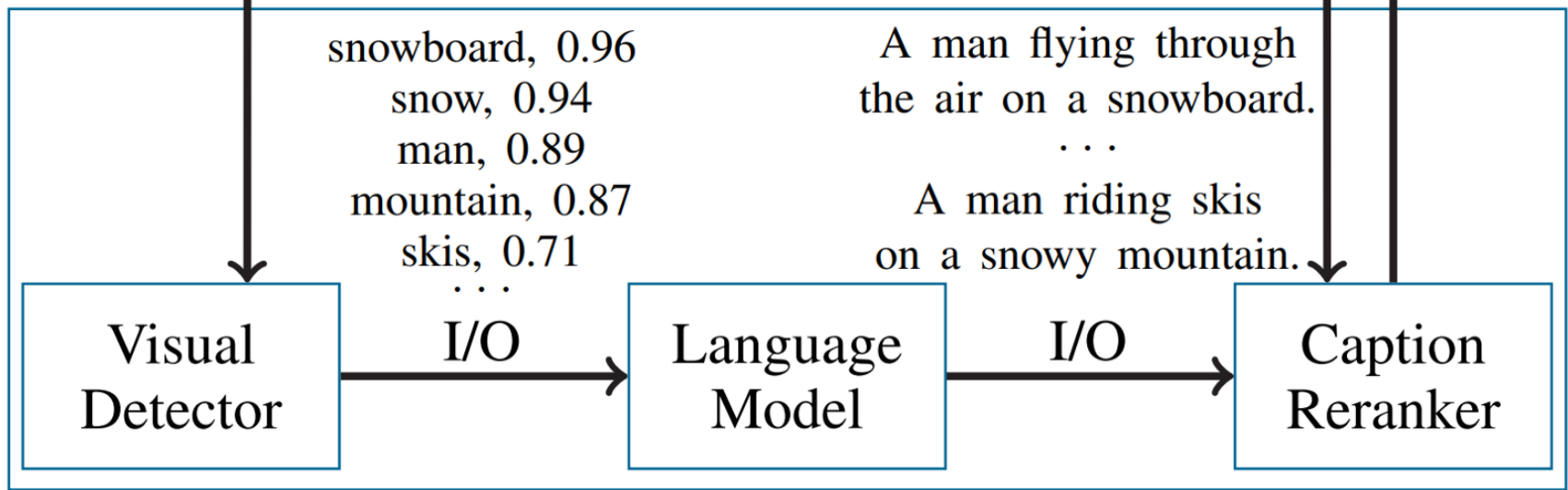
Using insights of how humans reason: Captions contain important objects in the image and their relations. Captions follow typical language/grammatical structure

STATE OF THE ART DECOMPOSITION (IN 2015)



#1

A man flying
through the air
on a snowboard.



Example and image from: Nushi, Besmira, Ece Kamar, Eric Horvitz, and Donald Kossmann. "[On human intellect and machine failures: troubleshooting integrative machine learning systems](#)." In Proc. AAAI. 2017.

BLAME ASSIGNMENT?



Visual Detector

- | | |
|--------------------|------|
| 1. teddy | 0.92 |
| 2. on | 0.92 |
| 3. cake | 0.90 |
| 4. bear | 0.87 |
| 5. stuffed | 0.85 |
| ... | |
| 15. blender | 0.57 |

Language Model

- | |
|---|
| 1. A teddy bear. |
| 2. A stuffed bear. |
| ... |
| 108. A blender sitting on top of a cake. |

Caption Reranker

- | |
|---|
| 1. A blender sitting on top of a cake. |
| 2. A teddy bear in front of a birthday cake. |
| 3. A cake sitting on top of a blender . |

Example and image from: Nushi, Besmira, Ece Kamar, Eric Horvitz, and Donald Kossmann. "[On human intellect and machine failures: troubleshooting integrative machine learning systems.](#)" In Proc. AAAI. 2017.

NONMONOTONIC ERRORS



Visual Detector

| | |
|----------|------|
| teddy | 0.92 |
| computer | 0.91 |
| bear | 0.90 |
| wearing | 0.87 |
| keyboard | 0.84 |
| glasses | 0.63 |

1. A teddy bear
sitting on top
of a computer.

Fixed Visual Detector

| | |
|----------|-----|
| teddy | 1.0 |
| bear | 1.0 |
| wearing | 1.0 |
| keyboard | 1.0 |
| glasses | 1.0 |

1. a person wearing
glasses and holding
a teddy bear sitting
on top of a keyboard.

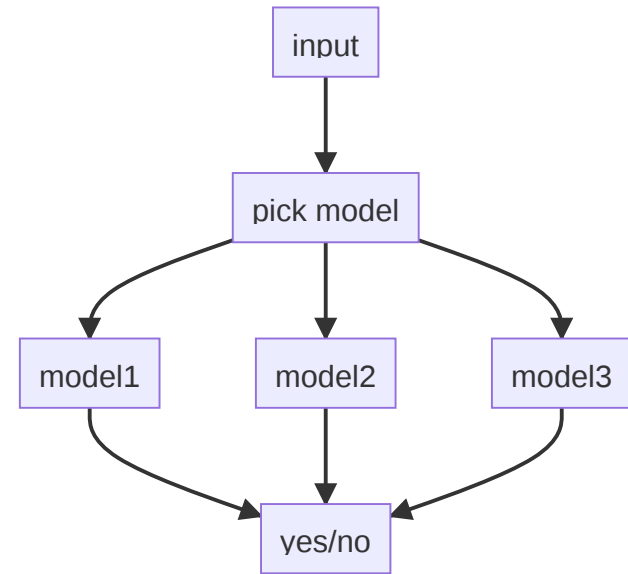
Example and image from: Nushi, Besmira, Ece Kamar, Eric Horvitz, and Donald Kossmann. "On human intellect and machine failures: troubleshooting integrative machine learning systems." In Proc. AAAI. 2017.

CHASING BUGS

- Update, clean, add, remove data
- Change modeling parameters
- Add regression tests
- Fixing one problem may lead to others, recognizable only later

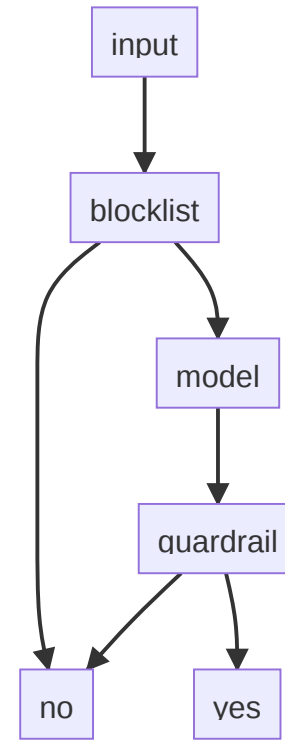
PARTITIONING CONTEXTS

- Separate models for different subpopulations
- Potentially used to address fairness issues
- ML approaches typically partition internally already



OVERRIDES

- Hardcoded heuristics (usually created and maintained by humans) for special cases
- Blocklists, guardrails
- Potential neverending attempt to fix special cases



IDEAS?



SUMMARY

- Provenance is important for debugging and accountability
- Data provenance, feature provenance, model provenance
- Reproducibility vs replicability
- Version everything
 - Strategies for data versioning at scale
 - Version the entire pipeline and dependencies
 - Adopt a pipeline view, modularize, automate
 - Containers and MLOps, many tools
- Strategies to fix models