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

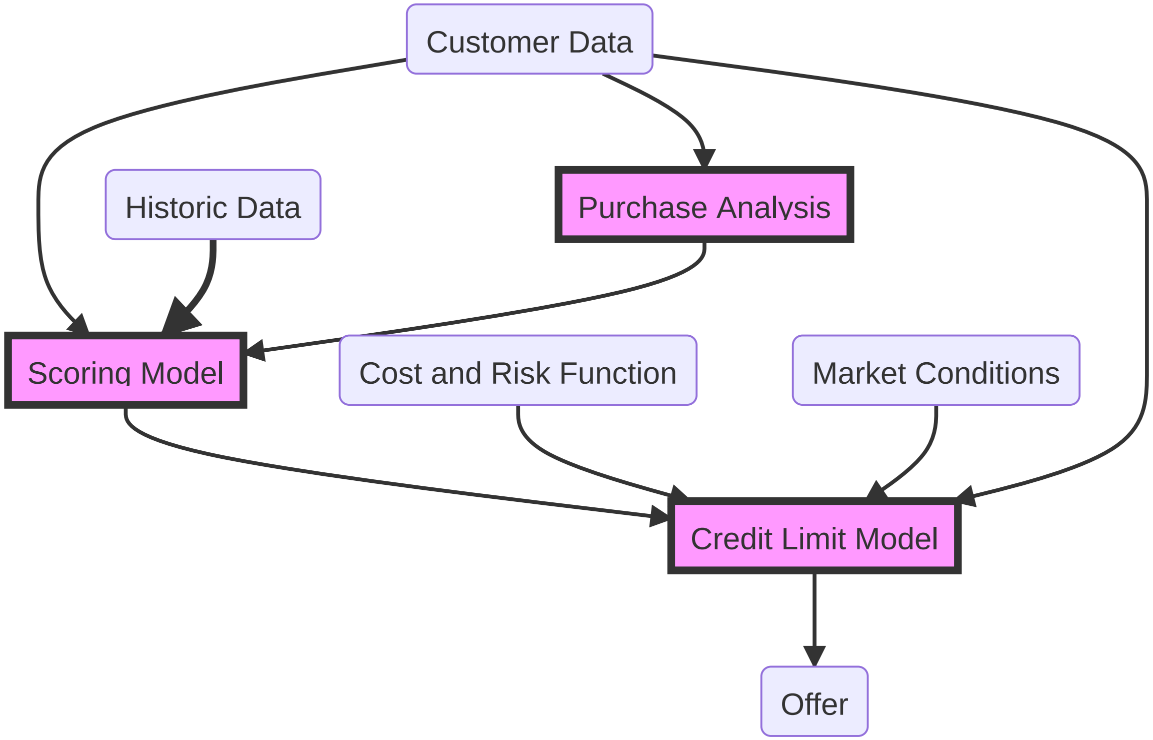
LEARNING GOALS

- 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


Customer Data
Historic Data
Purchase Analysis
Scoring Model
Cost and Risk Function
Market Conditions
Credit Limit Model
Offer

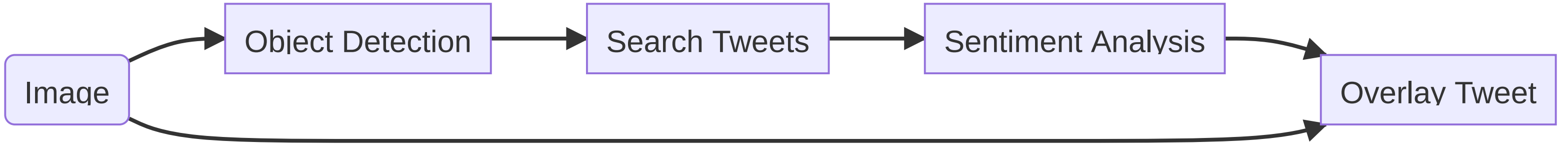
DEBUGGING?

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

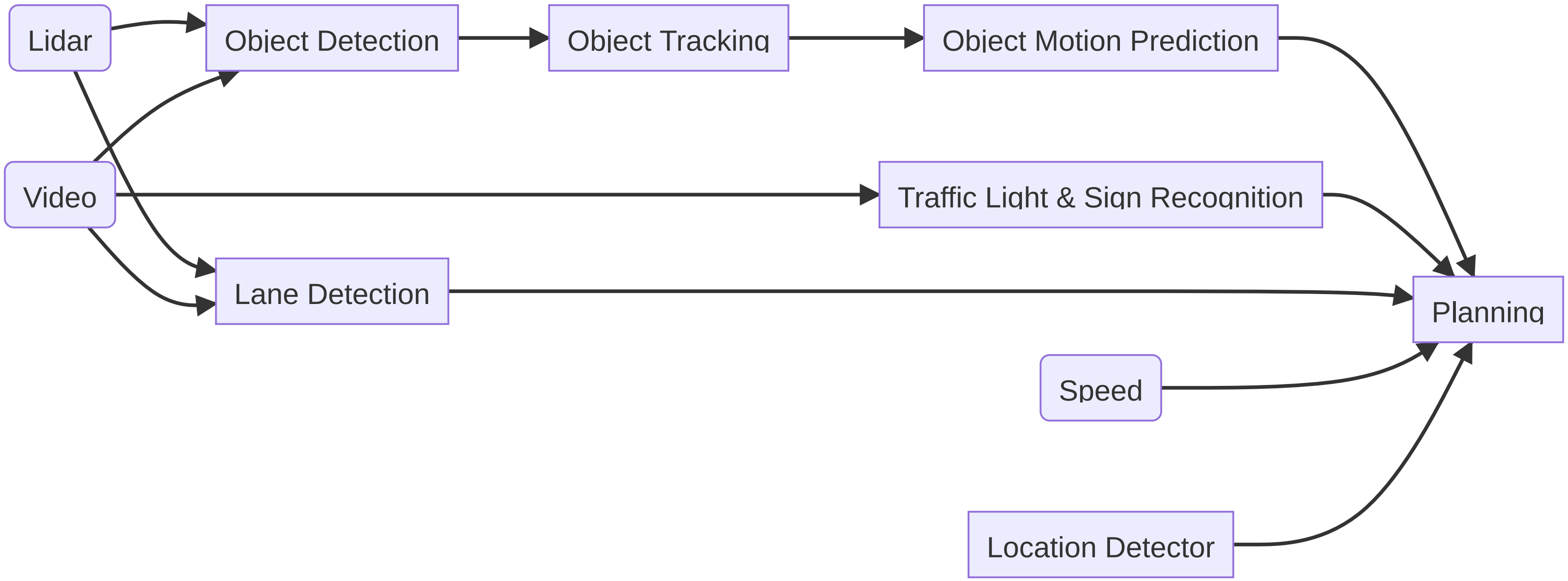


Version all models involved.

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 recommmendations?

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

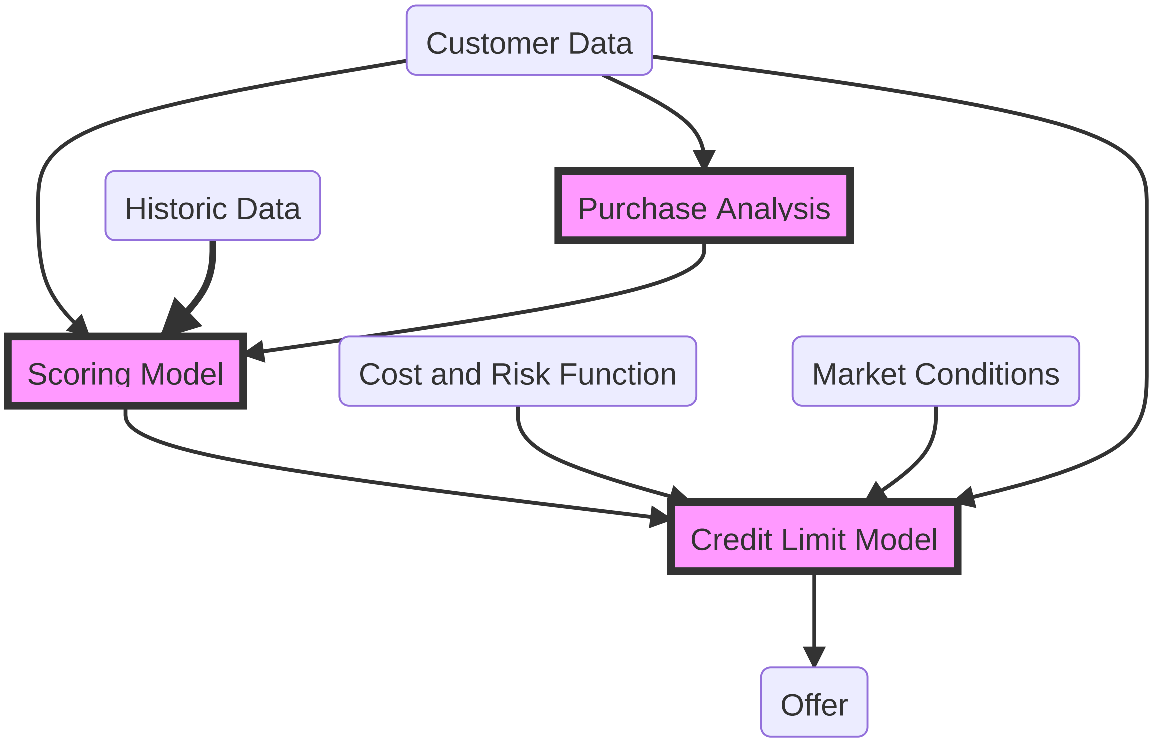
Kristie Bertucci. 16 NSFW Movies Streaming on Netflix. Gadget Reviews, 2020

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 drived from many sources through many steps, including other models



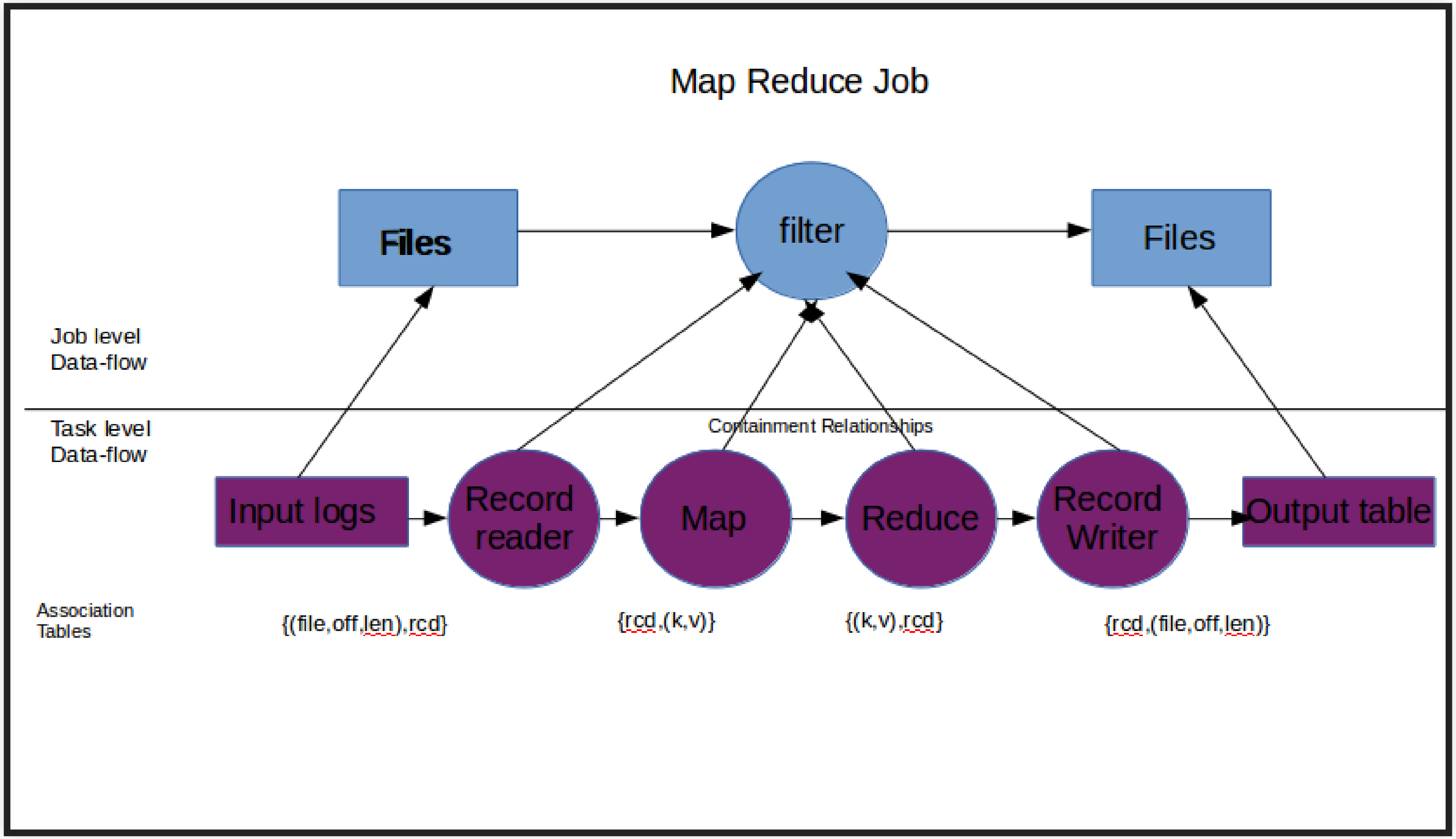
EXCURSION: PROVENANCE TRACKING IN DATABASES

- Whenever value is changed, record:
    - who changed it
    - time of change
    - history of previous values
    - possibly also justifcation 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?

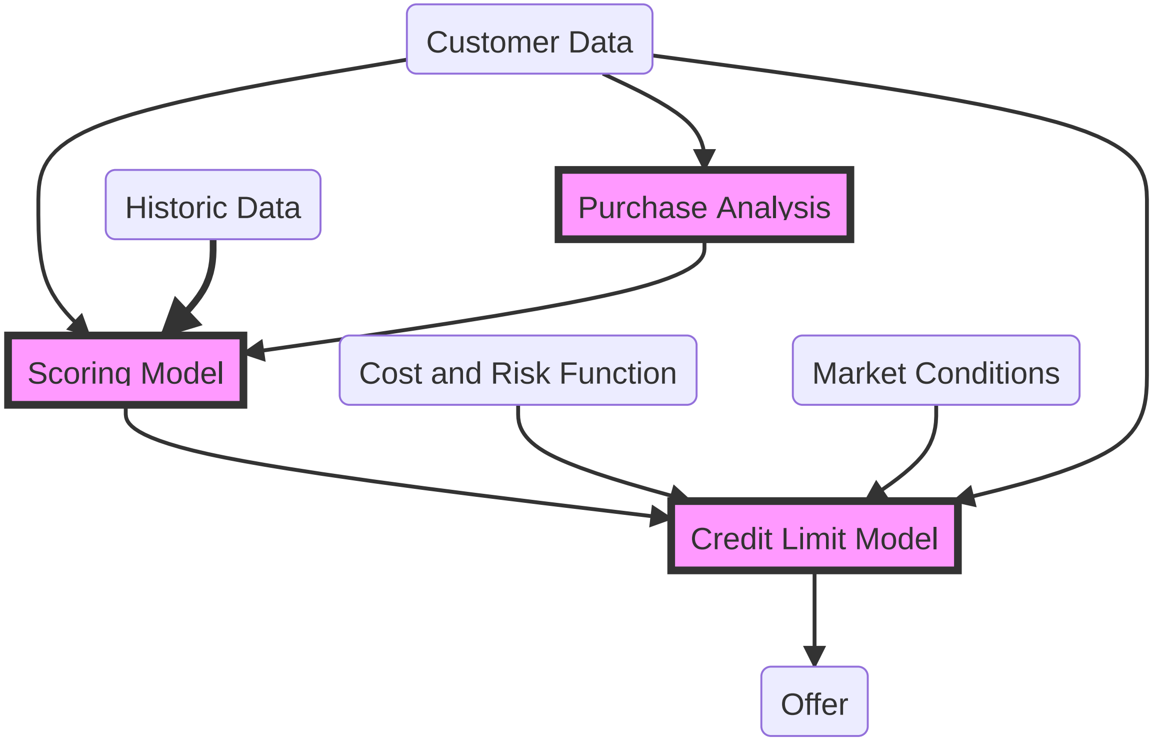
GOOD PRACTICE: FEATURE STORE

- Excapsulate 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?


Customer Data
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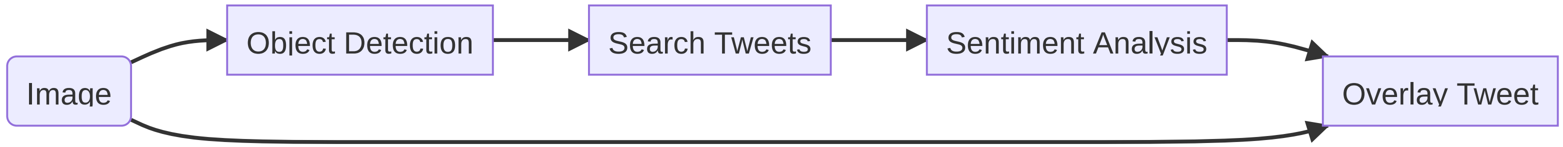
IN REAL SYSTEMS: TRACKING PROVENANCE ACROSS MULTIPLE MODELS

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

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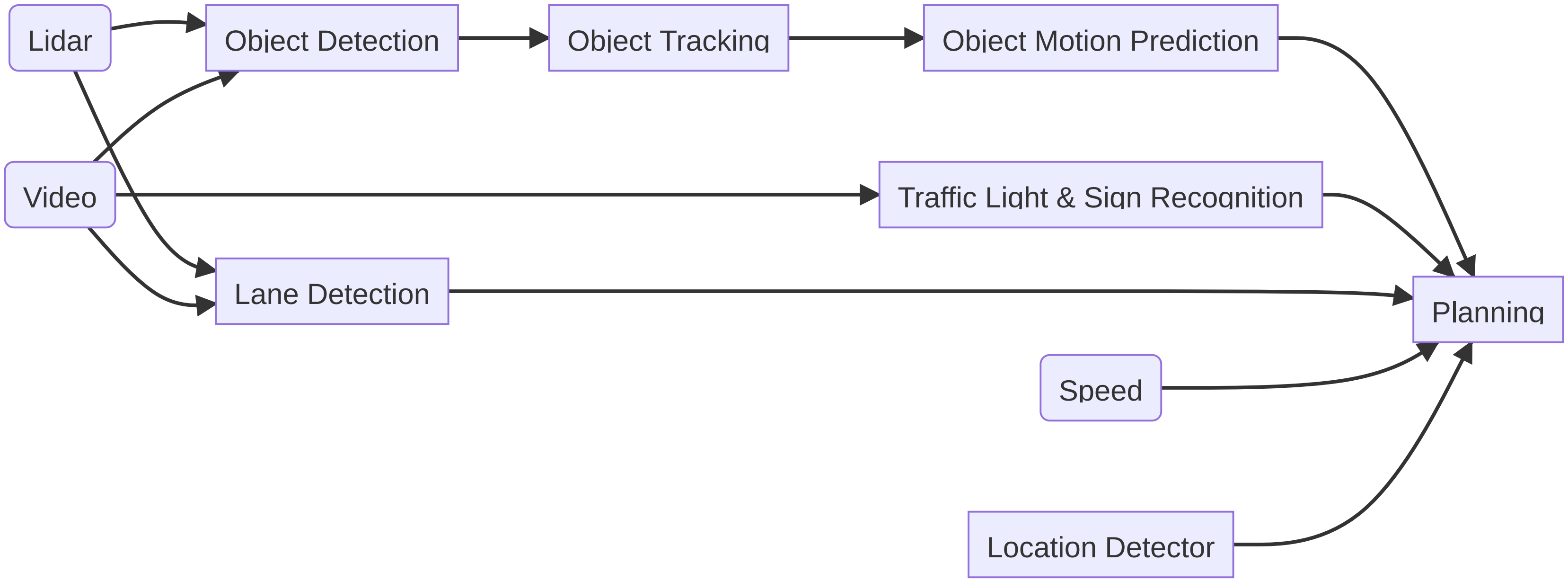


Example: Zong, W., Zhang, C., Wang, Z., Zhu, J., & Chen, Q. (2018). [Architecture design and implementation of an autonomous vehicle](). IEEE access, 6, 21956-21970.

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

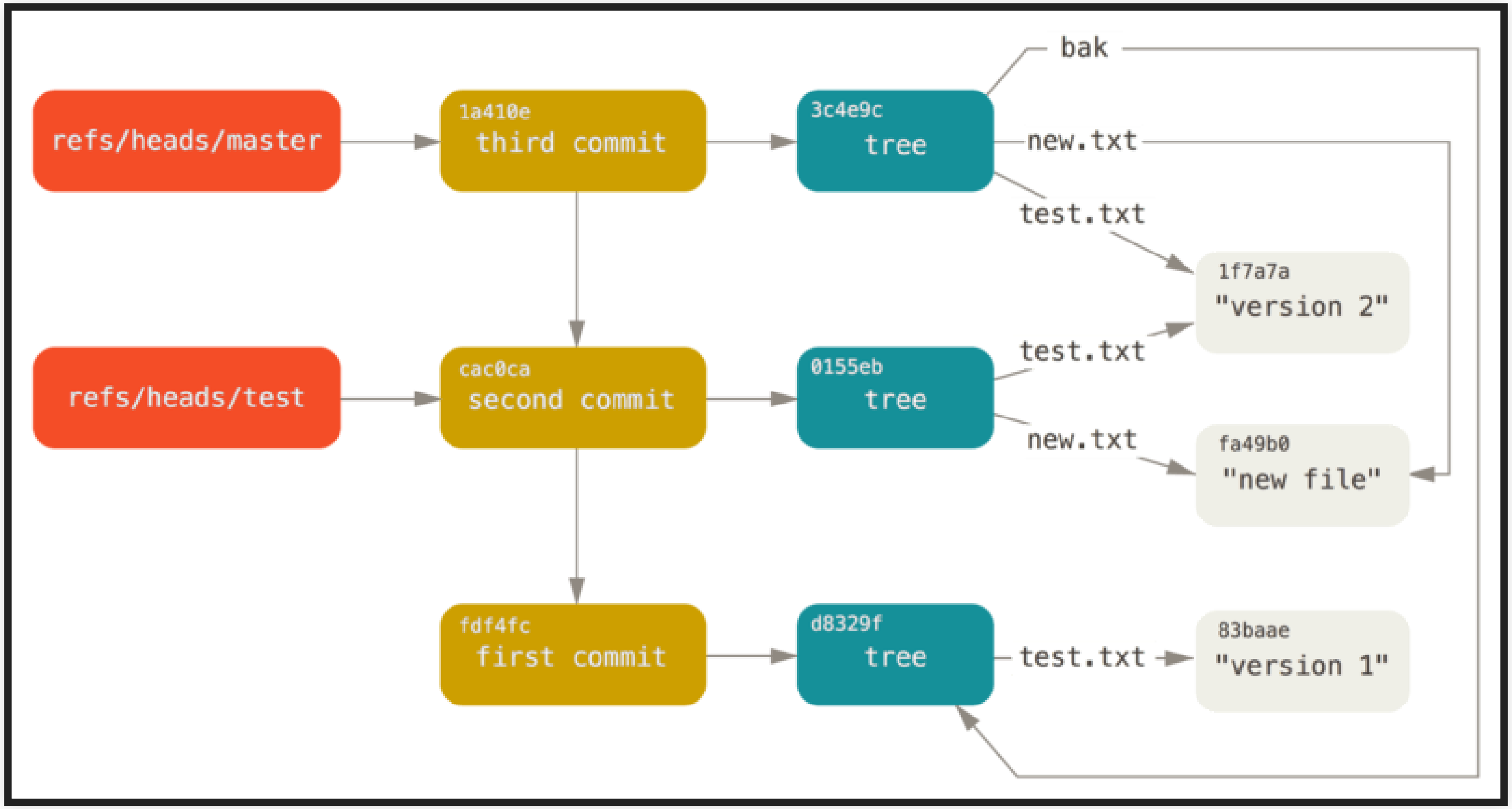
```
createUser(id=5, name="Christian", dpt="SCS")
updateUser(id=5, dpt="ISR")
deleteUser(id=5)
```

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



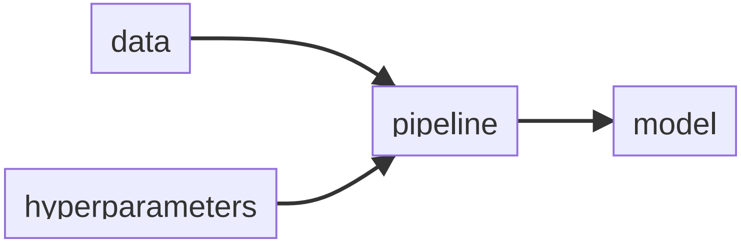
Scott Chacon and Ben Straub. Pro Git. 2014

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 reproducable 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

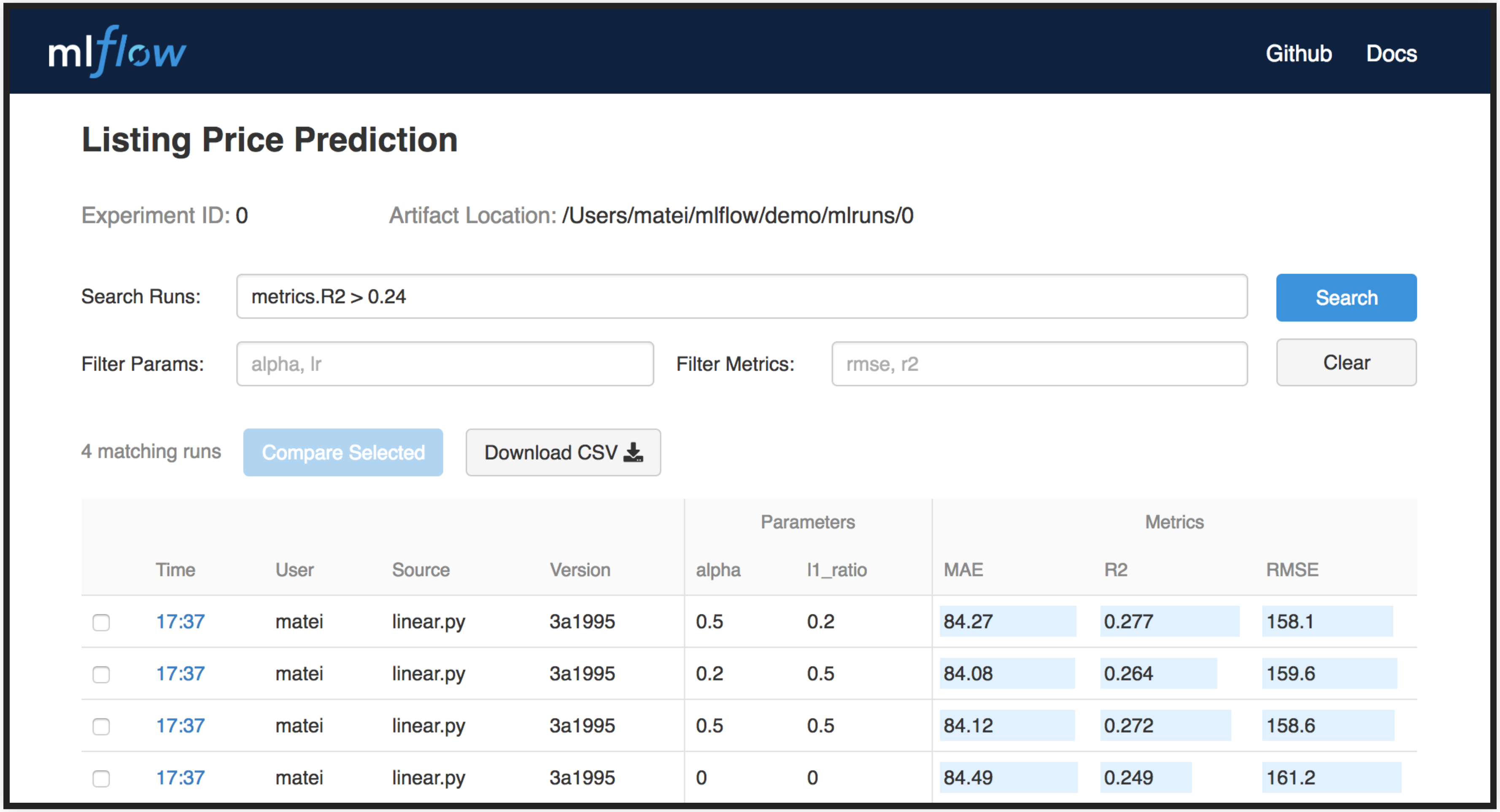
https://dvc.org/

DVC EXAMPLE

```yaml
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



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
```

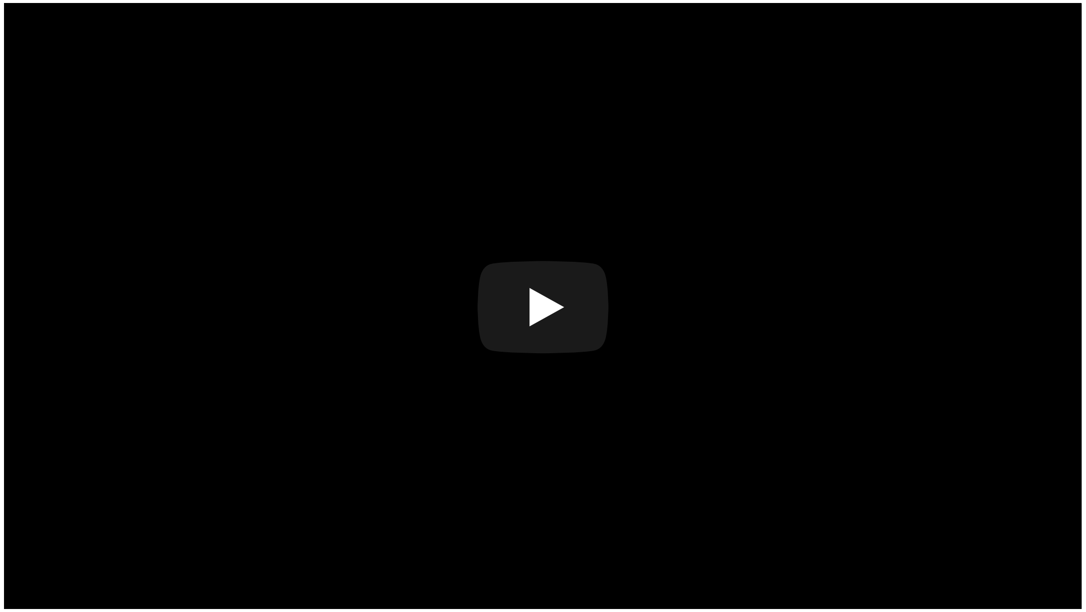
GOOGLE'S GOODS

- 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)
    - Kubernetis, Cortex, BentoML, ...
- Track which prediction has been performed with which model version (logging)

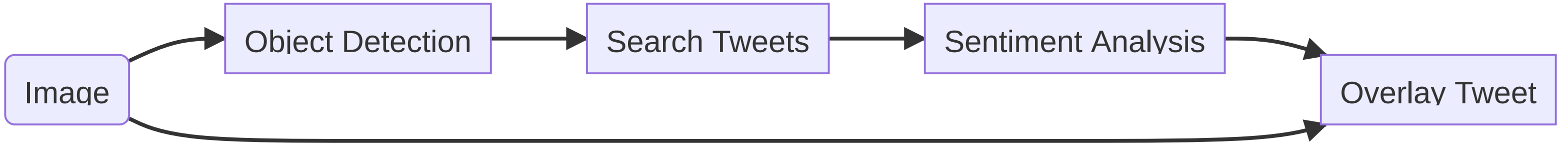
LOGGING AND AUDIT TRACES

- 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 `#lecture`:

- 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, nonexperiemental, 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

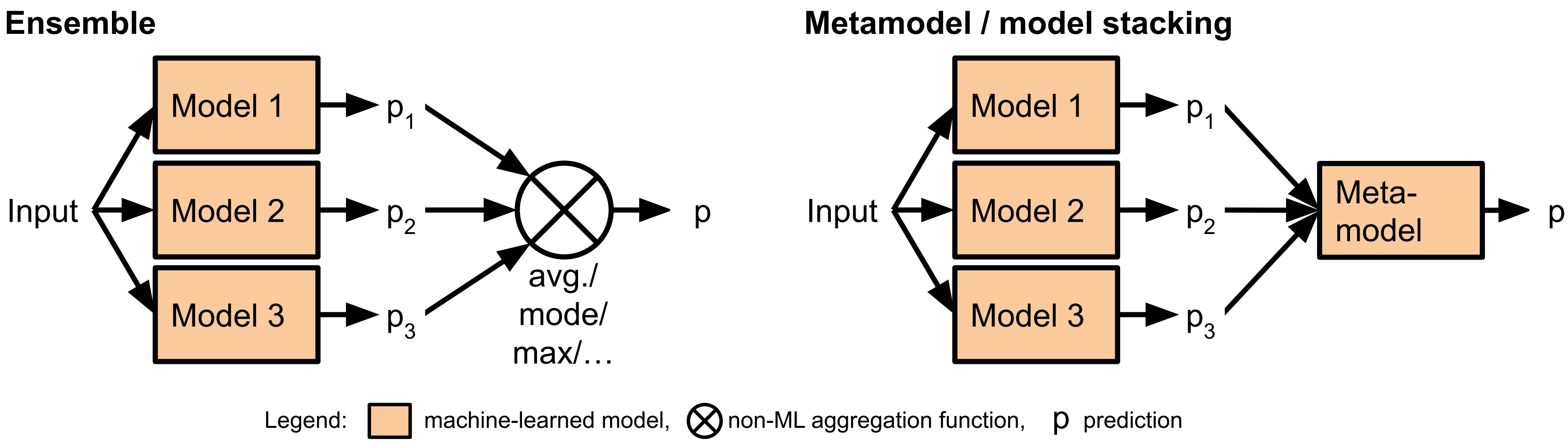
- Version pipeline and data (see above)
- Document each step
    - document intention and assumptions of the process (not just results)
    - e.g., document why data is cleaned a certain way
    - e.g., document why certain parameters chosen
- Ensure determinism of pipeline steps (-> test)
- Modularize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

DEBUGGING AND FIXING MODELS

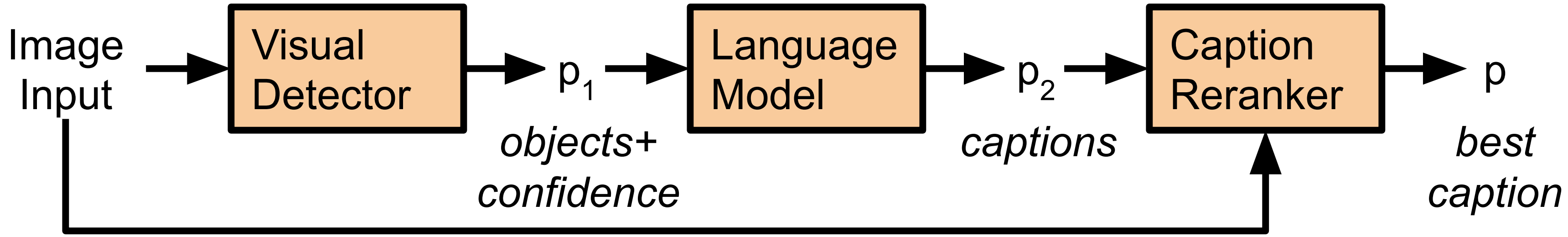
See also Hulten. Building Intelligent Systems. Chapter 21

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.

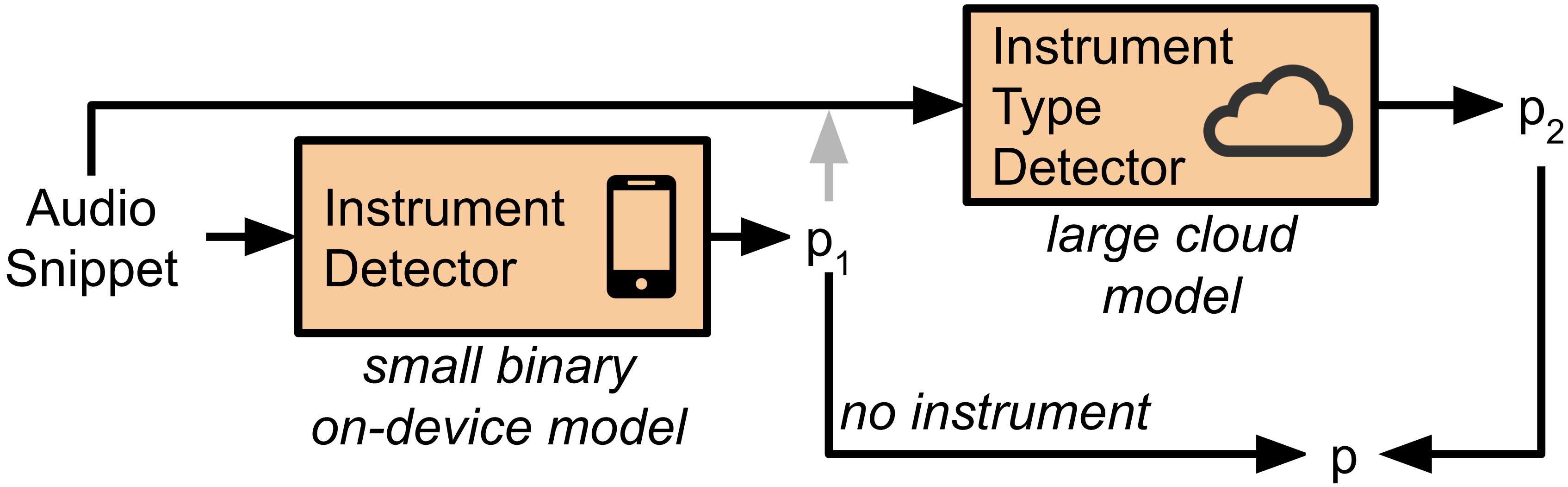
RECALL: COMPOSING MODELS: ENSEMBLE AND METAMODELS



RECALL: COMPOSING MODELS: DECOMPOSING THE PROBLEM, SEQUENTIAL



RECALL: COMPOSING MODELS: CASCADE/TWO-PHASE PREDICTION

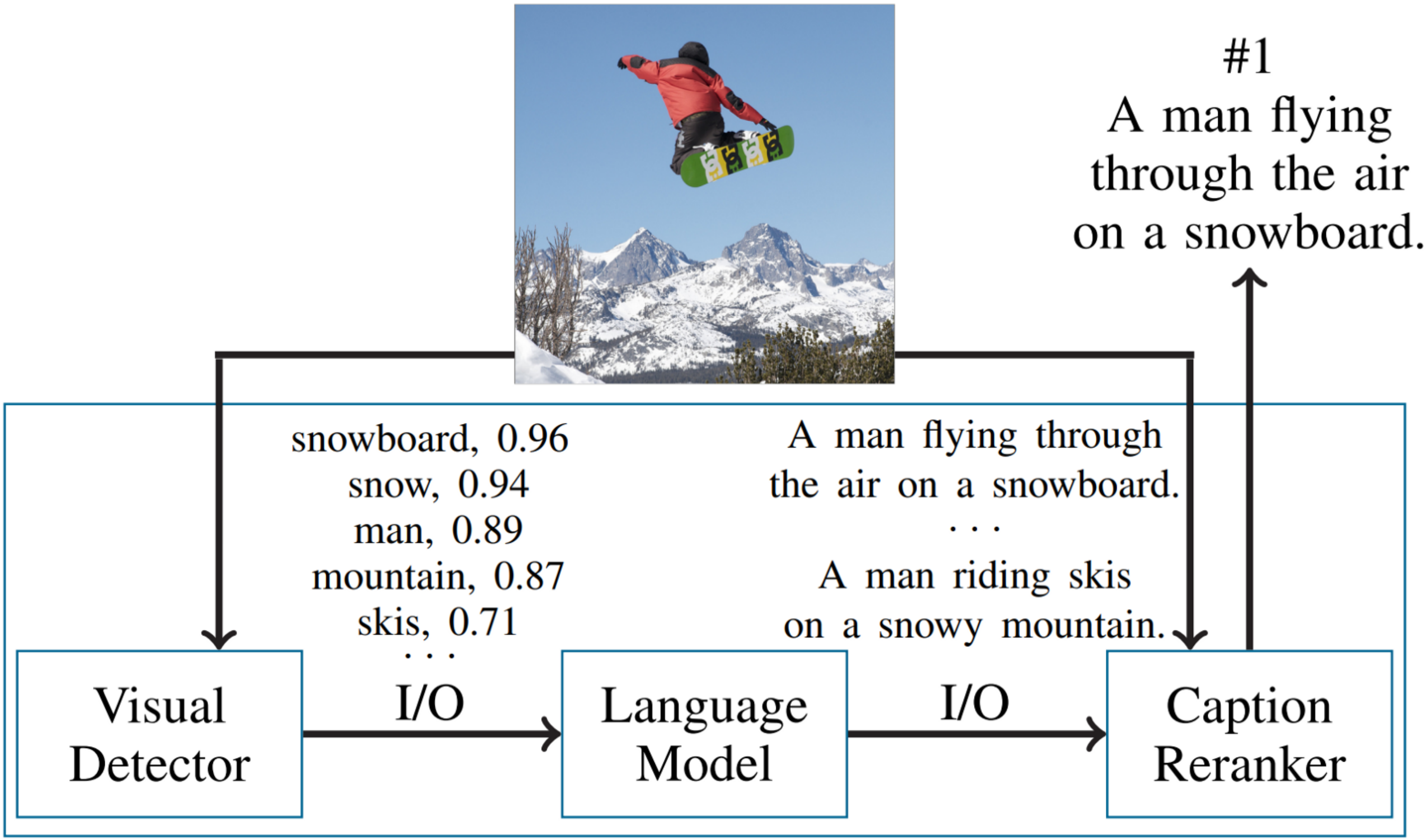


DECOMPOSING THE IMAGE CAPTIONING PROBLEM?

Speaker notes

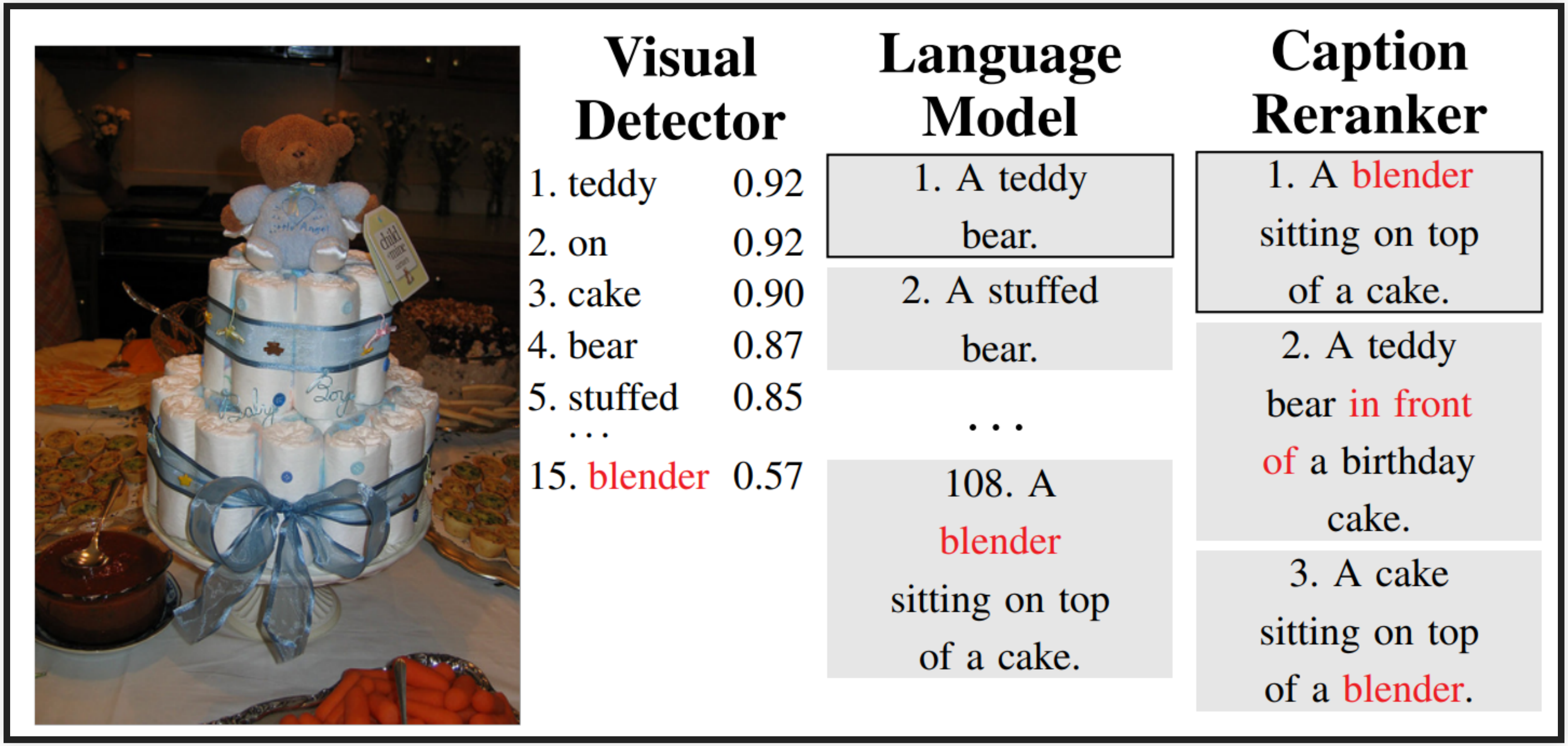
Using insights of how humans reason: Captions contain important objects in the image and their relations. Captions follow typical language/grammatical structure

STATE OF THE ART DECOMPOSITION (IN 2015)



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?



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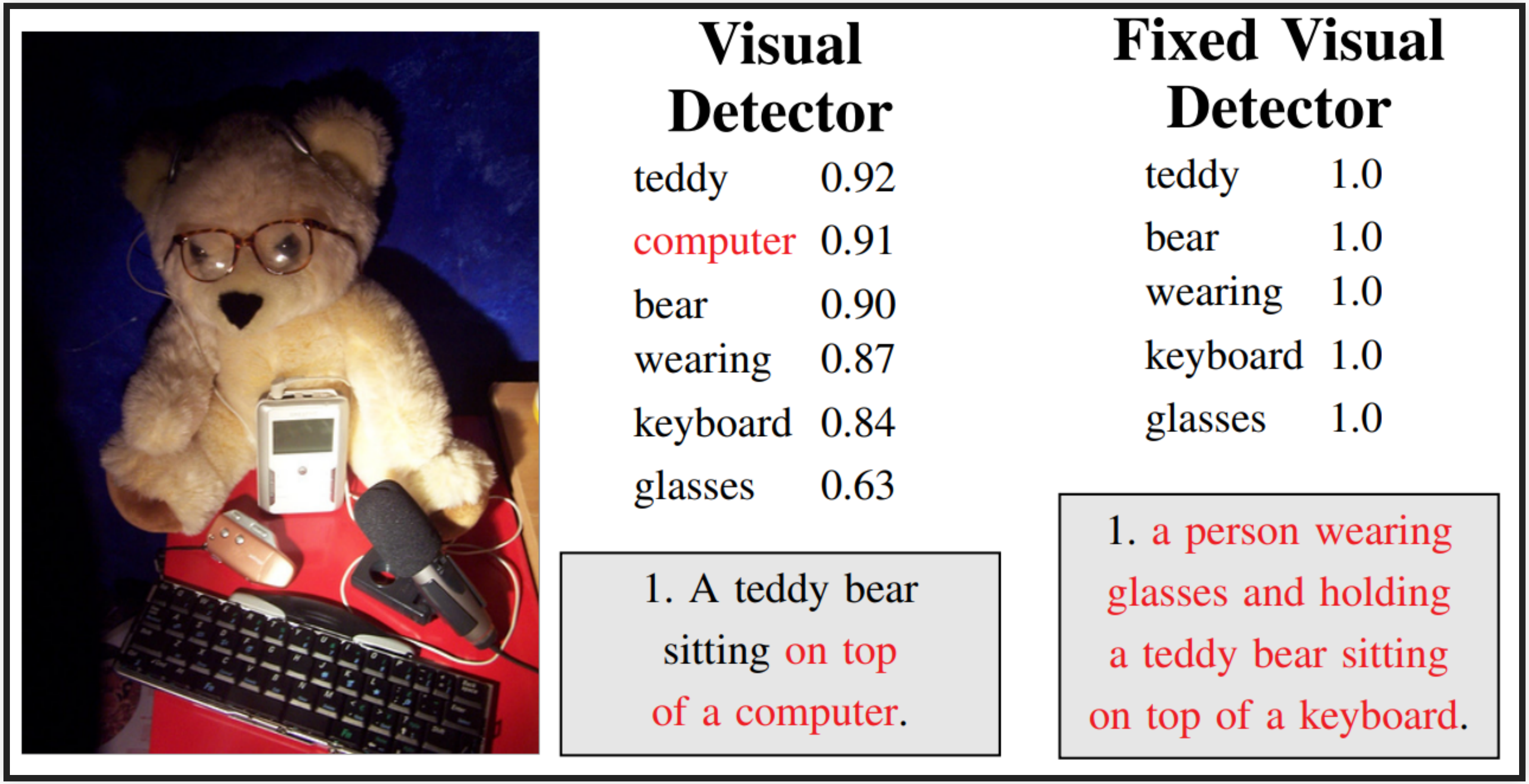
NONMONOTONIC ERRORS



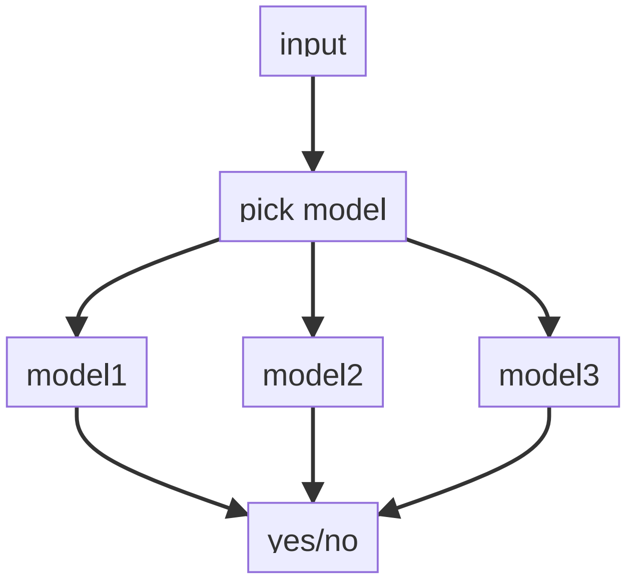
Example and image from: Nushi, Besmira, Ece Kamar, Eric Horvitz, and Donald Kossmann. "On human intellect and machine failures: troubleshooting integrative machine learning systems." In Proc. AAAI. 2017.

CHASING BUGS

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

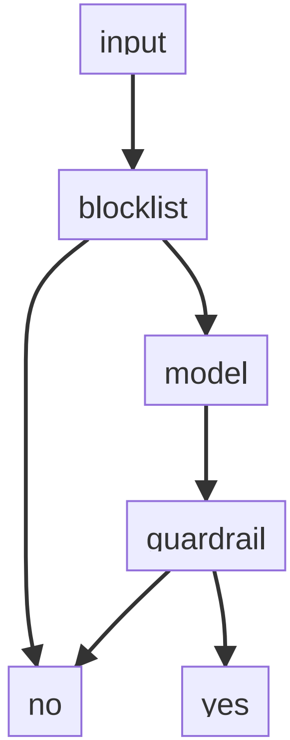
PARTITIONING CONTEXTS

- 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
- Reproducability 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