MODEL QUALITY

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Required reading:

- Hulten, Geoff. "Building Intelligent Systems: A Guide to Machine Learning Engineering." Apress, 2018, Chapter 19 (Evaluating Intelligence).
- Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. "Semantically equivalent adversarial rules for debugging NLP models." In Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pp. 856-865. 2018.

LEARNING GOALS

- Select a suitable metric to evaluate prediction accuracy of a model and to compare multiple models
- Select a suitable baseline when evaluating model accuracy
- Explain how software testing differs from measuring prediction accuracy of a model
- Curate validation datasets for assessing model quality, covering subpopulations as needed
- Use invariants to check partial model properties with automated testing
- Develop automated infrastructure to evaluate and monitor model quality

MODEL QUALITY

FIRST PART: MEASURING PREDICTION ACCURACY

the data scientist's perspective

SECOND PART: LEARNING FROM SOFTWARE TESTING

how software engineering tools may apply to ML

testing in production (next week)

"Programs which were written in order to determine the answer in the first place. There would be no need to write such programs, if the correct answer were known" (Weyuker, 1982).

MODEL QUALITY VS SYSTEM QUALITY

PREDICTION ACCURACY OF A MODEL

– *model:* $X \rightarrow Y$

– *validation data (tests?):* sets of (X, Y) pairs indicating desired outcomes for select inputs

For our discussion: any form of model, including machine learning models, symbolic AI components, hardcoded heuristics, composed models, ...

COMPARING MODELS

Compare two models (same or different implementation/learning technology) for the same task:

- Which one supports the system goals better?
- Which one makes fewer important mistakes?
- Which one is easier to operate?
- Which one is better overall?
- Is either one good enough?

ML ALGORITHM QUALITY VS MODEL QUALITY VS DATA QUALITY VS SYSTEM QUALITY

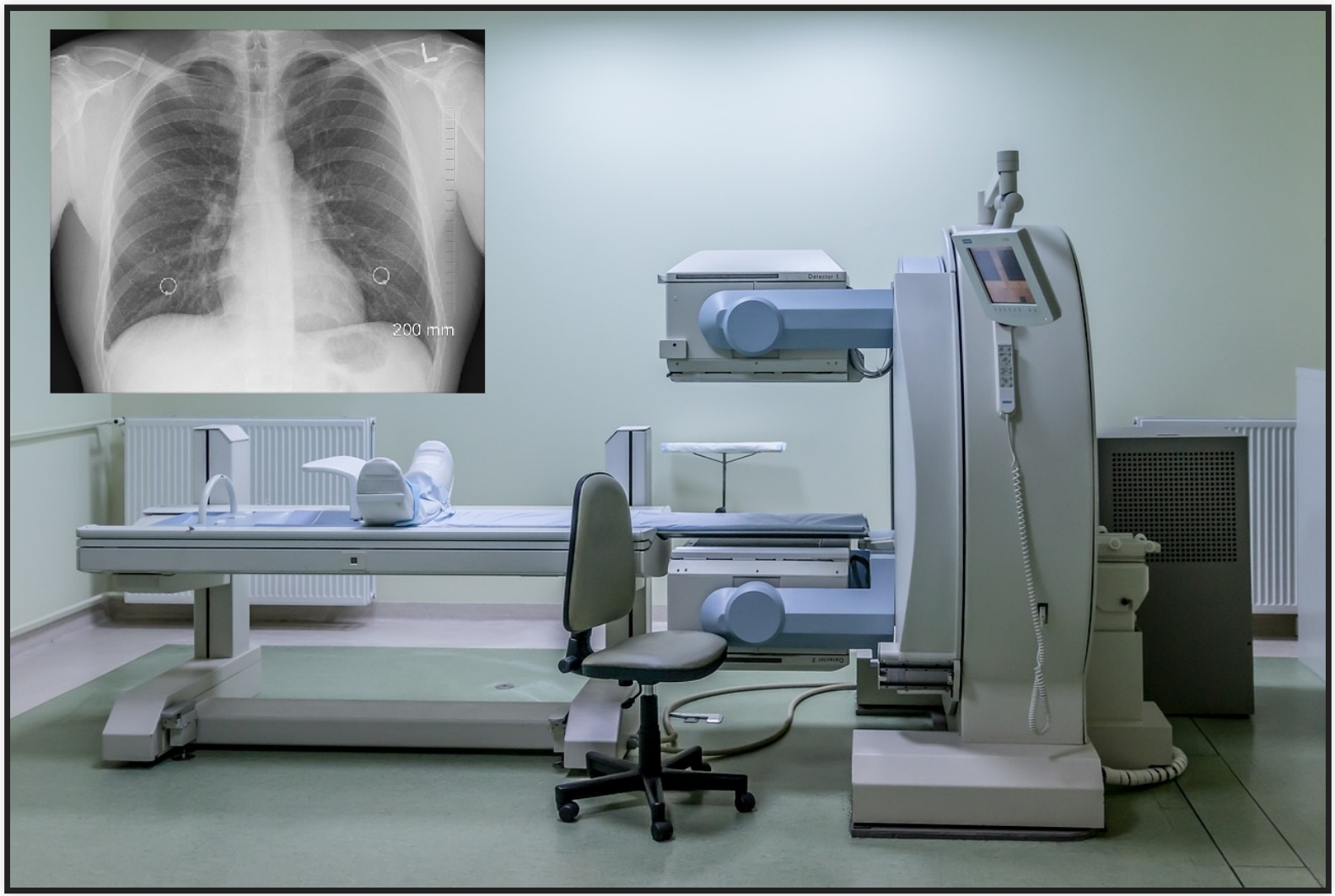
Todays focus is on the quality of the produced *model*, not the algorithm used to learn the model or the data used to train the model

i.e. assuming *Decision Tree Algorithm* and feature extraction are correctly implemented (according to specification), is the model learned from data any good?

The model is just one component of the entire system.

Focus on measuring quality, not debugging the source of quality problems (e.g., in data, in feature extraction, in learning, in infrastructure)

CASE STUDY: CANCER DETECTION



Speaker notes

Application to be used in hospitals to screen for cancer, both as routine preventative measure and in cases of specific suspicions. Supposed to work together with physicians, not replace.

THE SYSTEMS PERSPECTIVE

System is more than the model

Includes deployment, infrastructure, user interface, data infrastructure, payment services, and often much more

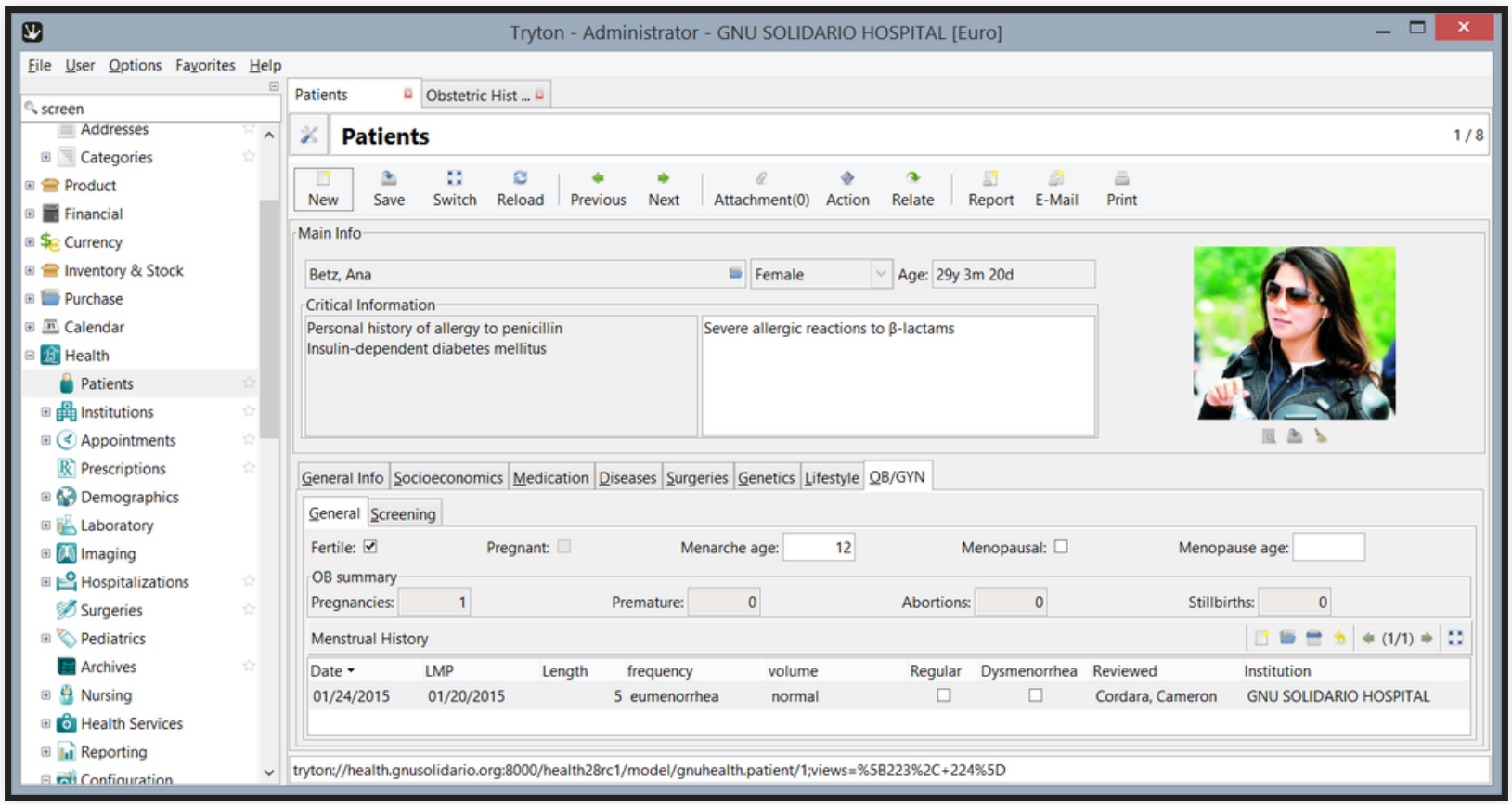
Systems have a goal:

- maximize sales
- save lifes
- entertainment
- connect people

Models can help or may be essential in those goals, but are only one part

Today: Narrow focus on prediction accuracy of the model

CANCER PREDICTION WITHIN A HEALTHCARE APPLICATION



MANY QUALITIES

Prediction accuracy of a model is important

But many other quality matters when building a system:

- Model size
- Inference time
- User interaction model
- Kinds of mistakes made
- How the system deals with mistakes
- Ability to incrementally learn
- Safety, security, fairness, privacy
- Explainability

Today: Narrow focus on prediction accuracy of the model

ON TERMINOLOGY: PERFORMANCE

In machine learning, "performance" typically refers to accuracy

"this model performs better" = it produces more accurate results

Be aware of ambiguity across communities.

When speaking of "time", be explicit: "learning time", "inference time", "latency", ...

(see also: performance in arts, job performance, company performance, performance test (bar exam) in law, software/hardware/network performance)

MEASURING PREDICTION ACCURACY FOR CLASSIFICATION TASKS

(The Data Scientists Toolbox)

CONFUSION/ERROR MATRIX

	Actually A	Actually B	Actually C
AI predicts A	**10**	6	2
AI predicts B	3	**24**	10
AI predicts C	5	22	**82**

$$\text{accuracy} = \frac{\text{correct predictions}}{\text{all predictions}}$$

$$\text{Example's accuracy} = \frac{10+24+82}{10+6+2+3+24+10+5+22+82} = .707$$

```
def accuracy(model, xs, ys):
  count = length(xs)
  countCorrect = 0
  for i in 1..count:
    predicted = model(xs[i])
    if predicted == ys[i]:
      countCorrect += 1
  return countCorrect / count
```

IS 99% ACCURACY GOOD?

IS 99% ACCURACY GOOD?

-> depends on problem; can be excellent, good, mediocre, terrible

10% accuracy can be good on some tasks (information retrieval)

Always compare to a base rate!

$$\text{Reduction in error} = \frac{(1 - accuracy_{\text{baseline}}) - (1 - accuracy_f)}{1 - accuracy_{\text{baseline}}}$$

- from 99.9% to 99.99% accuracy = 90% reduction in error
- from 50% to 75% accuracy = 50% reduction in error

BASELINES?

Suitable baselines for cancer prediction? For recidivism?

Speaker notes

Many forms of baseline possible, many obvious: Random, all true, all false, repeat last observation, simple heuristics, simpler model

TYPES OF MISTAKES

Two-class problem of predicting event A:

	Actually A	**Actually not A**
AI predicts A	True Positive (TP)	False Positive (FP)
AI predicts not A	False Negative (FN)	True Negative (TN)

True positives and true negatives: correct prediction

False negatives: wrong prediction, miss, Type II error

False positives: wrong prediction, false alarm, Type I error

MULTI-CLASS PROBLEMS VS TWO-CLASS PROBLEM

	Actually A	Actually B	Actually C
AI predicts A	**10**	6	2
AI predicts B	3	**24**	10
AI predicts C	5	22	**82**

MULTI-CLASS PROBLEMS VS TWO-CLASS PROBLEM

	Actually A	Actually B	Actually C
AI predicts A	**10**	6	2
AI predicts B	3	**24**	10
AI predicts C	5	22	**82**

	Act. A	Act. not A
AI predicts A	10	8
AI predicts not A	8	138

	Act. B	Act. not B
AI predicts B	24	13
AI predicts not B	28	99

Speaker notes

Individual false positive/negative classifications can be derived by focusing on a single value in a confusion matrix. False positives/recall/etc are always considered with regard to a single specific outcome.

CONSIDER THE BASELINE PROBABILITY

Predicting unlikely events -- 1 in 2000 has cancer (stats)

Random predictor

	Cancer	No c.
Cancer pred.	3	4998
No cancer pred.	2	4997

.5 accuracy

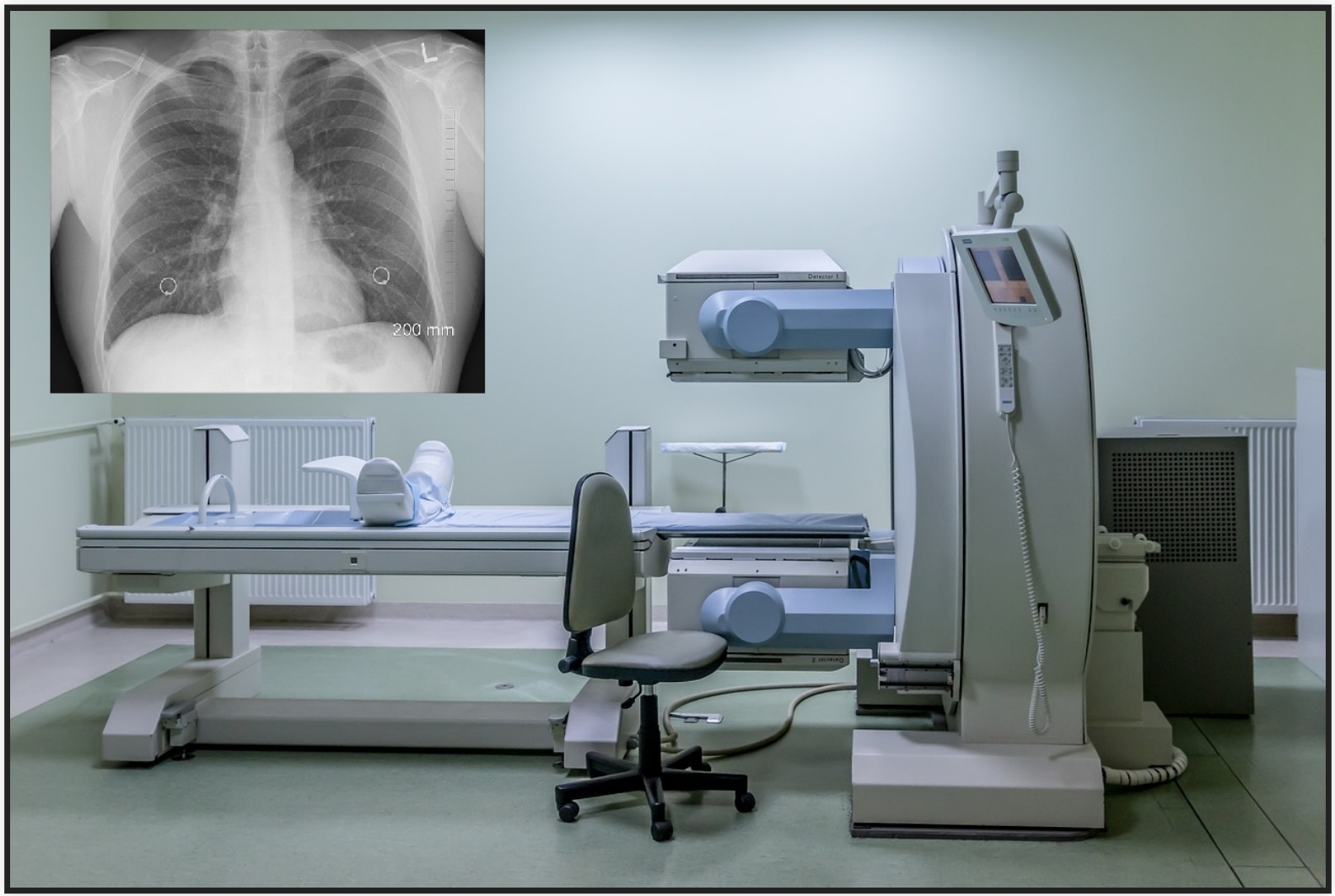
Never cancer predictor

	Cancer	No c.
Cancer pred.	0	0
No cancer pred.	5	9995

.999 accuracy

See also Bayesian statistics

TYPES OF MISTAKES IN IDENTIFYING CANCER?



MEASURES

Measuring success of correct classifications (or missing results):

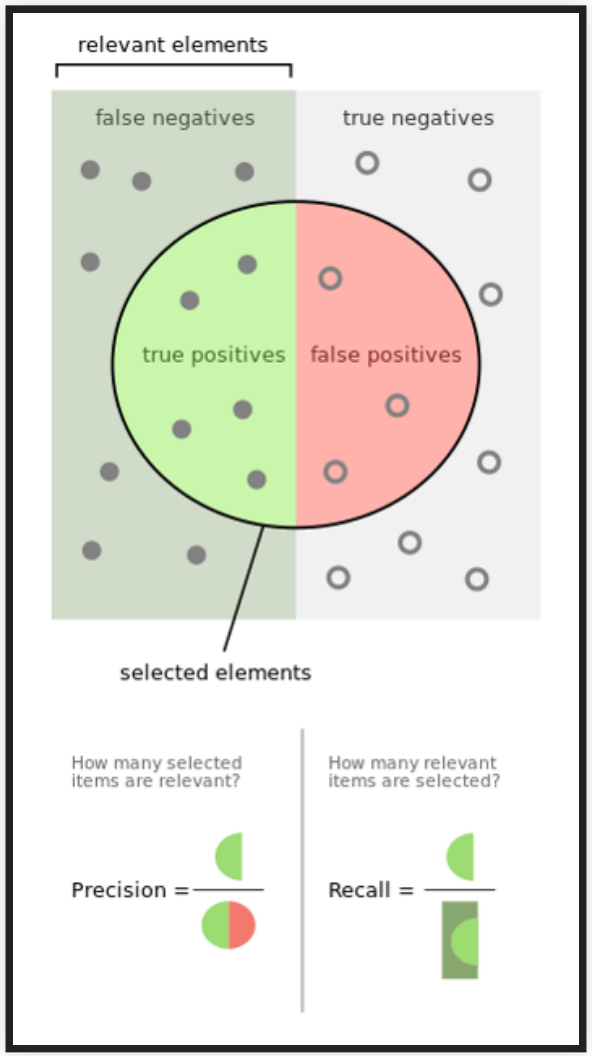
- Recall = TP/(TP+FN)
  - aka true positive rate, hit rate, sensitivity; *higher is better*
- False negative rate = FN/(TP+FN) = 1 - recall
  - aka miss rate; *lower is better*

Measuring rate of false classifications (or noise):

- Precision = TP/(TP+FP)
  - aka positive predictive value; *higher is better*
- False positive rate = FP/(FP+TN)
  - aka fall-out; *lower is better*

Combined measure (harmonic mean):

$$\text{F1 score} = 2\frac{recall * precision}{recall + precision}$$



FALSE POSITIVES AND FALSE NEGATIVES EQUALLY BAD?

Consider:

- Recognizing cancer
- Suggesting products to buy on e-commerce site
- Identifying human trafficking at the border
- Predicting high demand for ride sharing services
- Predicting recidivism chance
- Approving loan applications

No answer vs wrong answer?

EXTREME CLASSIFIERS

- Identifies every instance as negative (e.g., no cancer):
  - 0% recall (finds none of the cancer cases)
  - 100% false negative rate (misses all actual cancer cases)
  - undefined precision (no false predictions, but no predictions at all)
  - 0% false positive rate (never reports false cancer warnings)
- Identifies every instance as positive (e.g., has cancer):
  - 100% recall (finds all instances of cancer)
  - 0% false negative rate (does not miss any cancer cases)
  - low precision (also reports cancer for all noncancer cases)
  - 100% false positive rate (all noncancer cases reported as warnings)

CONSIDER THE BASELINE PROBABILITY

Predicting unlikely events -- 1 in 2000 has cancer (stats)

Random predictor

	Cancer	No c.
Cancer pred.	3	4998
No cancer pred.	2	4997

.5 accuracy, .6 recall, 0.001 precision

Never cancer predictor

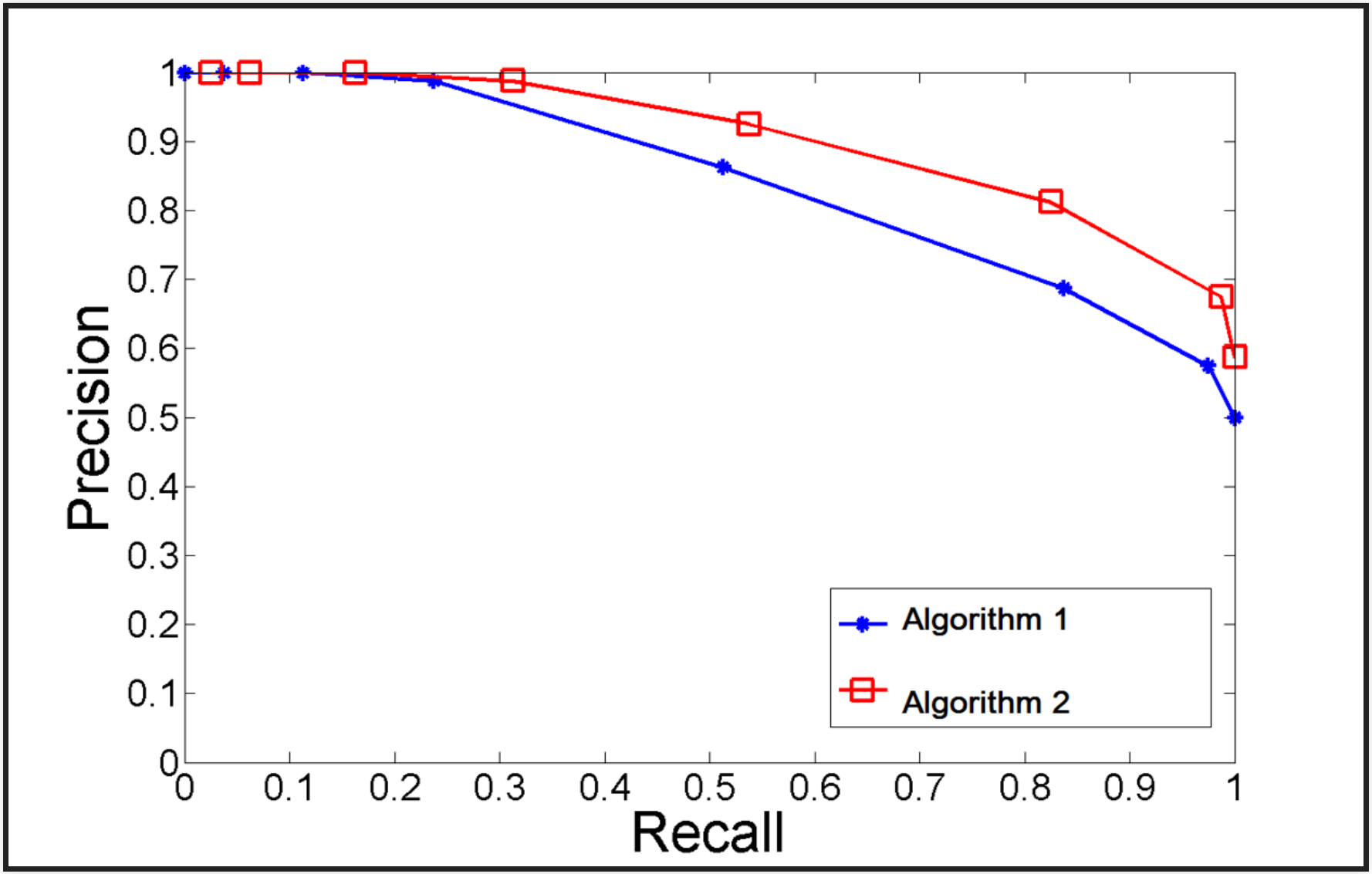
	Cancer	No c.
Cancer pred.	0	0
No cancer pred.	5	9995

.999 accuracy, 0 recall, .999 precision

See also Bayesian statistics

AREA UNDER THE CURVE

Turning numeric prediction into classification with threshold ("operating point")


Precision
Recall
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Algorithm 1
Algorithm 2

Speaker notes

The plot shows the recall precision/tradeoff at different thresholds (the thresholds are not shown explicitly). Curves closer to the top-right corner are better considering all possible thresholds. Typically, the area under the curve is measured to have a single number for comparison.

MORE ACCURACY MEASURES FOR CLASSIFICATION PROBLEMS

- Lift
- Break even point
- F1 measure, etc
- Log loss (for class probabilities)
- Cohen's kappa, Gini coefficient (improvement over random)

MEASURING PREDICTION ACCURACY FOR REGRESSION AND RANKING TASKS

(The Data Scientists Toolbox)

CONFUSION MATRIX FOR REGRESSION TASKS?

Rooms	Crime Rate	...	Predicted Price	Actual Price
3	.01	...	230k	250k
4	.01	...	530k	498k
2	.03	...	210k	211k
2	.02	...	219k	210k

Speaker notes

Confusion Matrix does not work, need a different way of measuring accuracy that can distinguish "pretty good" from "far off" predictions

COMPARING PREDICTED AND EXPECTED OUTCOMES

Mean Absolute Percentage Error

MAPE =

$$\frac{1}{n}\sum_{t=1}^{n}\left|\frac{A_t - F_t}{A_t}\right|$$

(A_t actual outcome, F_t predicted outcome, for row t)

Compute relative prediction error per row, average over all rows

Rooms	Crime Rate	...	Predicted Price	Actual Price
3	.01	...	230k	250k
4	.01	...	530k	498k
2	.03	...	210k	211k
2	.02	...	219k	210k

MAPE =

$$\frac{1}{4}(20/250 + 32/498 + 1/211 + 9/210) =$$

$$\frac{1}{4}(0.08 + 0.064 + 0.005 + 0.043) = 0.048$$

OTHER MEASURES FOR REGRESSION MODELS

- Mean Absolute Error (MAE) = $\frac{1}{n}\sum_{t=1}^{n}\left|A_t - F_t\right|$
- Mean Squared Error (MSE) = $\frac{1}{n}\sum_{t=1}^{n}\left(A_t - F_t\right)^2$
- Root Mean Square Error (RMSE) = $\sqrt{\frac{\sum_{t=1}^{n}(A_t - F_t)^2}{n}}$
- R^2 = percentage of variance explained by model
- ...

EVALUATING RANKINGS

Ordered list of results, true results should be ranked high

Common in information retrieval (e.g., search engines) and recommendations

Mean Average Precision

MAP@K = precision in first K results

Averaged over many queries

Rank	Product	Correct?
1	Juggling clubs	true
2	Bowling pins	false
3	Juggling balls	false
4	Board games	true
5	Wine	false
6	Audiobook	true

MAP@1 = 1, MAP@2 = 0.5, MAP@3 = 0.33, ...

OTHER RANKING MEASURES

- Mean Reciprocal Rank (MRR) (average rank for first correct prediction)
- Average precision (concentration of results in highest ranked predictions)
- MAR@K (recall)
- Coverage (percentage of items ever recommended)
- Personalization (how similar predictions are for different users/queries)
- Discounted cumulative gain
- ...

Speaker notes

Good discussion of tradeoffs at https://medium.com/swlh/rank-aware-recsys-evaluation-metrics-5191bba16832

MODEL QUALITY IN NATURAL LANGUAGE PROCESSING?

Highly problem dependent:

- Classify text into positive or negative -> classification problem
- Determine truth of a statement -> classification problem
- Translation and summarization -> comparing sequences (e.g ngrams) to human results with specialized metrics, e.g. BLEU and ROUGE
- Modeling text -> how well its probabilities match actual text, e.g., likelyhoold or perplexity

ALWAYS COMPARE AGAINST BASELINES!

Accuracy measures in isolation are difficult to interpret

Report baseline results, reduction in error

Example: Baselines for house price prediction? Baseline for shopping recommendations?

MEASURING GENERALIZATION

OVERFITTING IN CANCER DETECTION?

SEPARATE TRAINING AND VALIDATION DATA

Always test for generalization on *unseen* validation data

Accuracy on training data (or similar measure) used during learning to find model parameters

```
train_xs, train_ys, valid_xs, valid_ys = split(all_xs, all_ys)
model = learn(train_xs, train_ys)

accuracy_train = accuracy(model, train_xs, train_ys)
accuracy_valid = accuracy(model, valid_xs, valid_ys)
```

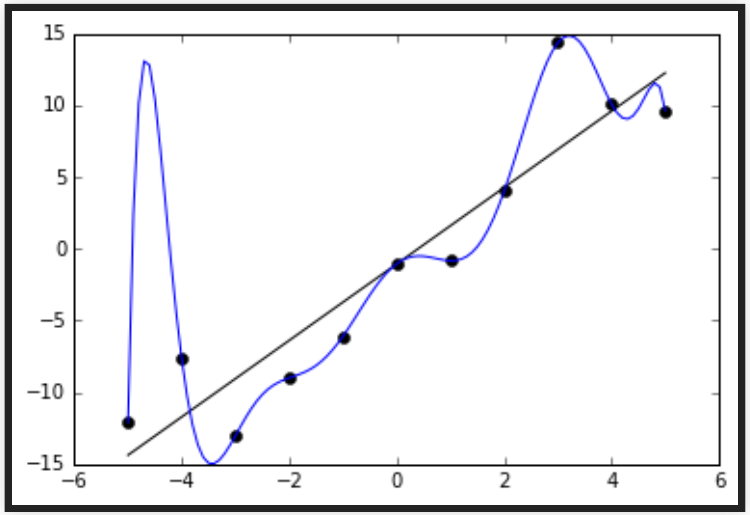
accuracy_train >> accuracy_valid = sign of overfitting

OVERFITTING/UNDERFITTING

Overfitting: Model learned exactly for the input data, but does not generalize to unseen data (e.g., exact memorization)

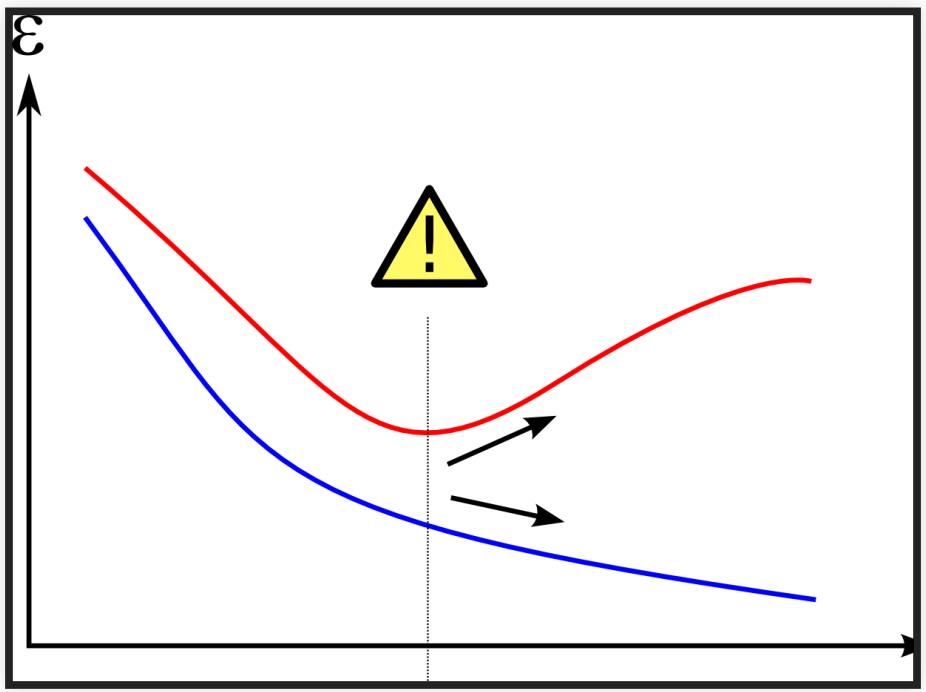
Underfitting: Model makes very general observations but poorly fits to data (e.g., brightness in picture)

Typically adjust degrees of freedom during model learning to balance between overfitting and underfitting: can better learn the training data with more freedom (more complex models); but with too much freedom, will memorize details of the training data rather than generalizing



DETECTING OVERFITTING

Change hyperparameter to detect training accuracy (blue)/validation accuracy (red) at different degrees of freedom



(CC SA 3.0 by Dake)

demo time

Speaker notes

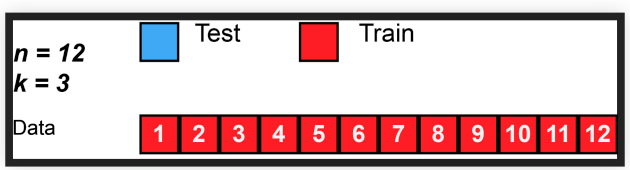
Overfitting is recognizable when performance of the evaluation set decreases.

Demo: Show how trees at different depth first improve accuracy on both sets and at some point reduce validation accuracy with small improvements in training accuracy

CROSSVALIDATION

- Motivation
  - Evaluate accuracy on different training and validation splits
  - Evaluate with small amounts of validation data
- Method: Repeated partitioning of data into train and validation data, train and evaluate model on each partition, average results
- Many split strategies, including
  - leave-one-out: evaluate on each datapoint using all other data for training
  - k-fold: k equal-sized partitions, evaluate on each training on others
  - repeated random sub-sampling (Monte Carlo)

demo time



(Graphic CC MBanuelos22 BY-SA 4.0)

SEPARATE TRAINING, VALIDATION AND TEST DATA

Often a model is "tuned" manually or automatically on a validation set (hyperparameter optimization)

In this case, we can overfit on the validation set, separate test set is needed for final evaluation

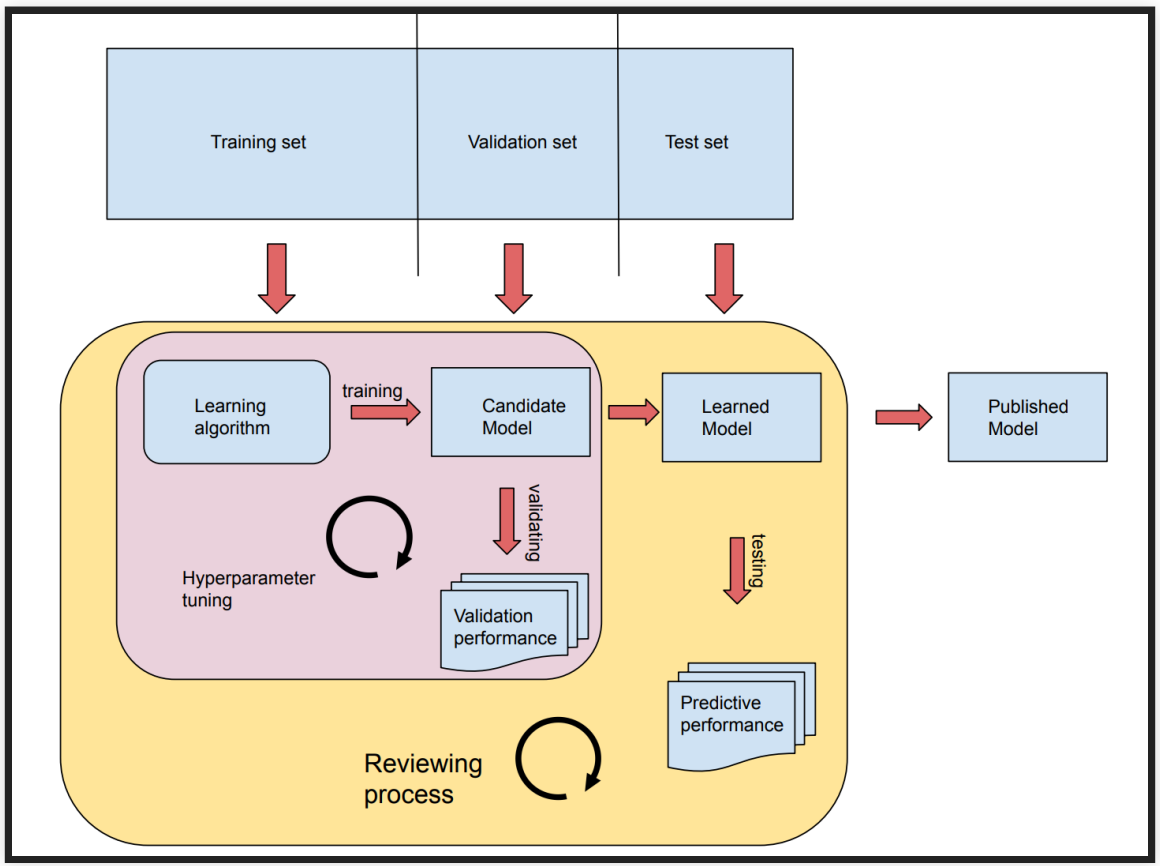
```
train_xs, train_ys, valid_xs, valid_ys, test_xs, test_ys =
            split(all_xs, all_ys)

best_model = null
best_model_accuracy = 0
for (hyperparameters in candidate_hyperparameters)
  candidate_model = learn(train_xs, train_ys, hyperparameter)
  model_accuracy = accuracy(model, valid_xs, valid_ys)
  if (model_accuracy > best_model_accuracy)
    best_model = candidate_model
    best_model_accuracy = model_accuracy

accuracy_test = accuracy(model, test_xs, test_ys)
```

ON TERMINOLOGY

- The decisions in a model are called *model parameter* of the model (constants in the resulting function, weights, coefficients), their values are usually learned from the data
- The parameters to the learning algorithm that are not the data are called *model hyperparameters*
- Degrees of freedom ~ number of model parameters

```
// max_depth and min_support are hyperparameters
def learn_decision_tree(data, max_depth, min_support): Model =
  ...

// A, B, C are model parameters of model f
def f(outlook, temperature, humidity, windy) =
   if A==outlook
      return B*temperature + C*windy > 10
```

ACADEMIC ESCALATION: OVERFITTING ON BENCHMARKS



(Figure by Andrea Passerini)

Speaker notes

If many researchers publish best results on the same benchmark, collectively they perform "hyperparameter optimization" on the test set

PRODUCTION DATA -- THE ULTIMATE UNSEEN VALIDATION DATA

more next week

ANALOGY TO SOFTWARE TESTING

(this gets messy)

SOFTWARE TESTING

- Program *p* with specification *s*
- Test consists of
  - Controlled environment
  - Test call, test inputs
  - Expected behavior/output (oracle)

```
assertEquals(4, add(2, 2));
assertEquals(??, factorPrime(15485863));
```

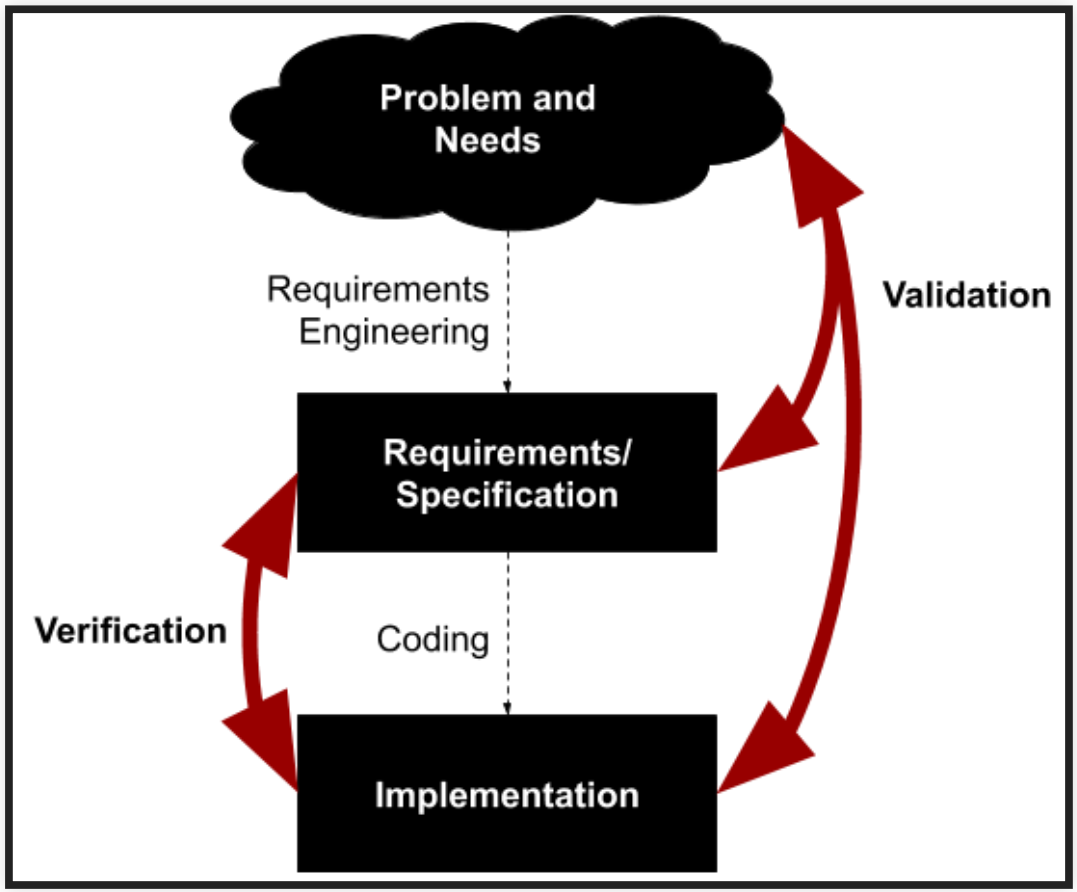
Testing is complete but unsound: Cannot guarantee the absence of bugs

SOFTWARE BUG

- Software's behavior is inconsistent with specification

```
// returns the sum of two arguments
int add(int a, int b) { ... }

assertEquals(4, add(2, 2));
```

VALIDATION VS VERIFICATION



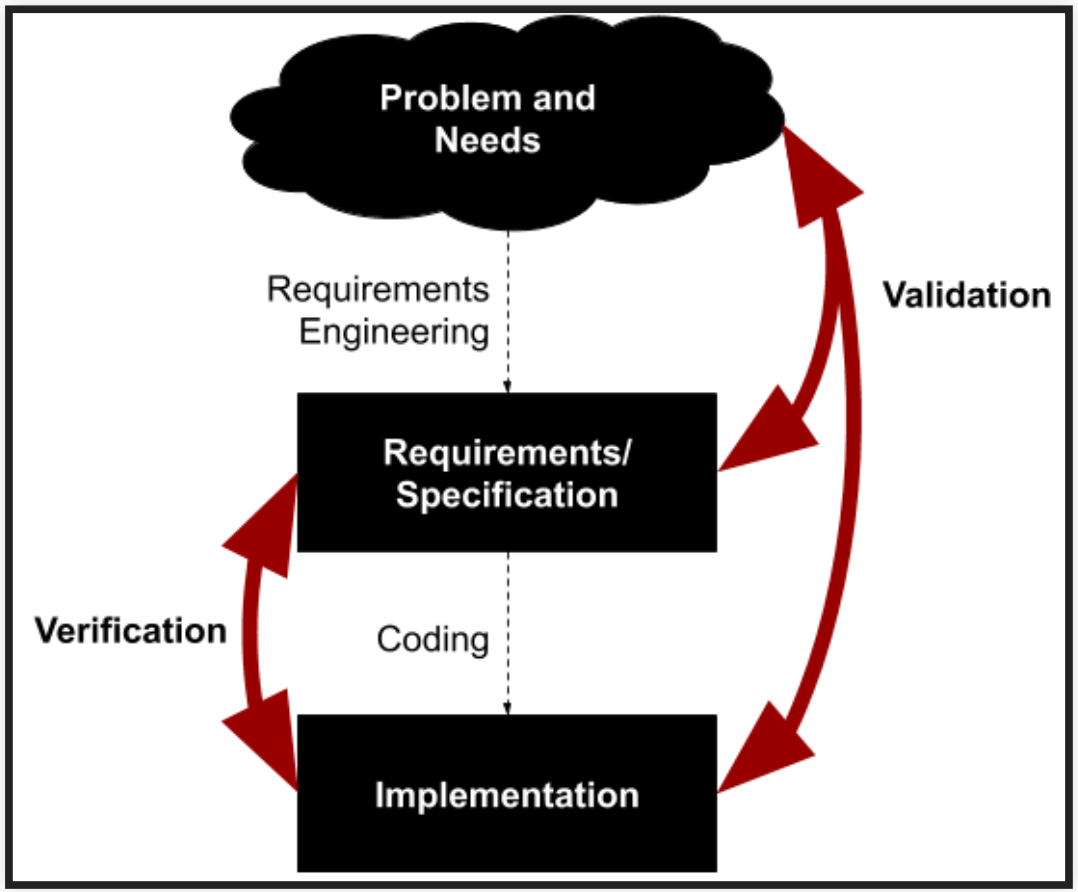
VALIDATION PROBLEM: CORRECT BUT USELESS?

- Correctly implemented to specification, but specifications are wrong
- Building the wrong system, not what user needs
- Ignoring assumptions about how the system is used

Speaker notes

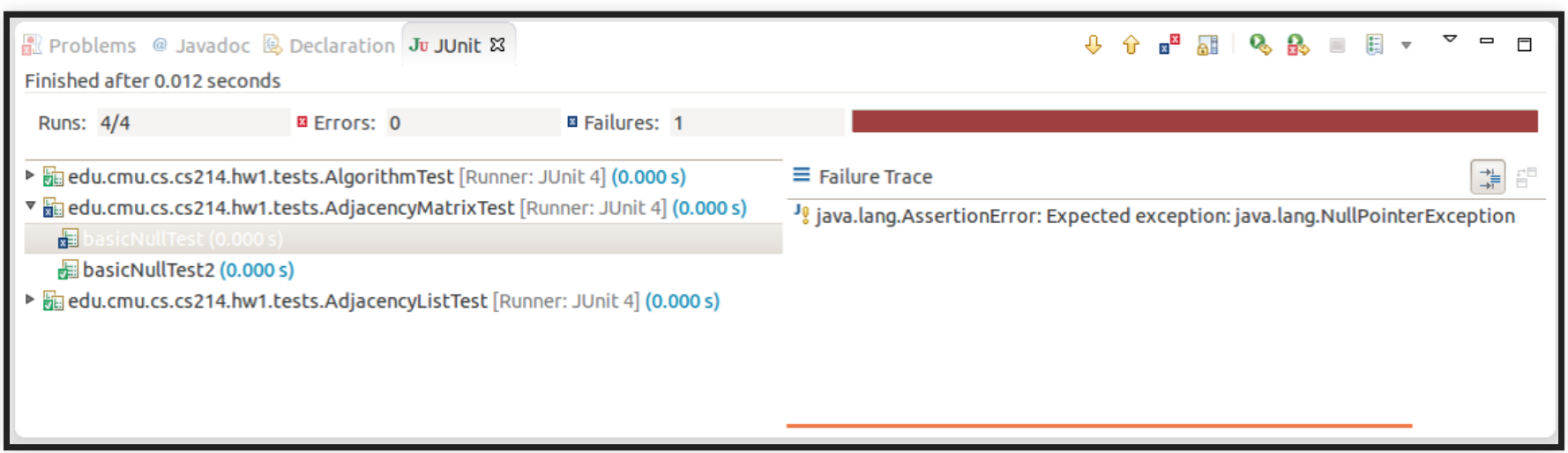
The Lufthansa flight 2904 crashed in Warsaw (overrun runway) because the plane's did not recognize that the airplane touched the ground. The software was implemented to specification, but the specifications were wrong, making inferences from on sensor values that were not reliable. More in a later lecture or at https://en.wikipedia.org/wiki/Lufthansa_Flight_2904

VALIDATION VS VERIFICATION



TEST AUTOMATION

```
@Test
public void testSanityTest(){
    //setup
    Graph g1 = new AdjacencyListGraph(10);
    Vertex s1 = new Vertex("A");
    Vertex s2 = new Vertex("B");
    //check expected behavior
    assertEquals(true, g1.addVertex(s1));
    assertEquals(true, g1.addVertex(s2));
    assertEquals(true, g1.addEdge(s1, s2));
    assertEquals(s2, g1.getNeighbors(s1)[0]);
}
```



TEST COVERAGE

Packages

All
net.sourceforge.cobertura.ant
net.sourceforge.cobertura.check
net.sourceforge.cobertura.coveragedat
net.sourceforge.cobertura.instrument
net.sourceforge.cobertura.merge
net.sourceforge.cobertura.reporting
net.sourceforge.cobertura.reporting.htr
net.sourceforge.cobertura.reporting.htr
net.sourceforge.cobertura.reporting.xm
net.sourceforge.cobertura.util

All Packages

Classes

AntUtil *(88%)*
Archive *(100%)*
ArchiveUtil *(80%)*
BranchCoverageData *(N/A)*
CheckTask *(0%)*
ClassData *(N/A)*
ClassInstrumenter *(94%)*
ClassPattern *(100%)*
CoberturaFile *(73%)*
CommandLineBuilder *(96%)*
CommonMatchingTask *(88%)*
ComplexityCalculator *(100%)*
ConfigurationUtil *(50%)*
CopyFiles *(87%)*
CoverageData *(N/A)*
CoverageDataContainer *(N/A)*
CoverageDataFileHandler *(N/A)*
CoverageRate *(0%)*
ExcludeClasses *(100%)*
FileFinder *(96%)*
FileLocker *(0%)*
FirstPassMethodInstrumenter *(100%)*
HTMLReport *(94%)*
HasBeenInstrumented *(N/A)*

Coverage Report - All Packages

Package	# Classes	Line Coverage		Branch Coverage		Complexity
All Packages	55	75%	1625/2179	64%	472/738	2.319
net.sourceforge.cobertura.ant	11	52%	170/330	43%	40/94	1.848
net.sourceforge.cobertura.check	3	0%	0/150	0%	0/76	2.429
net.sourceforge.cobertura.coveragedata	13	N/A	N/A	N/A	N/A	2.277
net.sourceforge.cobertura.instrument	10	90%	460/510	75%	123/164	1.854
net.sourceforge.cobertura.merge	1	86%	30/35	88%	14/16	5.5
net.sourceforge.cobertura.reporting	3	87%	116/134	80%	43/54	2.882
net.sourceforge.cobertura.reporting.html	4	91%	475/523	77%	156/202	4.444
net.sourceforge.cobertura.reporting.html.files	1	87%	39/45	62%	5/8	4.5
net.sourceforge.cobertura.reporting.xml	1	100%	155/155	95%	21/22	1.524
net.sourceforge.cobertura.util	9	60%	175/291	69%	70/102	2.892
someotherpackage	1	83%	5/6	N/A	N/A	1.2

Report generated by Cobertura 1.9 on 6/9/07 12:37 AM.

Header (80%)
IOUtil (62%)
Ignore (100%)
IgnoreBranches (0%)

CONTINUOUS INTEGRATION

Build #17 - wyvernla

https://travis-ci.org/wyvernlang/wyvern/builds/79099642

Travis CI Blog Status Help Jonathan Aldrich

Search all repositories

My Repositories +

wyvernlang/wyvern # 17

Duration: 16 sec

Finished: 3 days ago

wyvernlang / wyvern build passing

Current Branches Build History Pull Requests Build #17

Settings

SimpleWyvern-devel Asserting false (works on Linux, so its OK).

potanin authored and committed

17 passed

Commit fd7be1c

Compare 0e2af1f..fd7b

ran for 16 sec

3 days ago

This job ran on our legacy infrastructure. Please read our docs on how to upgrade

Remove Log Download Log

```
1  Using worker: worker-linux-027f0490-1.bb.travis-ci.org:travis-linux-2
2
3  Build system information                                   system_info
67
68 $ git clone --depth=50 --branch=SimpleWyvern-devel         git.checkout   0.81s
78 $ jdk_switcher use oraclejdk8
79 Switching to Oracle JDK8 (java-8-oracle), JAVA_HOME will be set to /usr/lib/jvm/java-8-oracle
80 $ java -Xmx32m -version
81 java version "1.8.0_31"
```

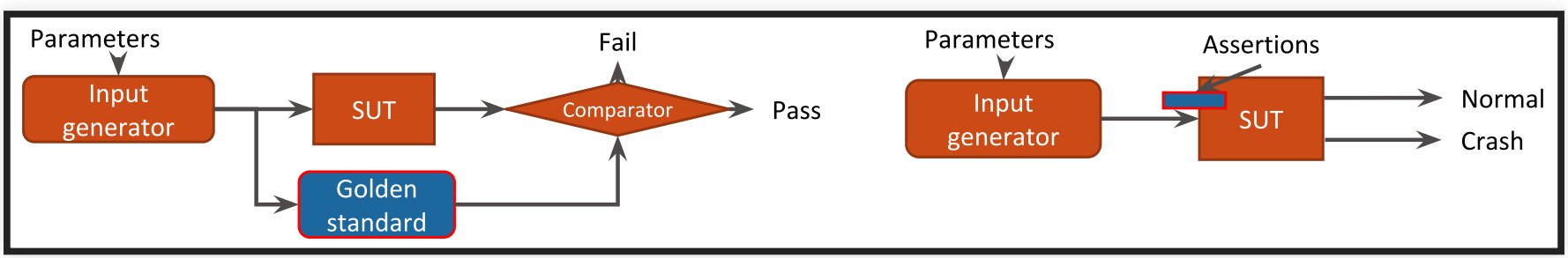
```
Java(TM) SE Runtime Environment (build 1.8.0_31-b13)
Java HotSpot(TM) 64-Bit Server VM (build 25.31-b07, mixed mode)
$ javac -J-Xmx32m -version
javac 1.8.0_31
$ cd tools                                                                    0.01s

The command "cd tools" exited with 0.
$ ant test                                                                    11.81s
Buildfile: /home/travis/build/wyvernlang/wyvern/tools/build.xml

copper-compose-compile:
    [mkdir] Created dir: /home/travis/build/wyvernlang/wyvern/tools/copper-composer/bin
    [javac] /home/travis/build/wyvernlang/wyvern/tools/build.xml:18: warning: 'includeantruntime'
was not set, defaulting to build.sysclasspath=last; set to false for repeatable builds
```

TEST CASE GENERATION & THE ORACLE PROBLEM

How do we know the expected output of a test?

```
assertEquals(??, factorPrime(15485863));
```

- Manually construct input-output pairs (does not scale, cannot automate)
- Comparison against gold standard (e.g., alternative implementation, executable specification)
- Checking of global properties only -- crashes, buffer overflows, code injections
- Manually written assertions -- partial specifications checked at runtime



AUTOMATED TESTING / TEST CASE GENERATION / FUZZING

- Many techniques to generate test cases
- Dumb fuzzing: generate random inputs
- Smart fuzzing (e.g., symbolic execution, coverage guided fuzzing): generate inputs to maximally cover the implementation
- Program analysis to understand the shape of inputs, learning from existing tests
- Minimizing redundant tests
- Abstracting/simulating/mocking the environment
- Typically looking for crashing bugs or assertion violations

SOFTWARE TESTING

"Testing shows the presence, not the absence of bugs" -- Edsger W. Dijkstra 1969

Software testing can be applied to many qualities:

- Functional errors
- Performance errors
- Buffer overflows
- Usability errors
- Robustness errors
- Hardware errors
- API usage errors

MODEL TESTING?

Rooms	Crime Rate	...	Actual Price
3	.01	...	250k
4	.01	...	498k
2	.03	...	211k
2	.02	...	210k

```
assertEquals(250000,
    model.predict([3, .01, ...])
assertEquals(498000,
    model.predict([4, .01, ...])
assertEquals(211000,
    model.predict([2, .03, ...])
assertEquals(210000,
    model.predict([2, .02, ...])
```

Fail the entire test suite for one wrong prediction?

IS LABELED VALIDATION DATA SOLVING THE ORACLE PROBLEM?

```
assertEquals(250000, model.predict([3, .01, ...]));
assertEquals(498000, model.predict([4, .01, ...]));
```

DIFFERENT EXPECTATIONS FOR PREDICTION ACCURACY

- Not expecting that all predictions will be correct (80% accuracy may be very good)
- Data may be mislabeled in training or validation set
- There may not even be enough context (features) to distinguish all training outcomes

- **Lack of specifications**
- **A wrong prediction is not necessarily a bug**

ANALOGY OF PERFORMANCE TESTING?

ANALOGY OF PERFORMANCE TESTING?

- Performance tests are not precise (measurement noise)
  - Averaging over repeated executions *of the same test*
  - Commonly using diverse benchmarks, i.e., *multiple inputs*
  - Need to control environment (hardware)
- No precise specification
  - Regression tests
  - Benchmarking as open-ended comparison
  - Tracking results over time

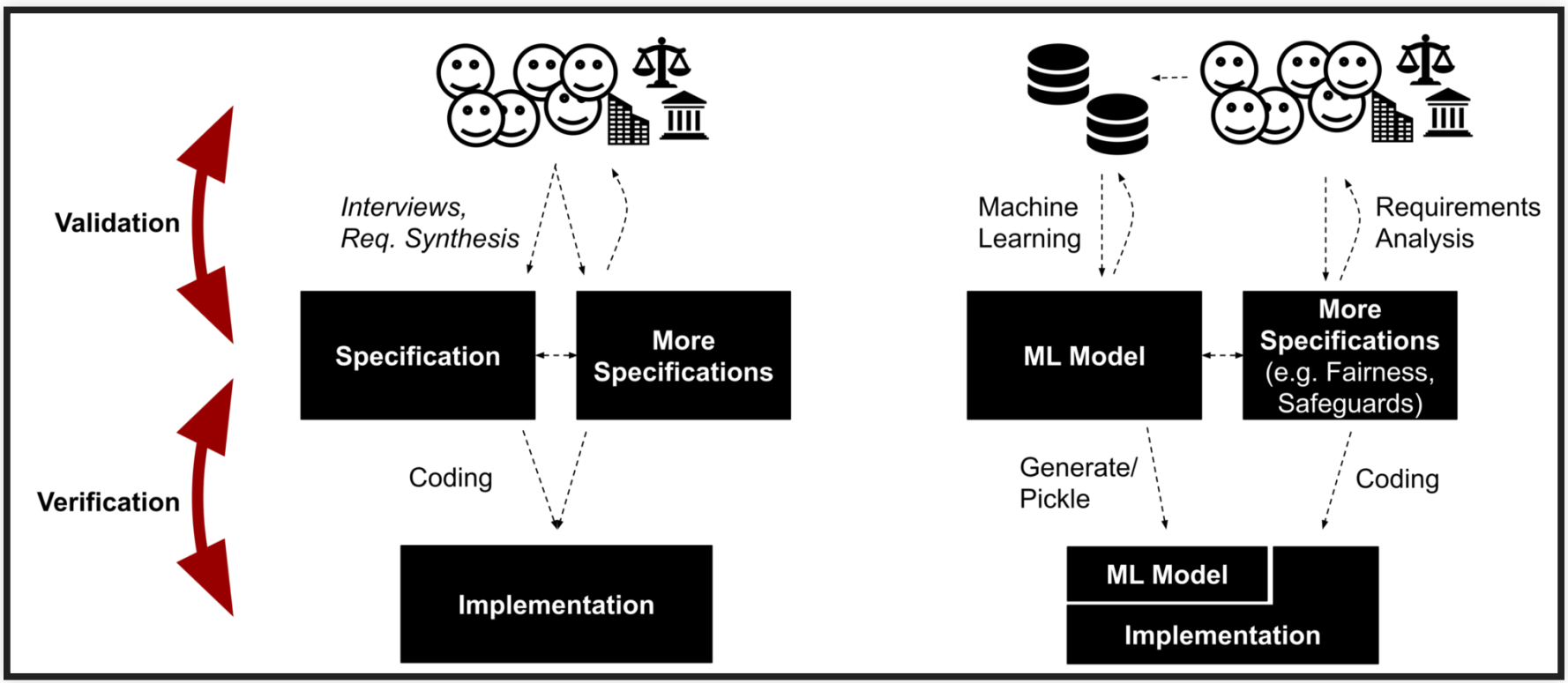
```
@Test(timeout=100)
public void testCompute() {
   expensiveComputation(...);
}
```

MACHINE LEARNING MODELS FIT, OR NOT

- A model is learned from given data in given procedure
    - The learning process is typically not a correctness concern
    - The model itself is generated, typically no implementation issues
- Is the data representative? Sufficient? High quality?
- Does the model "learn" meaningful concepts?

- **Is the model useful for a problem?** Does it *fit*?
- Do model predictions *usually* fit the users' expectations?
- Is the model *consistent* with other requirements? (e.g., fairness, robustness)

MY PET THEORY: MACHINE LEARNING IS REQUIREMENTS ENGINEERING



Long version: https://medium.com/@ckaestne/machine-learning-is-requirements-engineering-8957aee55ef4

TERMINOLOGY SUGGESTIONS

- Avoid term *model bug*, no agreement, no standardization
- *Performance* or *accuracy* are better fitting terms than *correct* for model quality
- Careful with the term *testing* for measuring *prediction accuracy*, be aware of different connotations
- *Verification/validation* analogy may help frame thinking, but will likely be confusing to most without longer explanation

CURATING VALIDATION DATA

(Learning from Software Testing)

SOFTWARE TEST CASE DESIGN

- Opportunistic/exploratory testing: Add some unit tests, without much planning
- Black-box testing: Derive test cases from specifications
  - Boundary value analysis
  - Equivalence classes
  - Combinatorial testing
  - Random testing
- White-box testing: Derive test cases to cover implementation paths
  - Line coverage, branch coverage
  - Control-flow, data-flow testing, MCDC, ...

- Test suite adequacy often established with specification or code coverage

EXAMPLE: BOUNDARY VALUE TESTING

- Analyze the specification, not the implementation!
- Key Insight: Errors often occur at the boundaries of a variable value
- For each variable select (1) minimum, (2) min+1, (3) medium, (4) max-1, and (5) maximum; possibly also invalid values min-1, max+1

- Example: nextDate(2015, 6, 13) = (2015, 6, 14)
    - **Boundaries?**

EXAMPLE: EQUIVALENCE CLASSES

- Idea: Typically many values behave similarly, but some groups of values are different
- Equivalence classes derived from specifications (e.g., cases, input ranges, error conditions, fault models)
- Example nextDate(2015, 6, 13)
    - leap years, month with 28/30/31 days, days 1-28, 29, 30, 31
- Pick 1 value from each group, combine groups from all variables

EXERCISE

```
/**
 * Compute the price of a bus ride:
 *  * Children under 2 ride for free, children under 18 and
 *    senior citizen over 65 pay half, all others pay the
 *    full fare of $3.
 *  * On weekdays, between 7am and 9am and between 4pm and
*     7pm a peak surcharge of $1.5 is added.
 *  * Short trips under 5min during off-peak time are free.
 */
def busTicketPrice(age: Int,
                   datetime: LocalDateTime,
                   rideTime: Int)
```

suggest test cases based on boundary value analysis and equivalence class testing

EXAMPLE: WHITE-BOX TESTING

```
int divide(int A, int B) {
  if (A==0)
    return 0;
  if (B==0)
    return -1;
  return A / B;
}
```

minimum set of test cases to cover all lines? all decisions? all path?

Packages

All
net.sourceforge.cobertura.ant
net.sourceforge.cobertura.check
net.sourceforge.cobertura.coveragedat
net.sourceforge.cobertura.instrument
net.sourceforge.cobertura.merge
net.sourceforge.cobertura.reporting
net.sourceforge.cobertura.reporting.htr
net.sourceforge.cobertura.reporting.htr
net.sourceforge.cobertura.reporting.xm
net.sourceforge.cobertura.util

All Packages

Classes

AntUtil *(88%)*
Archive *(100%)*
ArchiveUtil *(80%)*
BranchCoverageData *(N/A)*
CheckTask *(0%)*
ClassData *(N/A)*

Coverage Report - All Packages

Package	# Classes	Line Coverage		Branch Coverage		Complexity
All Packages	55	75%	1625/2179	64%	472/738	2.319
net.sourceforge.cobertura.ant	11	52%	170/330	43%	40/94	1.848
net.sourceforge.cobertura.check	3	0%	0/150	0%	0/76	2.429
net.sourceforge.cobertura.coveragedata	13	N/A	N/A	N/A	N/A	2.277
net.sourceforge.cobertura.instrument	10	90%	460/510	75%	123/164	1.854
net.sourceforge.cobertura.merge	1	86%	30/35	88%	14/16	5.5
net.sourceforge.cobertura.reporting	3	87%	116/134	80%	43/54	2.882
net.sourceforge.cobertura.reporting.html	4	91%	475/523	77%	156/202	4.444
net.sourceforge.cobertura.reporting.html.files	1	87%	39/45	62%	5/8	4.5
net.sourceforge.cobertura.reporting.xml	1	100%	155/155	95%	21/22	1.524
net.sourceforge.cobertura.util	9	60%	175/291	69%	70/102	2.892
someotherpackage	1	83%	5/6	N/A	N/A	1.2

Report generated by Cobertura 1.9 on 6/9/07 12:37 AM.

ClassInstrumenter *(94%)*
ClassPattern *(100%)*
CoberturaFile *(73%)*
CommandLineBuilder *(96%)*
CommonMatchingTask *(88%)*
ComplexityCalculator *(100%)*
ConfigurationUtil *(50%)*
CopyFiles *(87%)*
CoverageData *(N/A)*
CoverageDataContainer *(N/A)*
CoverageDataFileHandler *(N/A)*
CoverageRate *(0%)*
ExcludeClasses *(100%)*
FileFinder *(96%)*
FileLocker *(0%)*
FirstPassMethodInstrumenter *(100%)*
HTMLReport *(94%)*
HasBeenInstrumented *(N/A)*
Header *(80%)*
IOUtil *(62%)*
Ignore *(100%)*
IgnoreBranches *(0%)*

REGRESSION TESTING

- Whenever bug detected and fixed, add a test case
- Make sure the bug is not reintroduced later
- Execute test suite after changes to detect regressions
    - Ideally automatically with continuous integration tools

WHEN CAN WE STOP TESTING?

- Out of money? Out of time?
- Specifications, code covered?
- Finding few new bugs?
- High mutation coverage?

MUTATION ANALYSIS

- Start with program and passing test suite
- Automatically insert small modifications ("mutants") in the source code
  - a+b -> a-b
  - a<b -> a<=b
  - ...
- Can program detect modifications ("kill the mutant")?
- Better test suites detect more modifications ("mutation score")

```
int divide(int A, int B) {
  if (A==0)      // A!=0, A<0, B==0
    return 0;    // 1, -1
  if (B==0)      // B!=0, B==1
    return -1;   // 0, -2
  return A / B; // A*B, A+B
}
assert(1, divide(1,1));
assert(0, divide(0,1));
assert(-1, divide(1,0));
```

SELECTING VALIDATION DATA FOR MODEL QUALITY?

TEST ADEQUACY ANALOGY?

- Specification coverage (e.g., use cases, boundary conditions):
  - No specification!
  - ~> Do we have data for all important use cases and subpopulations?
  - ~> Do we have representatives data for all output classes?
- White-box coverage (e.g., branch coverage)
  - All path of a decision tree?
  - All neurons activated at least once in a DNN? (several papers "neuron coverage")
  - Linear regression models??
- Mutation scores
  - Mutating model parameters? Hyper parameters?
  - When is a mutant killed?

Does any of this make sense?

VALIDATION DATA REPRESENTATIVE?

- Validation data should reflect usage data
- Be aware of data drift (face recognition during pandemic, new patterns in credit card fraud detection)
- "*Out of distribution*" predictions often low quality (it may even be worth to detect out of distribution data in production, more later)

(note, similar to requirements validation: did we hear all/representative stakeholders)

NOT ALL INPUTS ARE EQUAL

"Call mom" "What's the weather tomorrow?" "Add asafetida to my shopping list"

NOT ALL INPUTS ARE EQUAL

There Is a Racial Divide in Speech-Recognition Systems, Researchers Say: Technology from Amazon, Apple, Google, IBM and Microsoft misidentified 35 percent of words from people who were black. White people fared much better. -- NYTimes March 2020

Tweet

NOT ALL INPUTS ARE EQUAL

some random mistakes vs rare but biased mistakes?

- A system to detect when somebody is at the door that never works for people under 5ft (1.52m)
- A spam filter that deletes alerts from banks

Consider separate evaluations for important subpopulations; monitor mistakes in production

IDENTIFY IMPORTANT INPUTS

Curate Validation Data for Specific Problems and Subpopulations:

- *Regression testing:* Validation dataset for important inputs ("call mom") -- expect very high accuracy -- closest equivalent to **unit tests**
- *Uniformness/fairness testing:* Separate validation dataset for different subpopulations (e.g., accents) -- expect comparable accuracy
- *Setting goals:* Validation datasets for challenging cases or stretch goals -- accept lower accuracy

Derive from requirements, experts, user feedback, expected problems etc. Think *blackbox testing*.

IMPORTANT INPUT GROUPS FOR CANCER DETECTION?

HOW MUCH VALIDATION DATA?

- Problem dependent
- Statistics can give confidence interval for results
  - e.g. Sample Size Calculator: 384 samples needed for ±5% confidence interval (95% conf. level; 1M population)
- Experience and heuristics. Example: Hulten's heuristics for stable problems:
  - 10s is too small
  - 100s sanity check
  - 1000s usually good
  - 10000s probably overkill
  - Reserve 1000s recent data points for evaluation (or 10%, whichever is more)
  - Reserve 100s for important subpopulations

BLACK-BOX TESTING TECHNIQUES AS INSPIRATION?

- Boundary value analysis
- Partition testing & equivalence classes
- Combinatorial testing
- Decision tables

Use to identify subpopulations (validation datasets), not individual tests.

AUTOMATED (RANDOM) TESTING

(if it wasn't for that darn oracle problem)

AUTOMATED SOFTWARE TESTING / TEST CASE GENERATION

- Many techniques to generate test cases
- Dumb fuzzing: generate random inputs
- Smart fuzzing (e.g., symbolic execution, coverage guided fuzzing): generate inputs to maximally cover the implementation
- Program analysis to understand the shape of inputs, learning from existing tests
- Minimizing redundant tests
- Abstracting/simulating/mocking the environment

TEST GENERATION EXAMPLE (SYMBOLIC EXECUTION)

Code:

```
void foo(a, b, c) {
    int x=0, y=0, z=0;
    if (a) x=-2;
    if (b<5) {
        if (!a && c) y=1;
        z=2;
    }
    assert(x+y+z!=3)
}
```

Paths:

- $a \wedge (b < 5)$: x=-2, y=0, z=2
- $a \wedge \neg(b < 5)$: x=-2, y=0, z=0
- $\neg a \wedge (\neg a \wedge c)$: x=0, z=1, z=2
- $\neg a \wedge (b < 5) \wedge \neg(\neg a \wedge c)$: x=0, z=0, z=2
- $\neg a \wedge (b < 5) \wedge \neg(\neg a \wedge c)$: x=0, z=0, z=2
- $\neg a \wedge \neg(b < 5)$: x=0, z=0, z=0

Speaker notes

example source: http://web.cs.iastate.edu/~weile/cs641/9.SymbolicExecution.pdf

AUTOMATED MODEL VALIDATION DATA GENERATION?

```
model.predict([3, .01, ...])
model.predict([4, .04, ...])
model.predict([5, .01, ...])
model.predict([1, .02, ...])
```

- Completely random data generation (uniform sampling from each feature's domain)
- Using knowledge about feature distributions (sample from each feature's distribution)
- Knowledge about dependencies among features and whole population distribution (e.g., model with probabilistic programming language)
- Mutate from existing inputs (e.g., small random modifications to select features)

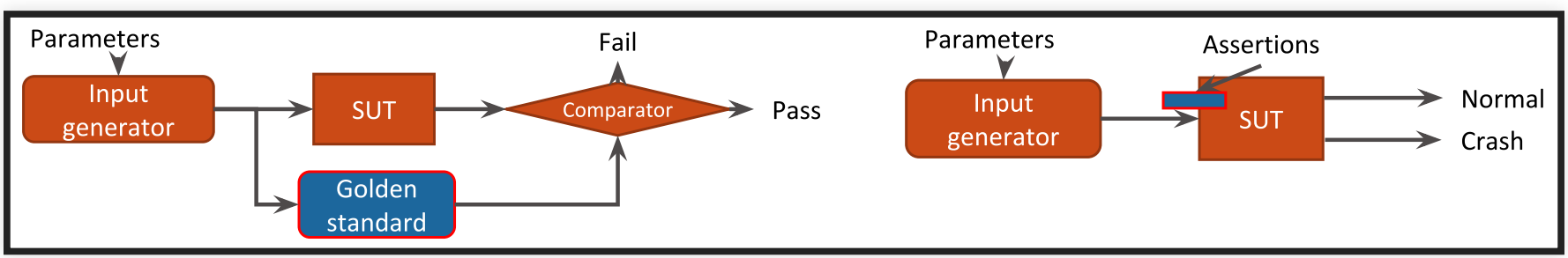
- **But how do we get labels?**

RECALL: THE ORACLE PROBLEM

How do we know the expected output of a test?

```
assertEquals(??, factorPrime(15485863));
```

- Manually construct input-output pairs (does not scale, cannot automate)
- Comparison against gold standard (e.g., alternative implementation, executable specification)
- Checking of global properties only -- crashes, buffer overflows, code injections
- Manually written assertions -- partial specifications checked at runtime



MACHINE LEARNED MODELS = UNTESTABLE SOFTWARE?

- Manually construct input-output pairs (does not scale, cannot automate)
  - **too expensive at scale**
- Comparison against gold standard (e.g., alternative implementation, executable specification)
  - **no specification, usually no other "correct" model**
  - comparing different techniques useful? (see ensemble learning)
- Checking of global properties only -- crashes, buffer overflows, code injections
  - **??**
- Manually written assertions -- partial specifications checked at runtime
  - **??**

INVARIANTS IN MACHINE LEARNED MODELS?

EXAMPLES OF INVARIANTS

- Credit rating should not depend on gender:
  - $\forall x.\ f(x[\text{gender} \leftarrow \text{male}]) = f(x[\text{gender} \leftarrow \text{female}])$
- Synonyms should not change the sentiment of text:
  - $\forall x.\ f(x) = f(\text{replace}(x, \text{"is not"}, \text{"isn't"}))$
- Negation should swap meaning:
  - $\forall x \in \text{"X is Y"}.\ f(x) = 1 - f(\text{replace}(x, \text{" is "}, \text{" is not "}))$
- Robustness around training data:
  - $\forall x \in \text{training data}.\ \forall y \in \text{mutate}(x, \delta).\ f(x) = f(y)$
- Low credit scores should never get a loan (sufficient conditions for classification, "anchors"):
  - $\forall x.\ x.\text{score} < 649 \Rightarrow \neg f(x)$

Identifying invariants requires domain knowledge of the problem!

METAMORPHIC TESTING

Formal description of relationships among inputs and outputs (*Metamorphic Relations*)

In general, for a model f and inputs x define two functions to transform inputs and outputs g_I and g_O such that:

$$\forall x.\ f(g_I(x)) = g_O(f(x))$$

e.g. $g_I(x) = \text{replace}(x, \text{" is "}, \text{" is not "})$ and $g_O(x) = \neg x$

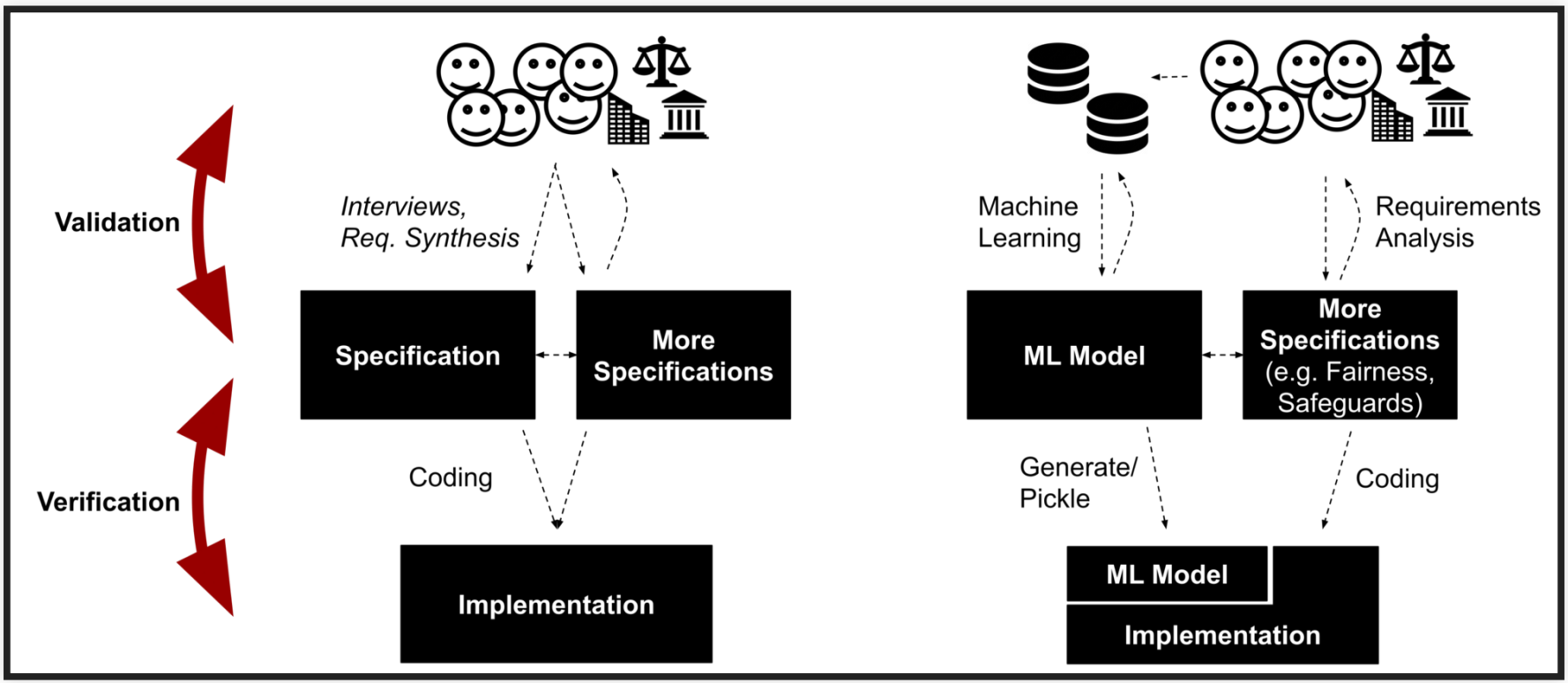
ON TESTING WITH INVARIANTS/ASSERTIONS

- Defining good metamorphic relations requires knowledge of the problem domain
- Good metamorphic relations focus on parts of the system
- Invariants usually cover only one aspect of correctness
- Invariants and near-invariants can be mined automatically from sample data (see *specification mining* and *anchors*)

Further reading:

- Segura, Sergio, Gordon Fraser, Ana B. Sanchez, and Antonio Ruiz-Cortés. "A survey on metamorphic testing." IEEE Transactions on software engineering 42, no. 9 (2016): 805-824.
- Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. "Anchors: High-precision model-agnostic explanations." In Thirty-Second AAAI Conference on Artificial Intelligence. 2018.

INVARIANT CHECKING ALIGNS WITH REQUIREMENTS VALIDATION



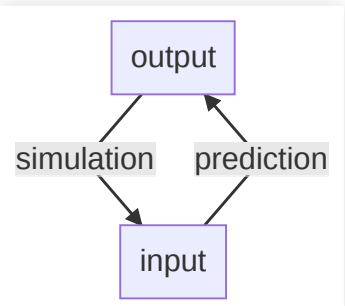
APPROACHES FOR CHECKING IN VARIANTS

- Generating test data (random, distributions) usually easy
- For many techniques gradient-based techniques to search for invariant violations (see adversarial ML)
- Early work on formally verifying invariants for certain models (e.g., small deep neural networks)

Further readings: Singh, Gagandeep, Timon Gehr, Markus Püschel, and Martin Vechev. "An abstract domain for certifying neural networks." Proceedings of the ACM on Programming Languages 3, no. POPL (2019): 1-30.

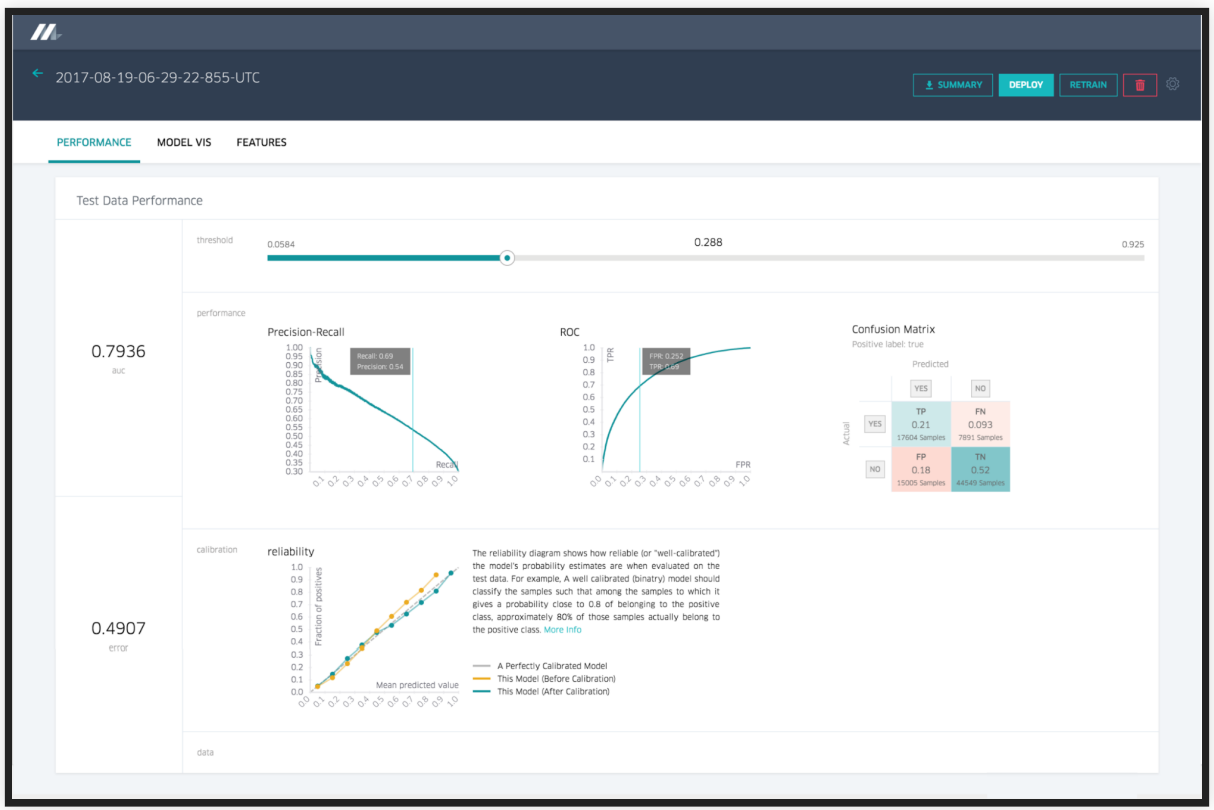
ONE MORE THING: SIMULATION-BASED TESTING

- Derive input-output pairs from simulation, esp. in vision systems
- Example: Vision for self-driving cars:
    - Render scene -> add noise -> recognize -> compare recognized result with simulator state
- Quality depends on quality of the simulator and how well it can produce inputs from outputs:
    - examples: render picture/video, synthesize speech, ...
    - Less suitable where input-output relationship unknown, e.g., cancer detection, housing price prediction, shopping recommendations



Further readings: Zhang, Mengshi, Yuqun Zhang, Lingming Zhang, Cong Liu, and Sarfraz Khurshid. "DeepRoad: GAN-based metamorphic testing and input validation framework for autonomous driving systems." In Proceedings of the 33rd ACM/IEEE International Conference on Automated Software Engineering, pp. 132-142. 2018.

CONTINUOUS INTEGRATION FOR MODEL QUALITY



CONTINUOUS INTEGRATION FOR MODEL QUALITY?

CONTINUOUS INTEGRATION FOR MODEL QUALITY

- Testing script
  - Existing model: Implementation to automatically evaluate model on labeled training set; multiple separate evaluation sets possible, e.g., for critical subcommunities or regressions
  - Training model: Automatically train and evaluate model, possibly using cross-validation; many ML libraries provide built-in support
  - Report accuracy, recall, etc. in console output or log files
  - May deploy learning and evaluation tasks to cloud services
  - Optionally: Fail test below quality bound (e.g., accuracy <.9; accuracy < accuracy of last model)
- Version control test data, model and test scripts, ideally also learning data and learning code (feature extraction, modeling, ...)
- Continuous integration tool can trigger test script and parse output, plot for comparisons (e.g., similar to performance tests)
- Optionally: Continuous deployment to production server

DASHBOARDS FOR MODEL EVALUATION RESULTS

2017-08-19-06-29-22-855-UTC

SUMMARY | DEPLOY | RETRAIN

PERFORMANCE | MODEL VIS | FEATURES

Test Data Performance

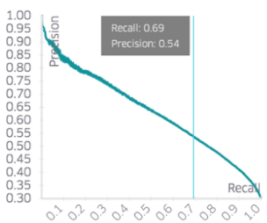
threshold

0.0584 — 0.288 — 0.925

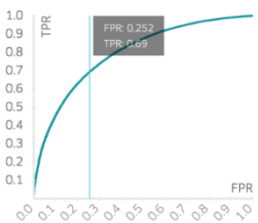
0.7936
auc

performance

Precision-Recall



ROC



Confusion Matrix

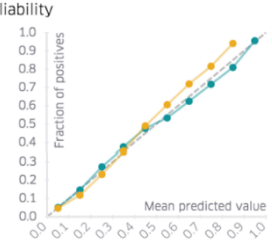
Positive label: true

Actual \ Predicted	YES	NO
YES	TP 0.21 17604 Samples	FN 0.093 7891 Samples
NO	FP 0.18 15005 Samples	TN 0.52 44549 Samples

0.4907
error

calibration

reliability

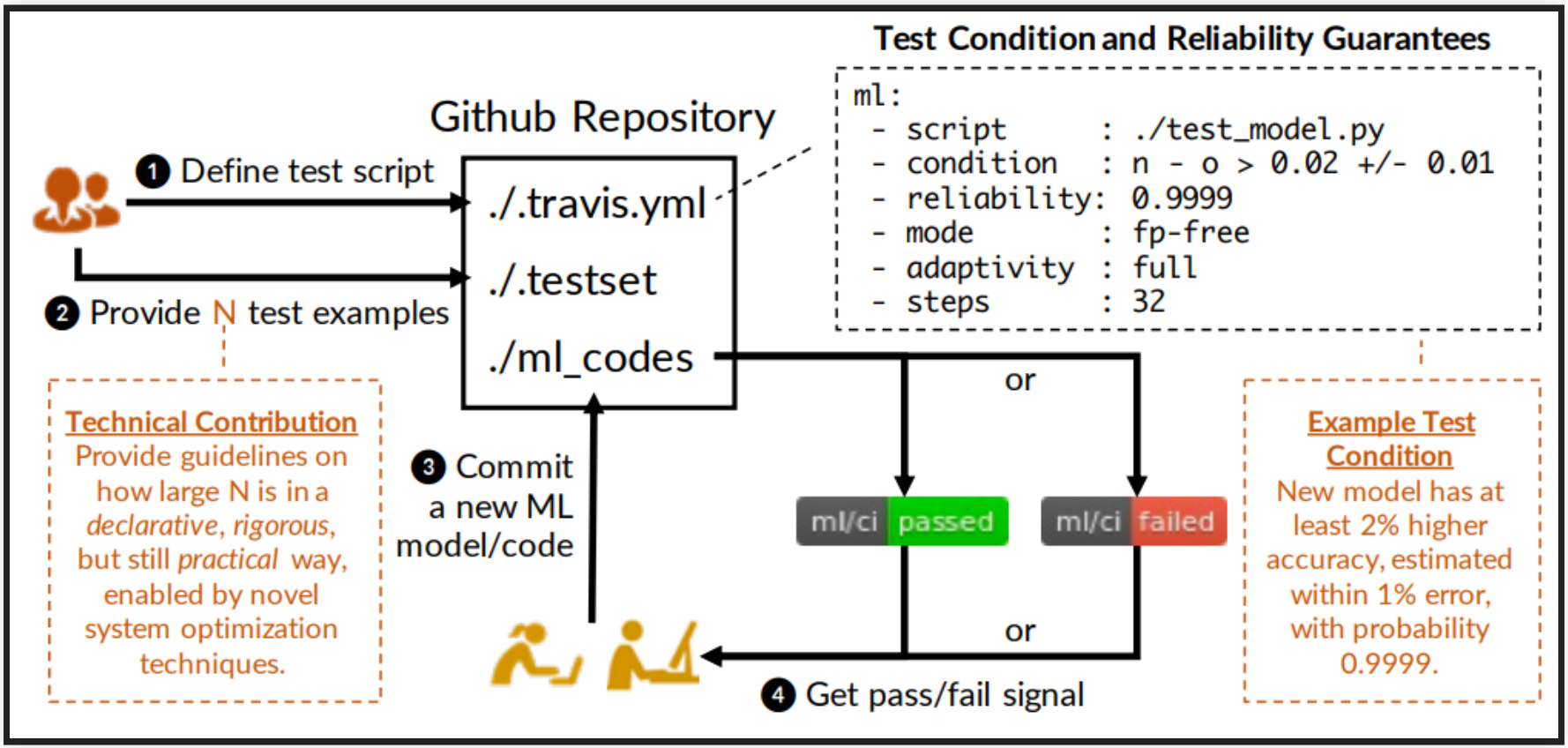


The reliability diagram shows how reliable (or "well-calibrated") the model's probability estimates are when evaluated on the test data. For example, A well calibrated (binatry) model should classify the samples such that among the samples to which it gives a probability close to 0.8 of belonging to the positive class, approximately 80% of those samples actually belong to the positive class. More Info

- A Perfectly Calibrated Model
- This Model (Before Calibration)
- This Model (After Calibration)

data

SPECIALIZED CI SYSTEMS



Renggli et. al, Continuous Integration of Machine Learning Models with ease.ml/ci: Towards a Rigorous Yet Practical Treatment, SysML 2019

DASHBOARDS FOR COMPARING MODELS

mlflow Github Docs

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
☐	17:37	matei	linear.py	3a1995	0.5	0.2	84.27	0.277	158.1
☐	17:37	matei	linear.py	3a1995	0.2	0.5	84.08	0.264	159.6
☐	17:37	matei	linear.py	3a1995	0.5	0.5	84.12	0.272	158.6
☐	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

COMMON PITFALLS OF EVALUATING MODEL QUALITY

EVALUATING ON TRAINING DATA

- surprisingly common in practice
- by accident, incorrect split -- or intentional using all data for training
- tuning on validation data (e.g., crossvalidation) without separate testing data

- Results in overfitting and misleading accuracy measures

USING MISLEADING QUALITY MEASURES

- using accuracy, when false positives are more harmful than false negatives
- comparing area under the curve, rather than relevant thresholds
- averaging over all populations, ignoring different results for subpopulations or different risks for certain predictions
- accuracy results on old static test data, when production data has shifted
- results on tiny validation sets
- reporting results without baseline
- ...

INDEPENDENCE OF DATA: TEMPORAL

Attempt to predict the stock price development for different companies based on twitter posts

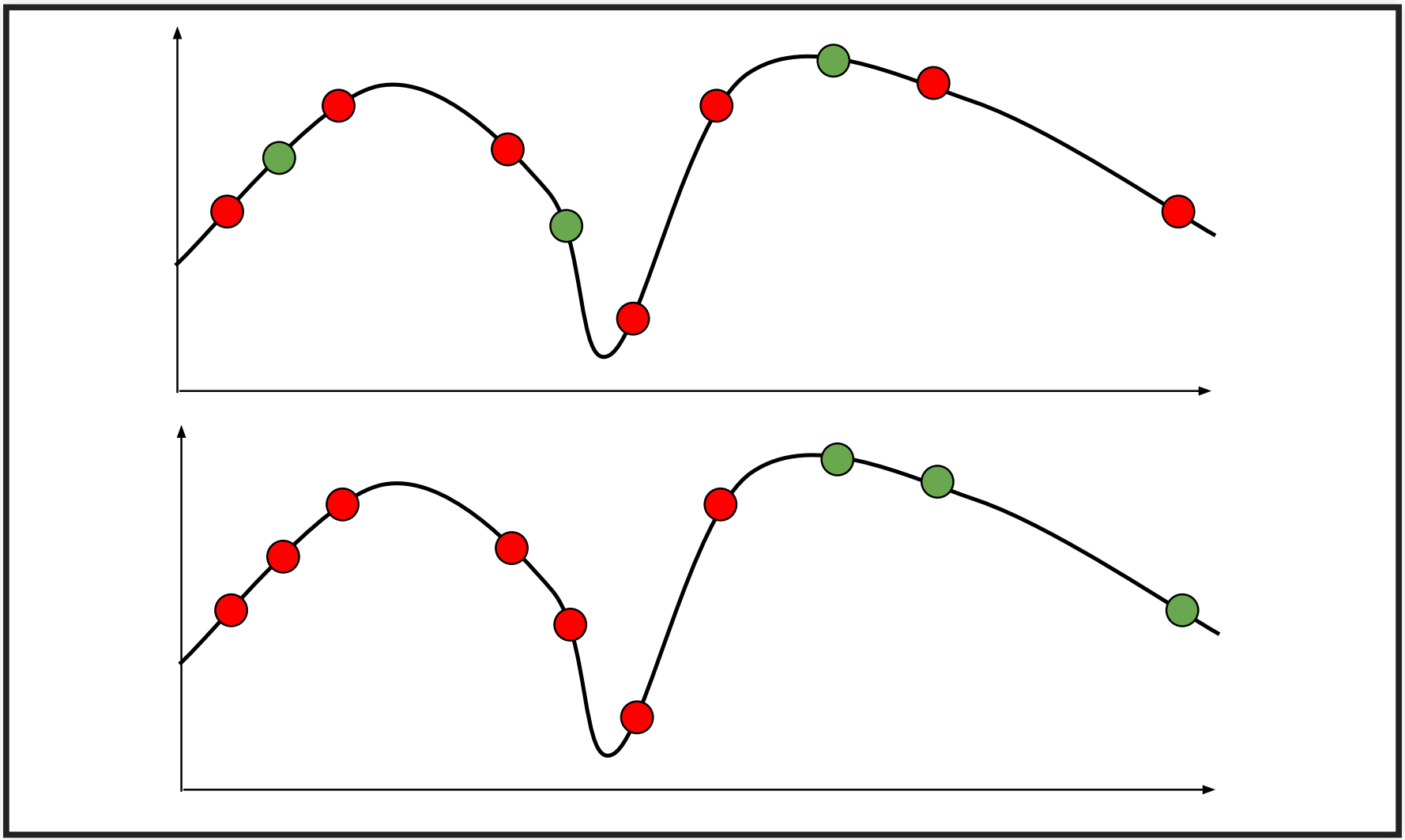
Data: stock prices of 1000 companies over 4 years and twitter mentions of those companies

Problems of random train--validation split?

Speaker notes

The model will be evaluated on past stock prices knowing the future prices of the companies in the training set. Even if we split by companies, we could observe general future trends in the economy during training

INDEPENDENCE OF DATA: TEMPORAL



Speaker notes

The curve is the real trend, red points are training data, green points are validation data. If validation data is randomly selected, it is much easier to predict, because the trends around it are known.

INDEPENDENCE OF DATA: RELATED DATAPOINTS

Kaggle competition on detecting distracted drivers

Relation of datapoints may not be in the data (e.g., driver)

https://www.fast.ai/2017/11/13/validation-sets/

Speaker notes

Many potential subtle and less subtle problems:

- Sales from same user
- Pictures taken on same day

SUMMARY

- Model prediction accuracy only one part of system quality
- Select suitable measure for prediction accuracy, depending on problem (recall, MAPE, AUC, MAP@K, ...)
- Use baselines for interpreting prediction accuracy
- Ensure independence of test and validation data
- Software testing is a poor analogy (model bug); validation may be a better analogy
- Still learn from software testing
    - Carefully select test data
    - Not all inputs are equal: Identify important inputs (inspiration from blackbox testing)
- Automated random testing
    - Feasible with invariants (e.g. metamorphic relations)
    - Sometimes possible with simulation
- Automate the test execution with continuous integration