

Explainable AI

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What is the problem?

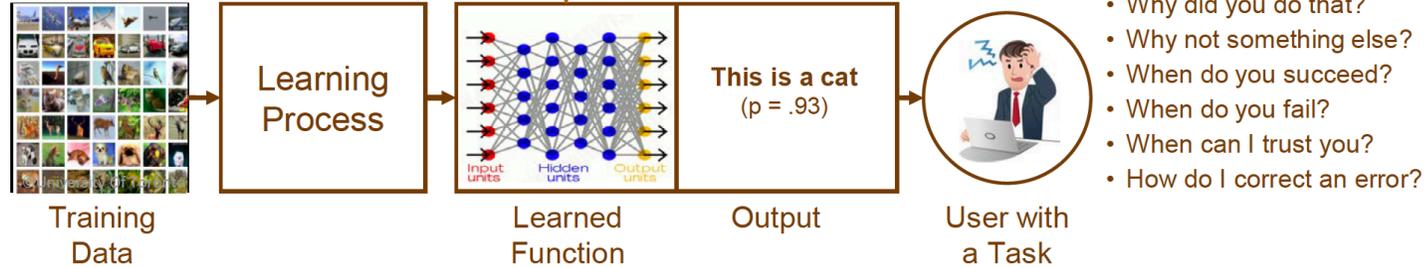
- Artificial intelligence and machine learning (AI/ML) systems have exceeded human performance in nearly every application where they have been tried
- AI is starting to be incorporated into consumer products. This trend is accelerating, and AI will be increasingly used in safety-critical systems
- AI systems are good, but sometimes make mistakes, and human users will not trust their decisions without explanation
- There is a tradeoff between AI accuracy and explainability: the most accurate methods, such as convolutional neural nets (CNNs), provide no explanations; understandable methods, such as rule-based, tend to be less accurate

What is the current state of the art?



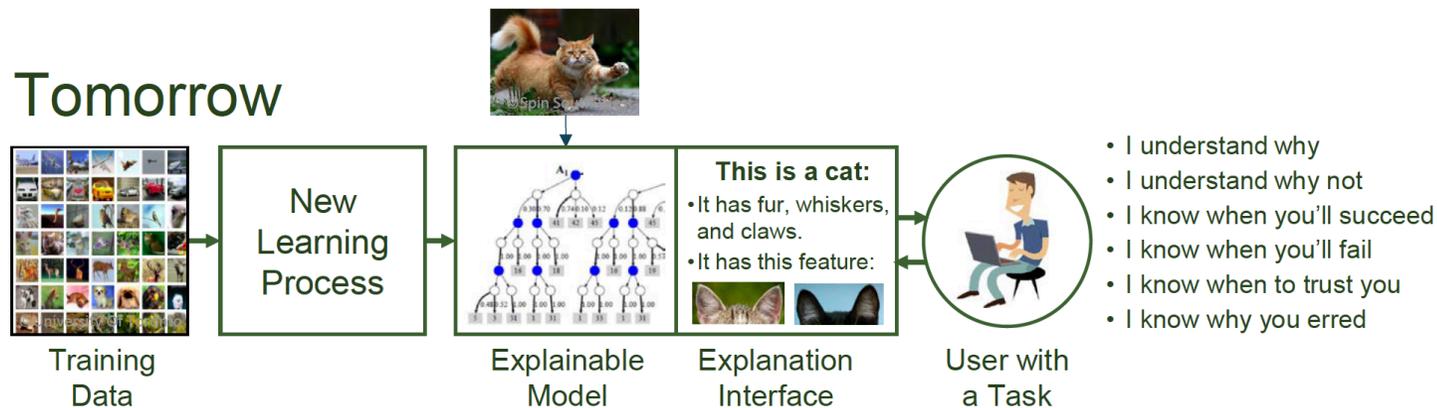
Explainable AI – What Are We Trying To Do?

Today



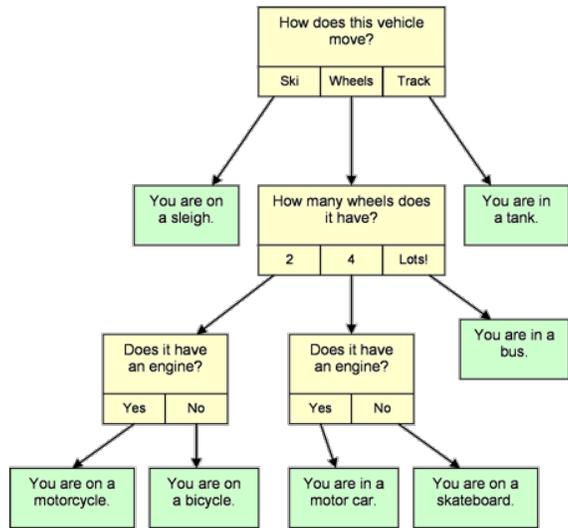
Black-box statistical predictions are inadequate

Tomorrow



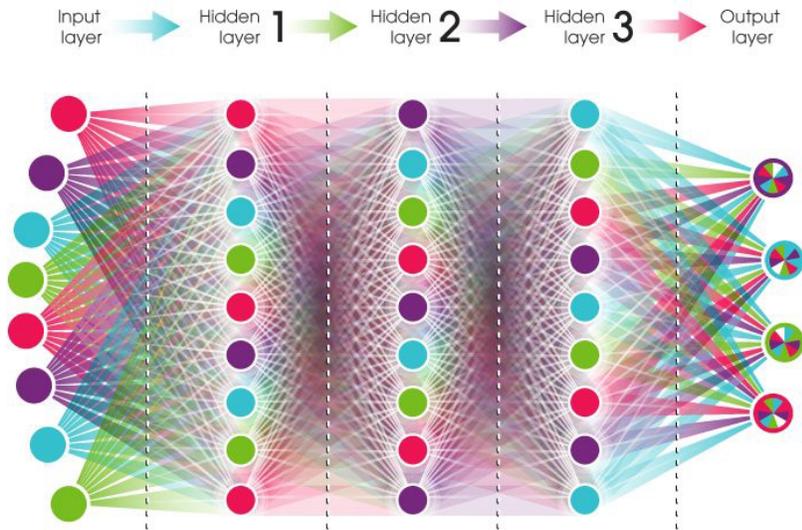
Explanations must be understandable to non-specialist

Tradeoff:



- OR -

DEEP NEURAL NETWORK



Expert system:

Good for explanations,
not so good for accuracy

Neural nets:

Good for accuracy,
not so good for explanations

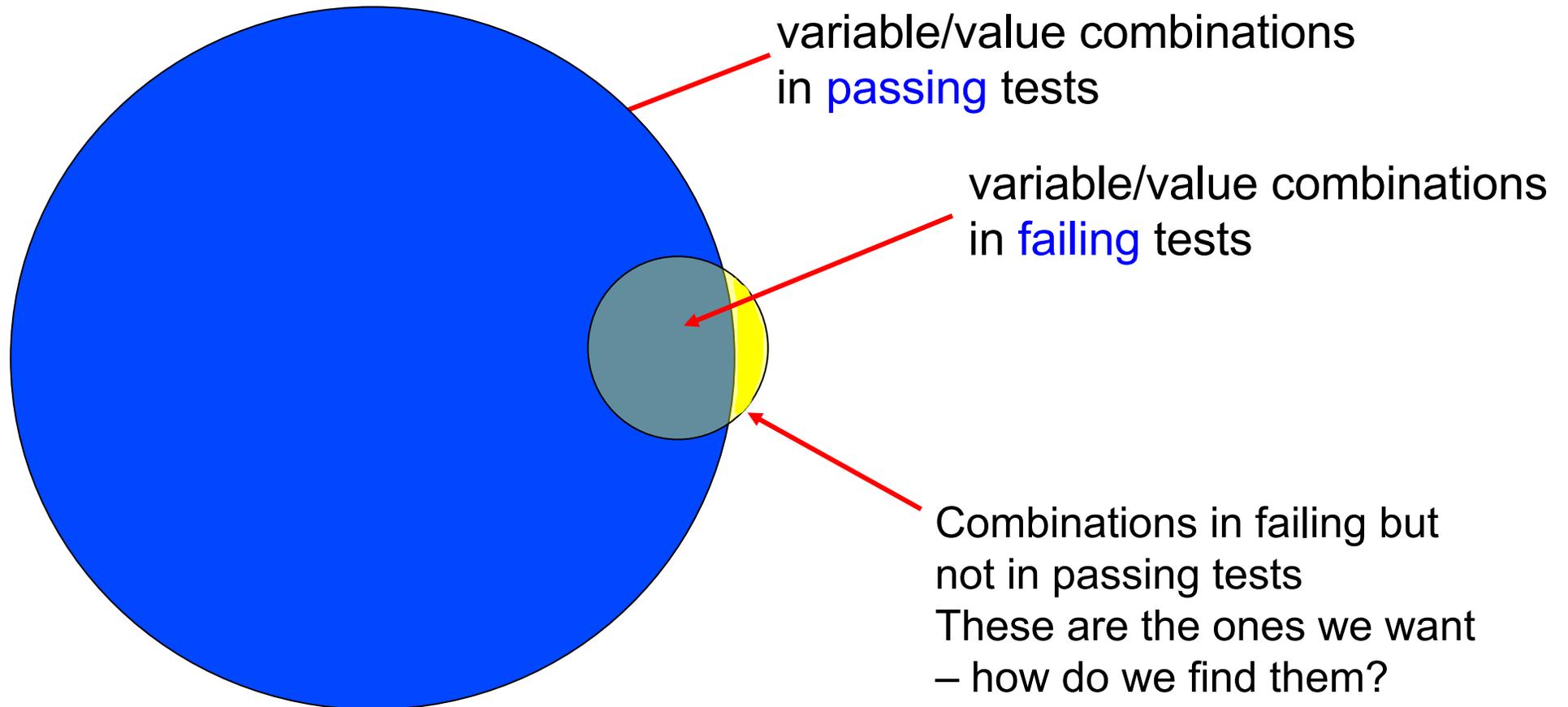
**How do we get the
best of both worlds?**

What can NIST do?

- The classification problem in machine learning is closely related to the problem of fault location in combinatorial testing for software.
- The objective in both cases is to identify a small number of interactions, out of possibly billions or more, that trigger a failure (in combinatorial testing) or produce a conclusion (in machine learning).
- We have methods and tools for fault location in combinatorial testing that could be adapted to ML problems, to identify the rare combinations of variable values that produce conclusions in AI systems.
- This approach has not been applied to AI/ML before.
- NIST has established the leading project in combinatorial software testing

Fault location

Given: a set of tests that the SUT fails, which combinations of variables/values triggered the failure?

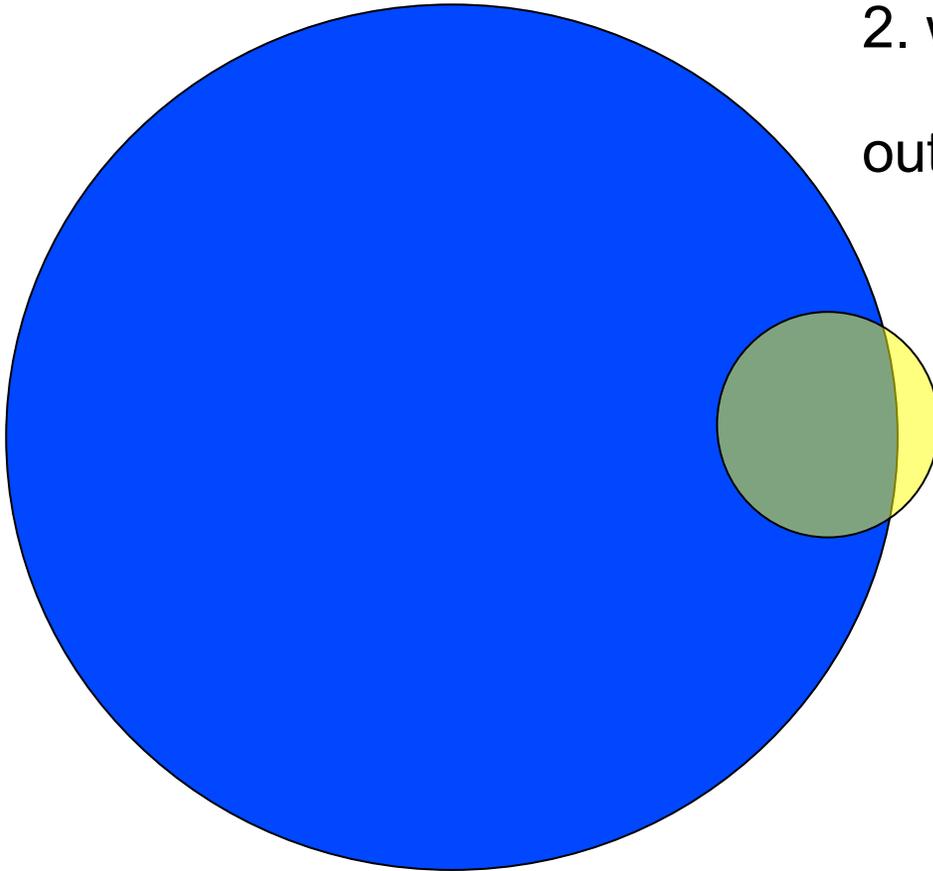


Fault location – what's the problem?

If they're in failing set but not in passing set:

1. which ones triggered the failure?
2. which ones don't matter?

out of $v^t \binom{n}{t}$ combinations



Example:

30 variables, 5 values each,
input configuration 5^{30}

→ 445,331,250 5-way combinations

142,506 combinations in each test

Find one or two out of >142,000 that
caused failure

Relevance to explainable AI

This is a cat:

- It has fur, whiskers, and claws.
- It has this feature:



Explanation Interface



User with a Task

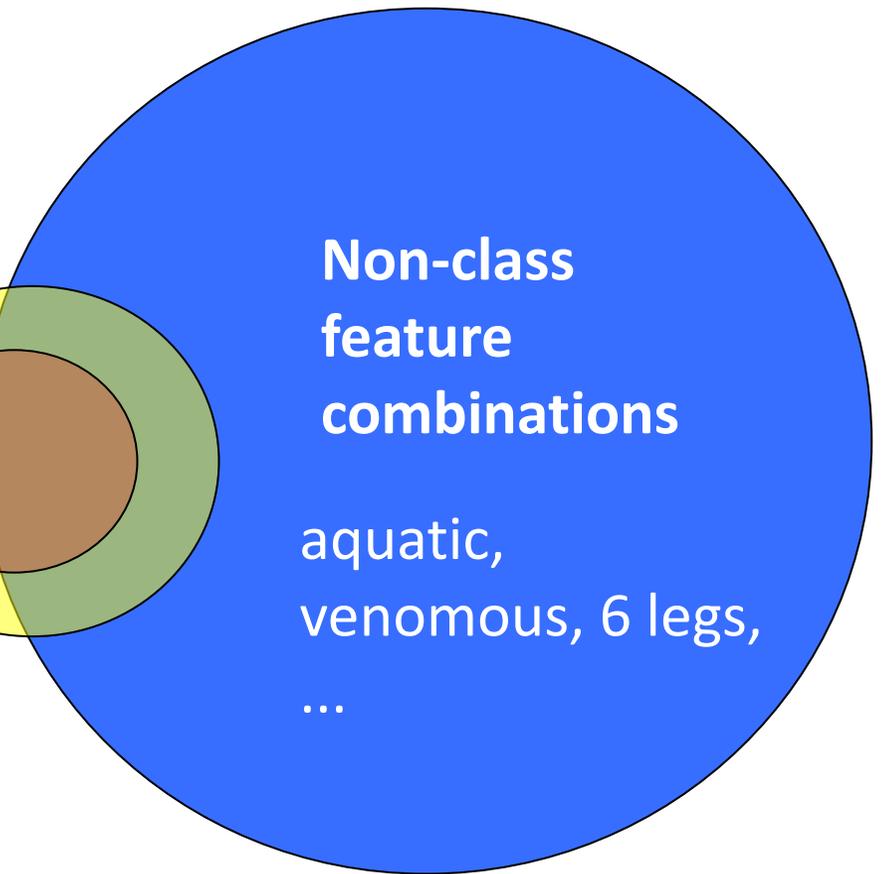
- I understand why
- I understand why not
- I know when you'll succeed
- I know when you'll fail
- I know when to trust you
- I know why you erred

Class feature combinations -
brown & furry,
black & furry,
whiskers, claws, ...
not aquatic, not
venomous, not 6
legs,

Individual feature combinations –
brown & furry,
whiskers, claws,
not aquatic, not
venomous, not 6
legs, ...

Animal shares features with cat class

Animal does not share features with non-cat classes



Why is this creature recognized as a reptile?

| | |
|----------------------|---|
| Class File: | Class file rep1.csv; rows=1; cols=16 |
| Nominal File: | Nominal file notreptile.csv; rows=96; cols=16 2-way: 120 3-way: 560 4-way: 1,820 5-way: 4,368 6-way: 8,008 |
| Class File Contents: | hair 0 feathers 0 eggs 1 milk 0 airborne 0 aquatic 0 predator 0 toothed 0 backbone 1 breathes 1 venomous 0 fins 0 nlegs 0 tail 4 domestic 1 catsize 0 1 |



```
-----
0053 occurrences = 0.552 of cases, hair = 0
0076 occurrences = 0.792 of cases, feathers = 0
0055 occurrences = 0.573 of cases, eggs = 1
0055 occurrences = 0.573 of cases, milk = 0
0072 occurrences = 0.750 of cases, airborne = 0
0061 occurrences = 0.635 of cases, aquatic = 0
0044 occurrences = 0.458 of cases, predator = 0
0039 occurrences = 0.406 of cases, toothed = 0
0078 occurrences = 0.813 of cases, backbone = 1
0076 occurrences = 0.792 of cases, breathes = 1
0090 occurrences = 0.938 of cases, venomous = 0
0079 occurrences = 0.823 of cases, fins = 0
0036 occurrences = 0.375 of cases, nlegs = 4
0070 occurrences = 0.729 of cases, tail = 1
0083 occurrences = 0.865 of cases, domestic = 0
0043 occurrences = 0.448 of cases, catsize = 1
```

No single feature is sufficient explanation – shares features with non-reptiles

No pair of features sufficient – shares 2-way combinations w/ non-reptiles

```
0002 occurrences = 0.021 of cases, toothed, nlegs = 0, 4
0005 occurrences = 0.052 of cases, hair, nlegs = 0, 4
0005 occurrences = 0.052 of cases, milk, nlegs = 0, 4
0006 occurrences = 0.063 of cases, eggs, nlegs = 1, 4
0008 occurrences = 0.083 of cases, toothed, catsize = 0, 1
0011 occurrences = 0.115 of cases, milk, catsize = 0, 1
0012 occurrences = 0.125 of cases, eggs, catsize = 1, 1
0013 occurrences = 0.135 of cases, hair, catsize = 0, 1
0015 occurrences = 0.156 of cases, predator, catsize = 0, 1
```

3-way combinations produce rules to explain recognition of Testudo as a reptile

```
00000 occurrences = 0.000 of cases, aquatic,toothed,nlegs = 0,0,4
00000 occurrences = 0.000 of cases, eggs,aquatic,nlegs = 1,0,4
00000 occurrences = 0.000 of cases, hair,aquatic,nlegs = 0,0,4
00000 occurrences = 0.000 of cases, hair,nlegs,catsize = 0,4,1
00000 occurrences = 0.000 of cases, milk,aquatic,nlegs = 0,0,4
00000 occurrences = 0.000 of cases, milk,nlegs,catsize = 0,4,1
00000 occurrences = 0.000 of cases, predator,toothed,nlegs = 0,0,4
00001 occurrences = 0.010 of cases, eggs,nlegs,catsize = 1,4,1
00001 occurrences = 0.010 of cases, eggs,predator,nlegs = 1,0,4
00001 occurrences = 0.010 of cases, feathers,toothed,backbone = 0,0,1
```

Non-reptiles in the database do not have these 3-way combinations

Only reptiles have these combinations of features:

- not aquatic AND not toothed AND four legs
- egg-laying AND not aquatic AND four legs
- not hairy AND four legs AND cat size
- not milk-producing AND not aquatic AND four legs
- not milk-producing AND four legs AND cat size
- not predator AND not toothed AND four legs

Sample ML problem

- “Titanic survivors” – popular demo problem for ML
- Predict which passengers survive, using attributes:
- Passenger class: 1st, 2nd, 3rd
- Sex
- Age: 14 and under, 15 to 20, 21 to 70, over 70
- Number of siblings or spouses onboard
- Number of parents or children onboard
- Embarkation point: Southampton, England; Queenstown, Ireland; Cherbourg, France
- Input configuration $2^1 3^2 4^1 5^2$

Example using prototype

– what factors explain this passenger's survival?

First class passenger, female aged 21 to 70, no siblings, spouse, parents, or children onboard, from England

What factors differentiate passenger from casualties?

Consider 2-way combinations of factors:
1st class female passengers (like this one) were only 0.6% of casualties

No single factor is adequate explanation:
15% of dead were 1st class;
16% were female;
61% aged 21 to 70

Survival explained by being female passenger traveling first class. Neither of these two factors alone is enough.

The screenshot shows a software interface with the following sections:

- File Information:**
 - Class File: Class file ts1.csv; rows=1; cols=6
 - Nominal File: Nominal file td.csv; rows=809; cols=6 || 2-way: 15 3-way: 20 4-way: 15 5-way: 6 6-way: 1
 - Class File Contents: pclass sex age sibsp parch embarked
1 female 21to70 0 0 S
- 2-Way Combinations:** (Selected tab)
 - Enabled
 - Combinations = 15, Settings = 289
 - List of combinations with occurrence rates and factor descriptions:

| Combination ID | Occurrences | Rate of Cases | Factors |
|----------------|---------------------|---------------|---------------------------|
| 0005 | occurrences = 0.006 | of cases | pclass, sex = 1, female |
| 0065 | occurrences = 0.080 | of cases | sex, age = female, 21to70 |
| 0065 | occurrences = 0.080 | of cases | sex, sibsp = female, 0 |
| 0075 | occurrences = 0.093 | of cases | sex, parch = female, 0 |
| 0078 | occurrences = 0.096 | of cases | pclass, embarked = 1, S |
| 0087 | occurrences = 0.108 | of cases | pclass, sibsp = 1, 0 |
| 0093 | occurrences = 0.115 | of cases | sex, embarked = female, S |
| 0095 | occurrences = 0.117 | of cases | pclass, age = 1, 21to70 |
| 0101 | occurrences = 0.125 | of cases | pclass, parch = 1, 0 |
| 0369 | occurrences = 0.456 | of cases | age, sibsp = 21to70, 0 |
| 0401 | occurrences = 0.496 | of cases | age, embarked = 21to70, S |
| 0431 | occurrences = 0.533 | of cases | age, parch = 21to70, 0 |
| 0432 | occurrences = 0.534 | of cases | sibsp, embarked = 0, S |
| 0496 | occurrences = 0.613 | of cases | parch, embarked = 0, S |
| 0551 | occurrences = 0.681 | of cases | sibsp, parch = 0, 0 |
| ----- | | | |
| 0123 | occurrences = 0.152 | of cases | pclass = 1 |
| 0127 | occurrences = 0.157 | of cases | sex = female |
| 0494 | occurrences = 0.611 | of cases | age = 21to70 |
| 0582 | occurrences = 0.719 | of cases | sibsp = 0 |
| 0666 | occurrences = 0.823 | of cases | parch = 0 |
| 0610 | occurrences = 0.754 | of cases | embarked = S |

Heatmap visualization of factor combinations

| Psngr class | Sex | Age | # sibling spouse | #parent child | embarked |
|-------------|-----|--------|------------------|---------------|----------|
| 1 | f | 21to70 | 0 | 0 | S |

Green to red -> **more significant** to **less significant** for explanation

| Heatmap | female | 21to070 | no sibling/spouse | no parents/children | Southampton |
|-----------------------|--------|---------|-------------------|---------------------|-------------|
| 1 st class | 0.0062 | 0.1174 | 0.1075 | 0.1248 | 0.0964 |
| female | | 0.0803 | 0.0803 | 0.0927 | 0.1150 |
| 21 to 70 | | | 0.4561 | 0.5328 | 0.4957 |
| no sibling/spouse | | | | 0.6811 | 0.5340 |
| no parents/children | | | | | 0.6131 |

Another example— what factors explain this passenger's survival?

First class passenger, male child, with one sibling, two parents onboard, from England

What factors differentiate passenger from casualties?

Consider 2-way combinations of factors:
1st class passengers with two parents onboard (like this one) were only 0.7% of casualties

No single factor is adequate explanation:

15% of dead were 1st class;

84% were male;

29% were children 14 and under

Survival explained by being child with parents traveling first class. No single factor alone is enough.

Easily seen in 3-way combinations:

...ncurrences = 0.001 of cases, pclass, age, parch = 1, 0to14, 2
...ncurrences = 0.001 of cases, pclass, age, sibsp = 1, 0to14, 1

The screenshot shows a software window titled "Class" with a "File Information" section and a "2-Way" combinations section. The "File Information" section displays:

- Class File: Class file ts2.csv; rows=1; cols=6
- Nominal File: Nominal file td.csv; rows=809; cols=6 || 2-way: 15 3-way: 20 4-way: 15 5-way: 6 6-way: 1
- Class File Contents: A table with columns pclass, sex, age, sibsp, parch, embarked and one row of data: 1, male, 0to14, 1, 2, S.

The "2-Way" section is set to "Enabled" and shows "Combinations = 15, Settings = 289". It lists 15 combinations of two factors with their respective occurrence rates. A blue arrow points from the text "Consider 2-way combinations of factors:" to the top of this list. Another blue arrow points from the text "Survival explained by being child with parents traveling first class. No single factor alone is enough." to the combination "0006 occurrences = 0.007 of cases, pclass, parch = 1, 2".

| Combination | Occurrences | Rate | Factors |
|-------------|-------------|-------|--------------------------|
| 0006 | occurrences | 0.007 | pclass, parch = 1, 2 |
| 0011 | occurrences | 0.014 | sibsp, parch = 1, 2 |
| 0021 | occurrences | 0.026 | pclass, age = 1, 0to14 |
| 0031 | occurrences | 0.038 | age, sibsp = 0to14, 1 |
| 0031 | occurrences | 0.038 | sex, parch = male, 2 |
| 0034 | occurrences | 0.042 | pclass, sibsp = 1, 1 |
| 0035 | occurrences | 0.043 | age, parch = 0to14, 2 |
| 0050 | occurrences | 0.062 | parch, embarked = 2, S |
| 0078 | occurrences | 0.096 | pclass, embarked = 1, S |
| 0116 | occurrences | 0.143 | sex, sibsp = male, 1 |
| 0116 | occurrences | 0.143 | sibsp, embarked = 1, S |
| 0118 | occurrences | 0.146 | pclass, sex = 1, male |
| 0142 | occurrences | 0.176 | age, embarked = 0to14, S |
| 0184 | occurrences | 0.227 | sex, age = male, 0to14 |
| 0517 | occurrences | 0.639 | sex, embarked = male, S |
| ----- | | | |
| 0123 | occurrences | 0.152 | pclass = 1 |
| 0682 | occurrences | 0.843 | sex = male |
| 0232 | occurrences | 0.287 | age = 0to14 |
| 0156 | occurrences | 0.193 | sibsp = 1 |
| 0056 | occurrences | 0.069 | parch = 2 |
| 0610 | occurrences | 0.754 | embarked = S |

Mapping combinations to expressions

- Report identifies t-way combinations that distinguish the predicted class from others
- Combinations can be mapped to expressions to produce a rule-based type of explanation

if (1st class passenger AND female) OR (female AND age 21to70) OR (female AND no siblings/spouses) then SURVIVE

if (1st class passenger AND age 14 or under AND parents onboard) OR (1st class passenger AND age 14 or under AND siblings onboard) then SURVIVE

As noted, **none of the single factors above is sufficient for explanation**

Example: empty vs. occupied rooms, using sensor data

Why do we conclude this room is occupied?

These levels of humidity and lighting are strong indication

Considering levels of lighting, CO2, and humidity ratio provide even stronger evidence:

Empty rooms don't have these levels

File Information

Class File: Class file o1.csv; rows=1; cols=5

Nominal File: Nominal file empty.csv; rows=7703; cols=5 || 2-way: 10 3-way: 10 4-way: 5 5-way: 1 6-way: 0

Class File Contents:

| | | | | |
|-------------|----------|-------|-----|---------------|
| Temperature | Humidity | Light | CO2 | HumidityRatio |
| B3 | B3 | B2 | B2 | B4 |

2-Way | 3-Way | 4-Way | 5-Way | 6-Way

Enabled

Combinations = 10, Settings = 210

| | | | |
|-------|---------------------|-----------|-------------------------------------|
| 0016 | occurrences = 0.002 | of cases, | Humidity, Light = B3, B2 |
| 0016 | occurrences = 0.002 | of cases, | Light, CO2 = B2, B2 |
| 0036 | occurrences = 0.005 | of cases, | Temperature, Light = B3, B2 |
| 0040 | occurrences = 0.005 | of cases, | CO2, HumidityRatio = B2, B4 |
| 0043 | occurrences = 0.006 | of cases, | Light, HumidityRatio = B2, B4 |
| 0054 | occurrences = 0.007 | of cases, | Temperature, CO2 = B3, B2 |
| 0078 | occurrences = 0.010 | of cases, | Humidity, CO2 = B3, B2 |
| 0205 | occurrences = 0.027 | of cases, | Temperature, HumidityRatio = B3, B4 |
| 0247 | occurrences = 0.032 | of cases, | Temperature, Humidity = B3, B3 |
| 0495 | occurrences = 0.064 | of cases, | Humidity, HumidityRatio = B3, B4 |
| ----- | | | |
| 0523 | occurrences = 0.068 | of cases, | Temperature = B3 |
| 2415 | occurrences = 0.314 | of cases, | Humidity = B3 |
| 0085 | occurrences = 0.011 | of cases, | Light = B2 |
| 0534 | occurrences = 0.069 | of cases, | CO2 = B2 |
| 2190 | occurrences = 0.284 | of cases, | HumidityRatio = B4 |

| | | | |
|-------|---------------------|-----------|---|
| 00003 | occurrences = 0.000 | of cases, | Light, CO2, HumidityRatio = B2, B2, B4 |
| 00005 | occurrences = 0.001 | of cases, | Humidity, Light, CO2 = B3, B2, B2 |
| 00008 | occurrences = 0.001 | of cases, | Temperature, Light, CO2 = B3, B2, B2 |
| 00011 | occurrences = 0.001 | of cases, | Humidity, Light, HumidityRatio = B3, B2, B4 |

A different example: lymph node pathology – why is this classified as malignant not metastatic?

- These combinations are characteristic of lymphoma that arises in lymph node instead of metastatic that spread to node from somewhere else

The screenshot shows a software window with a 'File Information' section at the top. Below it, there are tabs for '2Way', '3-Way', '4-Way', '5-Way', and '6-Way'. The '2Way' tab is selected, and a list of combinations is displayed. A blue arrow points from the text in the slide to the third line of the combinations list.

File Information

Class File: Class file mal1.csv; rows=1; cols=18

Nominal File: Nominal file meta.csv; rows=81; cols=18 || 2-way: 153 3-way: 816 4-way: 3,060 5-way: 8,568

Class File Contents:

| | | | | | | | |
|-----------|--------|------|------|--------|----------|-------|-------|
| lymphatic | affere | lymc | lyms | bypass | extravas | regen | early |
| 4 | 2 | 1 | 1 | 1 | 1 | 1 | 1 |

2Way | 3-Way | 4-Way | 5-Way | 6-Way

Enabled

Combinations = 153, Settings = 1358

```
0000 occurrences = 0.000 of cases, chnode, chstru = 4, 8
0000 occurrences = 0.000 of cases, chnode, disloc = 4, 1
0000 occurrences = 0.000 of cases, chnode, num = 4, 2
0000 occurrences = 0.000 of cases, chnode, spec = 4, 1
0000 occurrences = 0.000 of cases, defect, chnode = 2, 4
0000 occurrences = 0.000 of cases, extravas, chnode = 1, 4
0000 occurrences = 0.000 of cases, lymphatic, chnode = 4, 4
0001 occurrences = 0.012 of cases, bypass, chnode = 1, 4
0001 occurrences = 0.012 of cases, chang, chnode = 2, 4
0001 occurrences = 0.012 of cases, chnode, exclu = 4, 2
0001 occurrences = 0.012 of cases, lymc, chnode = 1, 4
0001 occurrences = 0.012 of cases, lymphatic, spec = 4, 1
0002 occurrences = 0.025 of cases, lyms, chnode = 1, 4
0002 occurrences = 0.025 of cases, affere, chnode = 2, 4
0002 occurrences = 0.025 of cases, dimin, chnode = 1, 4
0002 occurrences = 0.025 of cases, earlyup, chnode = 2, 4
0002 occurrences = 0.025 of cases, enlar, chnode = 2, 4
0002 occurrences = 0.025 of cases, regen, chnode = 1, 4
0002 occurrences = 0.025 of cases, spec, num = 1, 2
0003 occurrences = 0.037 of cases, lymphatic, disloc = 4, 1
0004 occurrences = 0.049 of cases, chstru, spec = 8, 1
0004 occurrences = 0.049 of cases, lymphatic, chstru = 4, 8
0005 occurrences = 0.062 of cases, lymphatic, chang = 4, 2
0006 occurrences = 0.074 of cases, chstru, num = 8, 2
```

Summary

- Combinatorial methods can provide explainable AI
- We have prototype that applies this approach
 - Determine combinations of variable values that differentiate an example from other possible conclusions
 - ➔ Feature combinations present shared with class
 - ➔ Feature combinations not shared with class not present
- Method can be applied to black-box functions such as CNNs
- Present explanation in the preferred form of rules, “if A & B, or C with D & E, then conclusion is X”

Summary

- Explainability is a critical problem in the acceptance of artificial intelligence/machine learning, especially for critical applications
- Human users will not trust AI if conclusions cannot be explained
- Methods from combinatorial software testing can be applied to solving the problem of explainable AI
- We have prototype that applies this approach
 - Determine combinations of variable values that differentiate an example from other possible conclusions
 - ➔ Feature combinations present shared with class
 - ➔ Feature combinations not shared with class not present
 - Present explanation in the preferred form of rules, “if A & B, or C with D & E, then conclusion is X”
- Method can be applied to black-box functions such as CNNs

What has been tried?

- Interpretable models – e.g. rule-based expert systems: “if patient has symptoms A and B, or has B with C and D, then illness is X”
 - best for explanations
 - hard to find rules
 - less accurate than other approaches
- Modify neural nets etc. to add explanations
 - reduces accuracy, complicates the system
 - explanations still not very understandable
- Model induction - infer explainable model from black-box
 - flexible for application, good explanations using only input, output
 - hard to produce the explainable model
- Our approach – derive rule predicates from inputs and outputs to CNNs and other black-box functions