

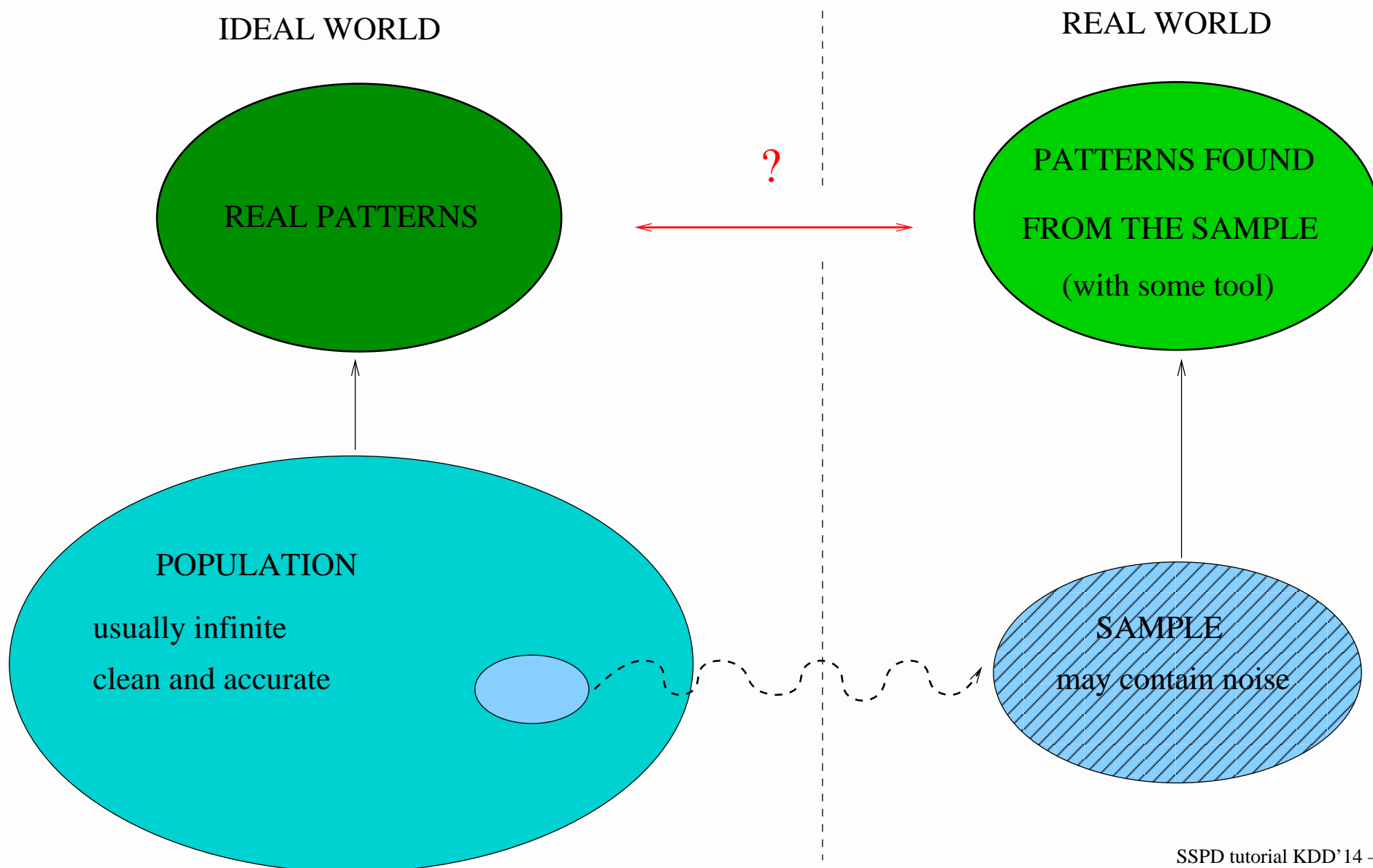
STATISTICALLY SOUND PATTERN DISCOVERY

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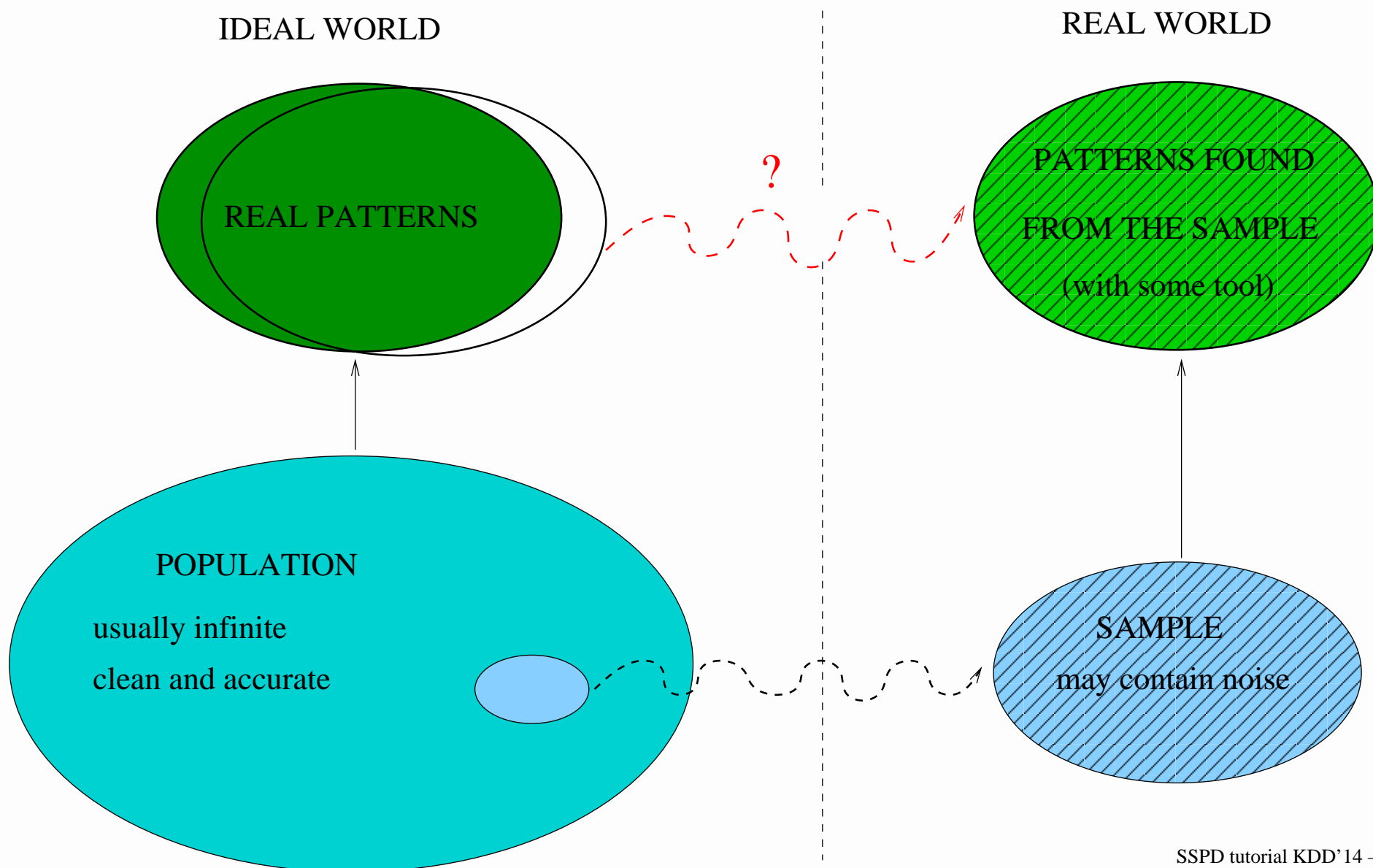
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[http://www.cs.joensuu.fi/pages/whamalai/kdd14/
sspdtutorial.html](http://www.cs.joensuu.fi/pages/whamalai/kdd14/sspdtutorial.html)

Statistically sound pattern discovery: Problem



Statistically sound pattern discovery: Problem



Statistically Sound vs. Unsound DM?

Pattern-type-first:

Given a desired classical pattern, invent a search method.

Method-first:

Invent a new pattern type which has an easy search method

e.g., an antimonotonic
“interestingness” property

Tricks to sell it:

- overload statistical terms
- don't specify exactly

Statistically Sound vs. Unsound DM?

Pattern-type-first:

Given a desired classical pattern, invent a search method.

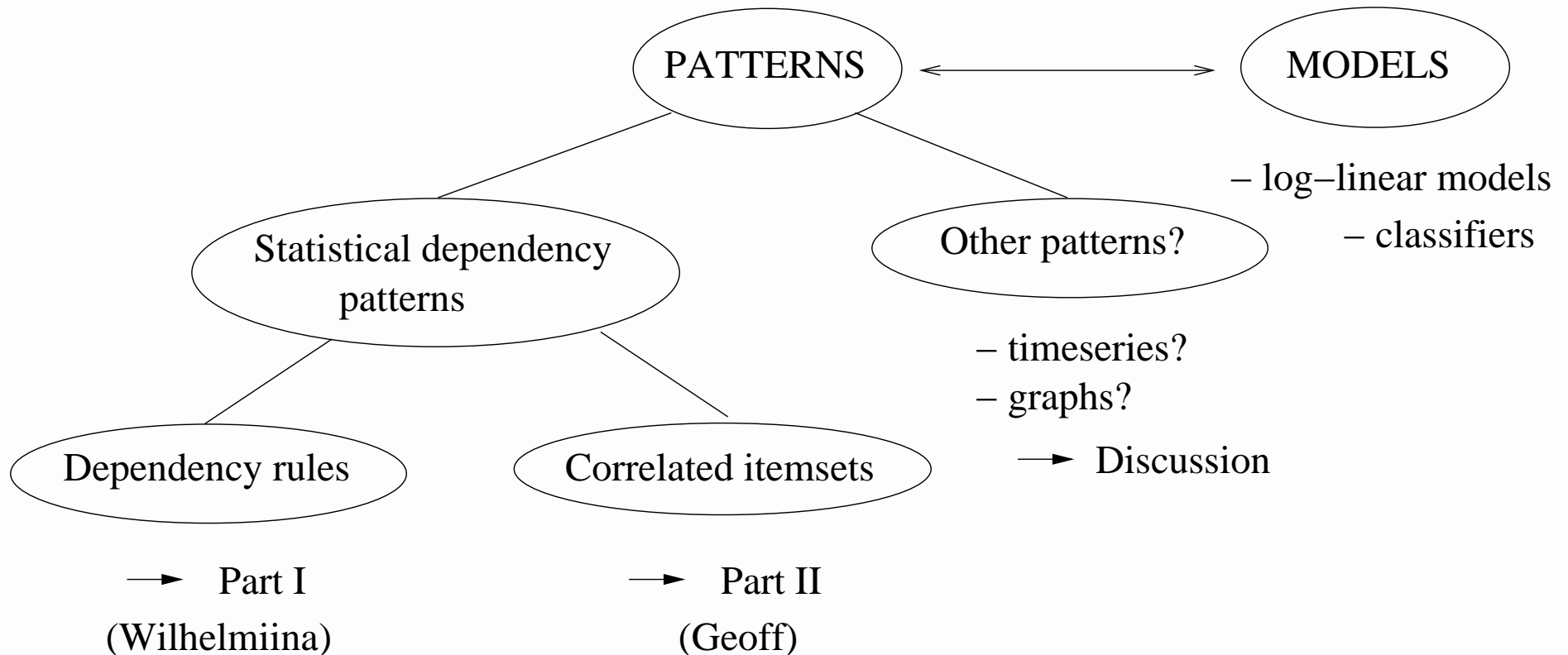
- + easy to interpret correctly
- + informative
- + likely to hold in future
- computationally demanding

Method-first:

Invent a new pattern type which has an easy search method

- difficult to interpret
- misleading “information”
- no guarantees on validity
- + computationally easy

Statistically sound pattern discovery: Scope



Contents

Overview (statistical dependency patterns)

Part I

- Dependency rules
- **Statistical significance testing**

Coffee break (10:00-10:30)

- Significance of improvement

Part II

- Correlated itemsets (self-sufficient itemsets)
- Significance tests for genuine set dependencies

Discussion

Statistical dependence: Many interpretations!

Events $(X = x)$ and $(Y = y)$ are statistically **independent**, if $P(X = x, Y = y) = P(X = x)P(Y = y)$.

- When variables (or variable-value combinations) are statistically **dependent**?
- When the dependency is genuine? → measures for the **strength** and **significance** of dependence
- How to define mutual dependence between three or more variables?

Statistical dependence: 3 main interpretations

Let A, B, C binary variables. Notate $\neg A \equiv (A = 0)$ and $A \equiv (A = 1)$

1. **Dependency rule** $AB \rightarrow C$: must be $\delta = P(ABC) - P(AB)P(C) > 0$ (positive dependence).

2. **Full probability model:**

$$\delta_1 = P(ABC) - P(AB)P(C),$$

$$\delta_2 = P(A\neg BC) - P(A\neg B)P(C),$$

$$\delta_3 = P(\neg ABC) - P(\neg AB)P(C) \text{ and}$$

$$\delta_4 = P(\neg A\neg BC) - P(\neg A\neg B)P(C).$$

- If $\delta_1 = \delta_2 = \delta_3 = \delta_4 = 0$, no dependence
- Otherwise decide from δ_i ($i = 1, \dots, 4$) (with some equation)

Statistical dependence: 3 interpretations

3. Correlated set ABC

- Starting point mutual independence:

$$P(A = a, B = b, C = c) = P(A = a)P(B = b)P(C = c) \text{ for all } a, b, c \in \{0, 1\}$$

- different variations (and names)! e.g.

(i) $P(ABC) > P(A)P(B)P(C)$ (positive dependence) or

(ii) $P(A = a, B = b, C = c) \neq P(A = a)P(B = b)P(C = c)$
for some $a, b, c \in \{0, 1\}$

+ extra criteria

In addition, **conditional independence** sometimes useful

$$P(B = b, C = c | A = a) = P(B = b | A = a)P(C = c | A = a)$$

Statistical dependence: no single correct definition

One of the most important problems in the philosophy of natural sciences is – in addition to the well-known one regarding the essence of the concept of probability itself – to make precise the premises which would make it possible to regard any given real events as independent.

A.N. Kolmogorov

Part I Contents

1. Statistical dependency rules
2. Variable- and value-based interpretations
3. Statistical significance testing
 - 3.1 Approaches
 - 3.2 Sampling models
 - 3.3 Multiple testing problem
4. Redundancy and significance of improvement
5. Search strategies

1. *Statistical dependency rules*

Requirements for a genuine statistical dependency rule
 $X \rightarrow A$:

- (i) Statistical dependence
- (ii) Statistically significant
 - likely not due to chance
- (iii) Non-redundant
 - not a side-product of another dependency
 - added value

Why?

Example: Dependency rules on atherosclerosis

1. Statistical dependencies:
smoking \rightarrow atherosclerosis
sports $\rightarrow \neg$ atherosclerosis
ABCA1-R219K \perp atherosclerosis ?
2. Statistical significance?
spruce sprout extract $\rightarrow \neg$ atherosclerosis ?
dark chocolate $\rightarrow \neg$ atherosclerosis
3. Redundancy?
stress, smoking \rightarrow atherosclerosis
smoking, coffee \rightarrow atherosclerosis ?
high cholesterol, sports \rightarrow atherosclerosis ?
male, male pattern baldness \rightarrow atherosclerosis ?

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2. Variable-based vs. Value-based interpretation

Meaning of dependency rule $X \rightarrow A$

1. Variable-based: dependency between binary **variables** X and A
 - Positive dependency $X \rightarrow A$ the same as $\neg X \rightarrow \neg A$
 - Equally strong as negative dependency between X and $\neg A$ (or $\neg X$ and A)
2. Value-based: positive dependency between **values** $X = 1$ and $A = 1$
 - different from $\neg X \rightarrow \neg A$ which may be weak!

Strength of statistical dependence

The most common measures:

1. Variable-based: leverage

$$\delta(X, A) = P(XA) - P(X)P(A)$$

2. Value-based: lift

$$\gamma(X, A) = \frac{P(XA)}{P(X)P(A)} = \frac{P(A|X)}{P(A)} = \frac{P(X|A)}{P(X)}$$

$P(A|X)$ = “confidence” of the rule

Remember: $X \equiv (X = 1)$ and $A \equiv (A = 1)$

Contingency table

	A	$\neg A$	All
X	$fr(XA) =$ $n[P(X)P(A) + \delta]$	$fr(X\neg A) =$ $n[P(X)P(\neg A) - \delta]$	$fr(X)$
$\neg X$	$fr(\neg XA) =$ $n[P(\neg X)P(A) - \delta]$	$fr(\neg X\neg A) =$ $n[P(\neg X)P(\neg A) + \delta]$	$fr(\neg X)$
All	$fr(A)$	$fr(\neg A)$	n

All value combinations have the same $|\delta|$!
 $\Leftrightarrow \gamma$ depends on the value combination

$fr(X)$ =absolute frequency of X
 $P(X)$ =relative frequency of X

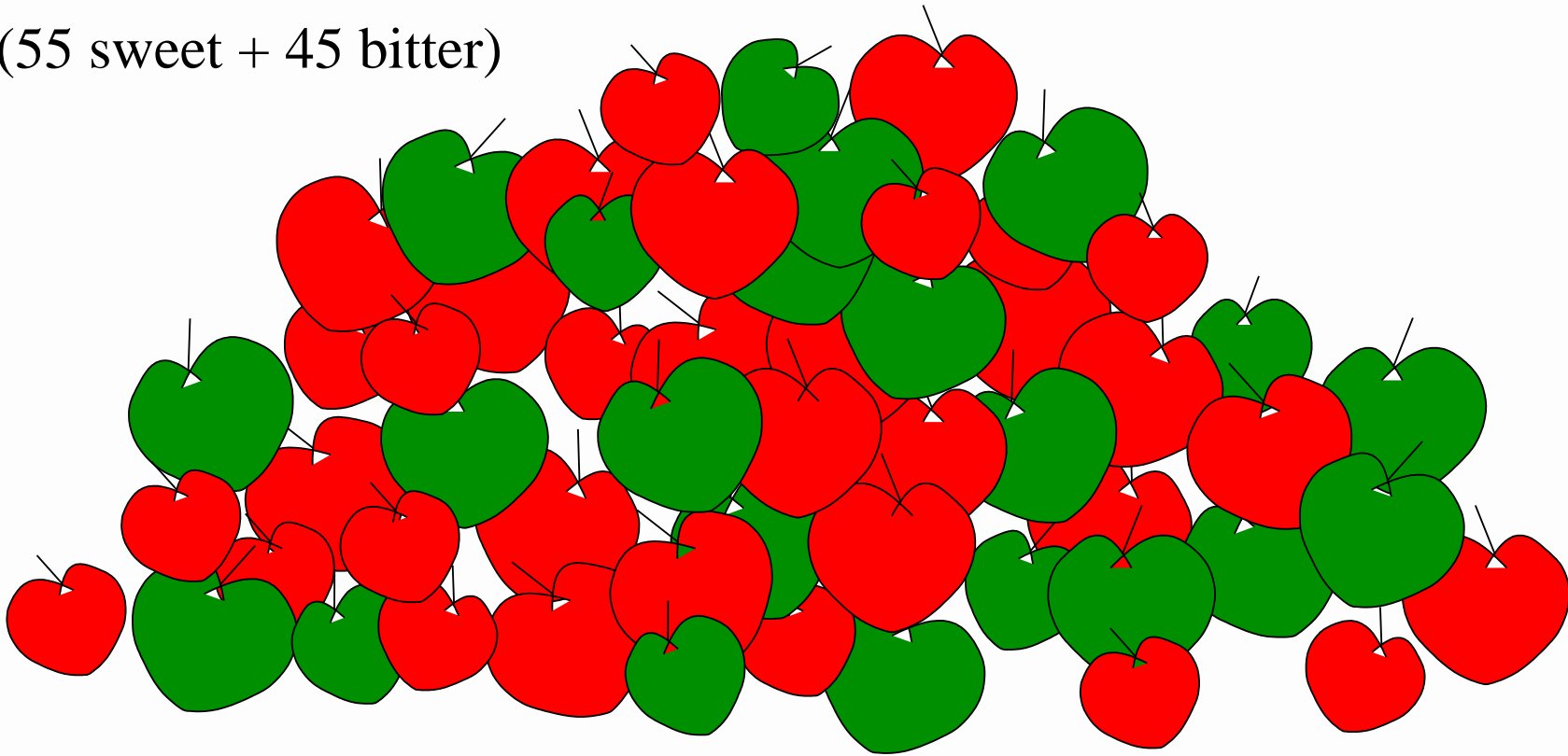
Example: The Apple problem

Variables: Taste, smell, colour, size, weight, variety, grower,

...

100 apples

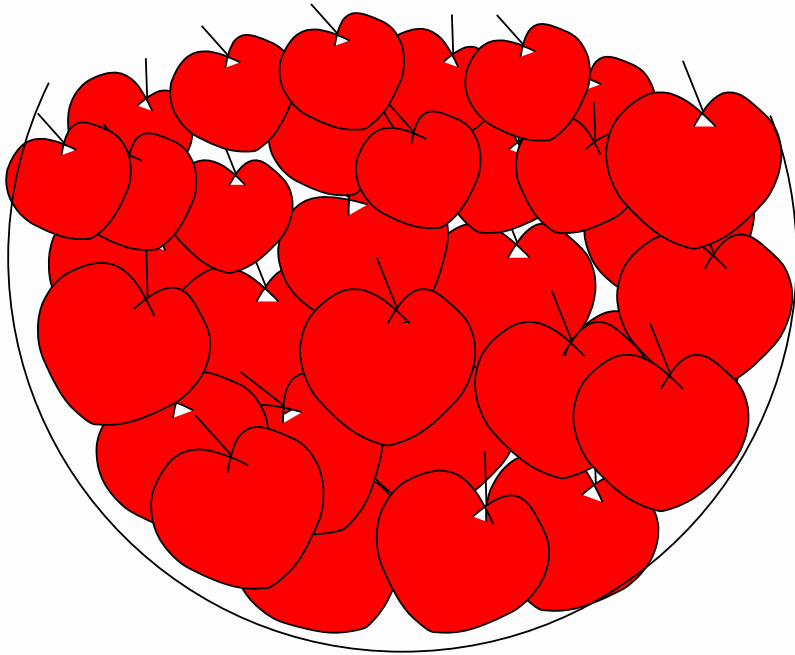
(55 sweet + 45 bitter)



Rule RED \rightarrow SWEET ($Y \rightarrow A$)

$$P(A|Y) = 0.92, P(\neg A|\neg Y) = 1.0$$
$$\delta = 0.22, \gamma = 1.67$$

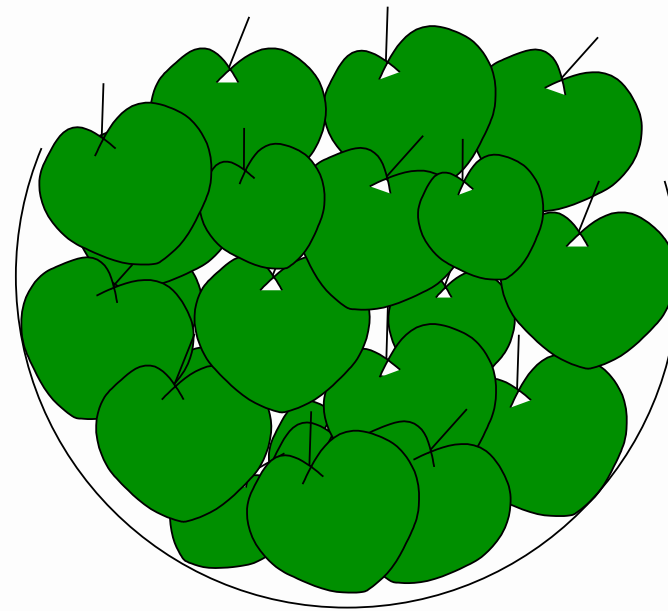
A =sweet, $\neg A$ =bitter
 Y =red, $\neg Y$ =green



Basket 1

60 red apples

(55 sweet)



Basket 2

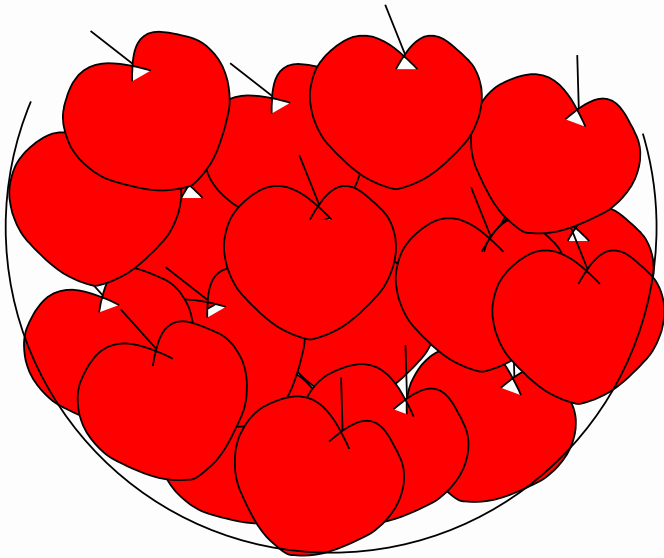
40 green apples

(all bitter)

Rule RED and BIG \rightarrow SWEET ($X \rightarrow A$)

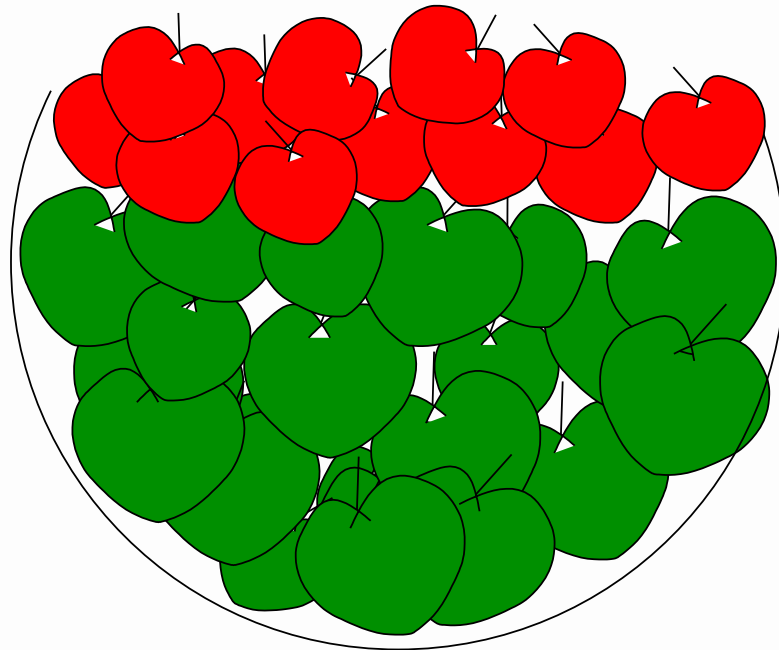
$$P(A|X) = 1.0, P(\neg A|\neg X) = 0.75$$
$$\delta = 0.18, \gamma = 1.82$$

$$X = (\text{red} \wedge \text{big})$$
$$\neg X = (\text{green} \vee \text{small})$$



Basket 1

40 large red apples
(all sweet)



Basket 2

40 green + 20 small red apples
(45 bitter)

When the value-based interpretation could be useful? Example

D =disease, X =allele combination

$P(X)$ small and $P(D|X) = 1.0$

$\Rightarrow \gamma(X, D) = P(D)^{-1}$ can be **large**

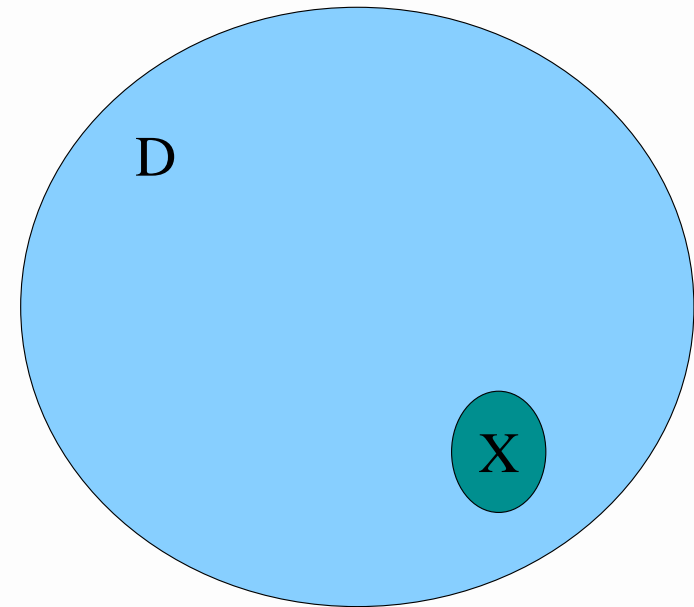
$P(D|\neg X) \approx P(D)$

$P(\neg D|\neg X) \approx P(\neg D)$

$\Rightarrow \delta(X, D) = P(X)P(\neg D)$ **small**.

Now dependency strong in the value-based but weak in the variable-based interpretation!

(Usually, **variable-based** dependencies tend to be more reliable)



Part I Contents

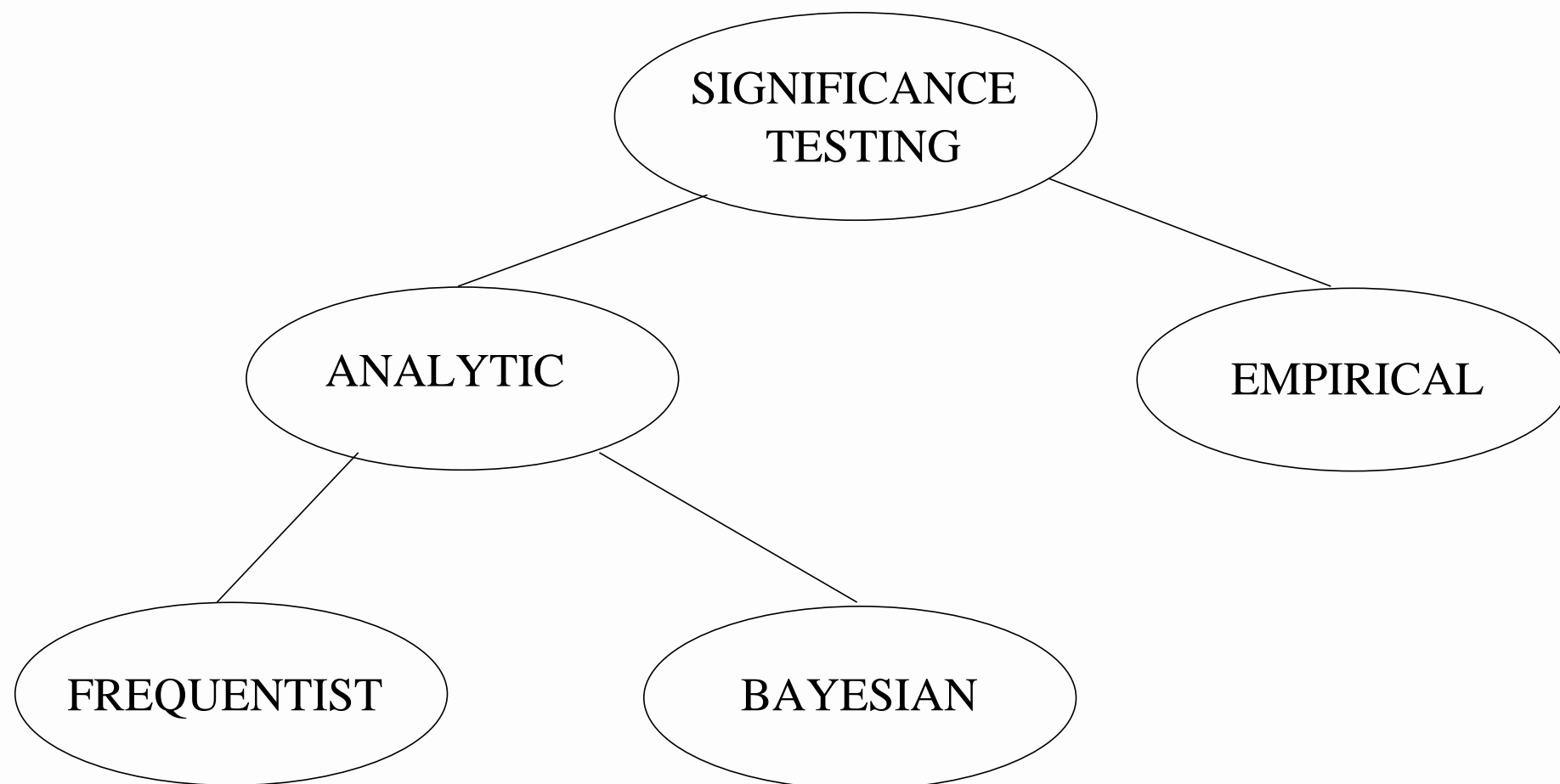
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3. *Statistical significance of $X \rightarrow A$*

What is the probability of the observed or a stronger dependency, if X and A were independent? If small probability, then $X \rightarrow A$ likely genuine (not due to chance).

- Significant $X \rightarrow A$ is likely to hold in future (in similar data sets)
- How to estimate the probability??
- How small the probability should be?
 - Fisherian vs. Neyman-Pearsonian schools
 - multiple testing problem

3.1 Main approaches



different schools

different sampling models

Analytic approaches

H_0 : X and A independent (null hypothesis)

H_1 : X and A positively dependent (research hypothesis)

- Frequentist: Calculate

$$p = P(\text{observed or stronger dependency} | H_0)$$

- Bayesian:

- (i) Set $P(H_0)$ and $P(H_1)$

- (ii) Calculate $P(\text{observed or stronger dependency} | H_0)$ and $P(\text{observed or stronger dependency} | H_1)$

- (iii) Derive (with Bayes' rule)

- $P(H_0 | \text{observed or stronger dependency})$ and $P(H_1 | \text{observed or stronger dependency})$

Analytic approaches: pros and cons

- + p -values relatively fast to calculate
- + can be used as search criteria
- How to define the distribution under H_0 ? (assumptions)
- If data not representative, the discoveries cannot be generalized to the whole population
 - describe only the sample data or other similar samples
 - random samples not always possible (infinite population)

Note: Differences between Fisherian vs. Neyman-Pearsonian schools

- significance testing vs. hypothesis testing
- role of nominal p -values (thresholds 0.05, 0.01)
- many textbooks represent a hybrid approach

→ see Hubbard & Bayarri

Empirical approach (randomization testing)

Generate random data sets according to H_0 and test how many of them contain the observed or stronger dependency $X \rightarrow A$.

- (i) Fix a permutation scheme (how to express H_0 + which properties of the original data should hold)
- (ii) Generate a random subset $\{d_1, \dots, d_b\}$ of all possible permutations
- (iii)

$$p = \frac{|\{d_i | \text{contains observed or stronger dependency}\}|}{b}$$

Empirical approach: pros and cons

- + no assumptions on any underlying parametric distribution
- + can test null hypotheses for which no closed form test exists
- + offers an approach to multiple testing problem → Later
- + data doesn't have to be a random sample
→ discoveries hold for the whole population ...
- ... **defined by the permutation scheme**
- often not clear (but critical), how to permute data!
- computationally heavy (*b*: efficiency vs. quality trade-off)
- How to apply during search??

Note: Randomization test vs. Fisher's exact test

When testing significance of $X \rightarrow A$

- a natural permutation scheme fixes $N = n$, $N_X = fr(X)$, $N_A = fr(A)$
- randomization test generates some random contingency tables with these constraints
- full permutation test = Fisher's exact test studies all contingency tables
 - faster to compute (analytically)
 - produces more reliable results

⇒ No need for randomization tests, here!

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 - 3.2 **Sampling models**
 - variable-based
 - value-based
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3.2 Sampling models

= defining the distribution under H_0

← What do we assume fixed?

- Variable-based dependencies: classical sampling models (Statistics)
- Value-based dependencies: several suggestions (Data mining)

Basic idea

Given a sampling model \mathcal{M}

\mathcal{T} = set of all possible contingency tables.

1. Define probability $P(T_i|\mathcal{M})$ for contingency tables $T_i \in \mathcal{T}$
2. Define an **extremeness relation** $T_i \geq T_j$
 - T_i contains at least as strong dependency $X \rightarrow A$ as T_j does
 - depends on the strength measure, e.g. δ (var-based) or γ (val-based)
3. Calculate $p = \sum_{T_i \geq T_0} P(T_i|\mathcal{M})$
(T_0 =our table)

Sampling models for variable-based dependencies

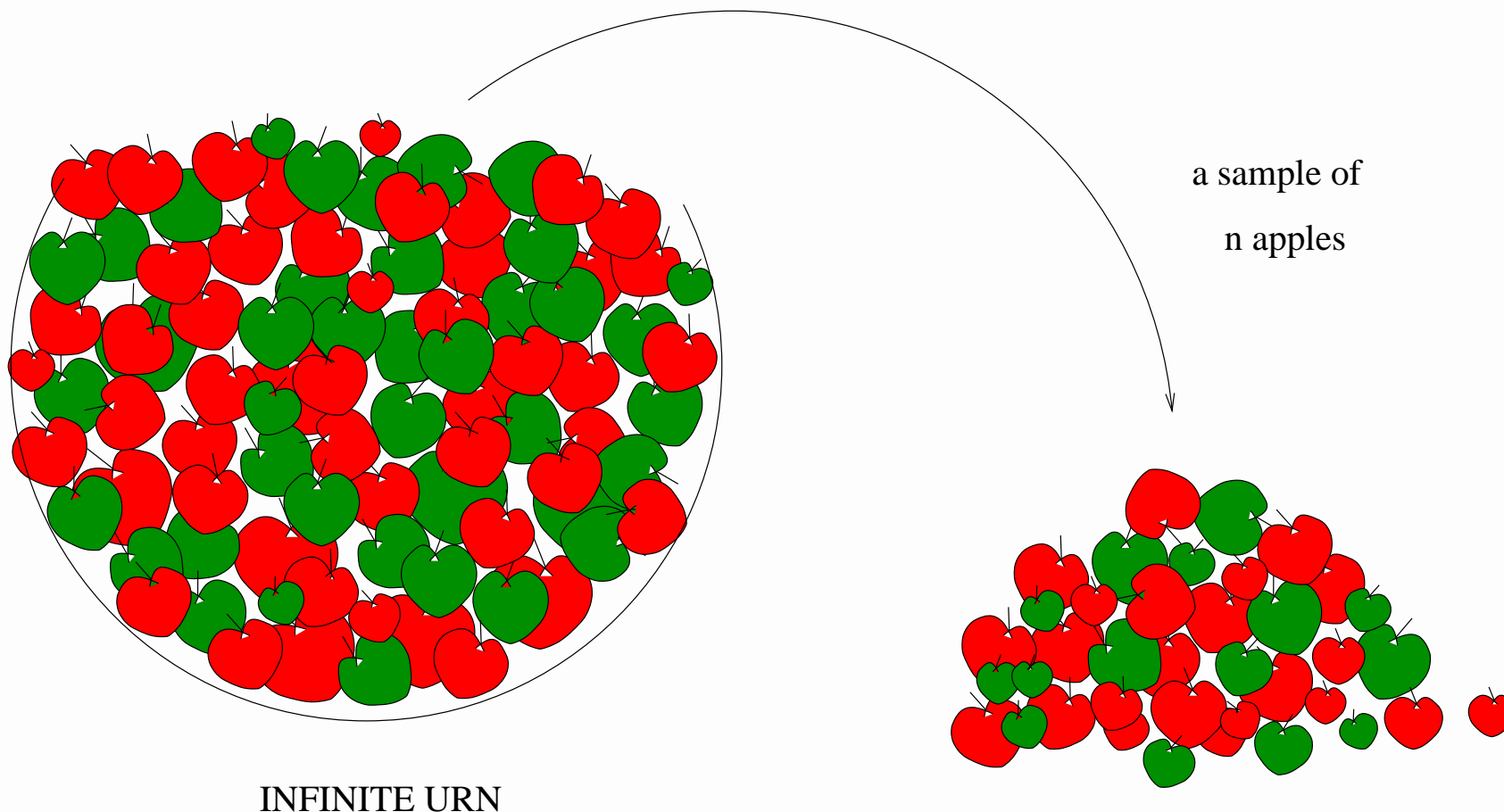
3 basic models:

1. Multinomial ($N = n$ fixed)
2. Double binomial ($N = n, N_X = fr(X)$ fixed)
3. Hypergeometric (\rightarrow Fisher's exact test)
($N = n, N_A = fr(A), N_X = fr(X)$ fixed)

+ asymptotic measures (like χ^2)

Multinomial model

Independence assumption: In the infinite urn, $p_{XA} = p_X p_A$.
(p_{XA} =probability of red sweet apples)



Multinomial model

T_i is defined by random variables $N_{XA}, N_{X\bar{A}}, N_{\bar{X}A}, N_{\bar{X}\bar{A}}$

$$P(N_{XA}, N_{X\bar{A}}, N_{\bar{X}A}, N_{\bar{X}\bar{A}} | n, p_X, p_A) = \binom{n}{N_{XA}, N_{X\bar{A}}, N_{\bar{X}A}, N_{\bar{X}\bar{A}}} p_X^{N_X} (1 - p_X)^{n - N_X} p_A^{N_A} (1 - p_A)^{n - N_A}.$$

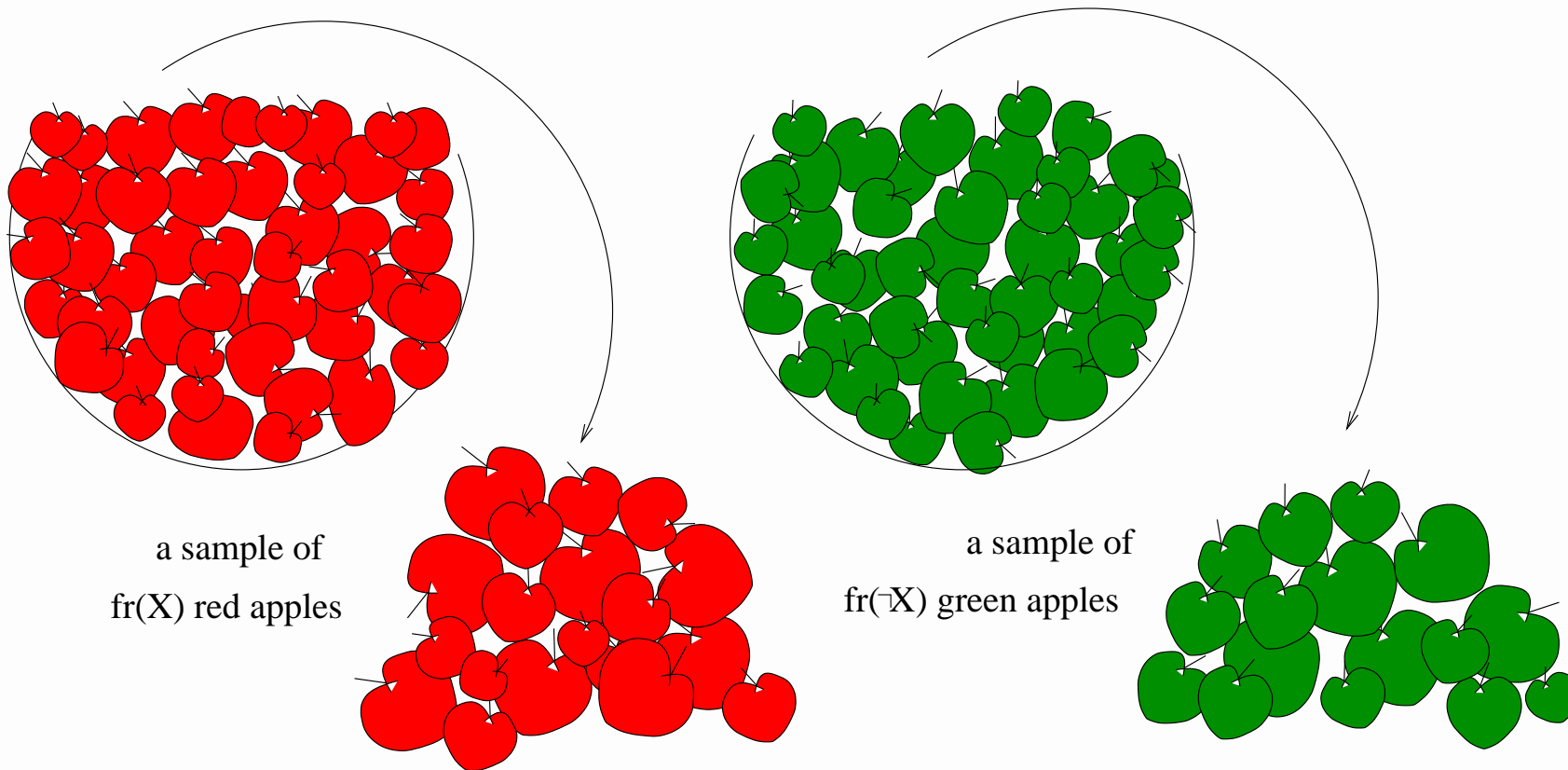
$$p = \sum_{T_i \geq T_0} P(N_{XA}, N_{X\bar{A}}, N_{\bar{X}A}, N_{\bar{X}\bar{A}} | n, p_X, p_A)$$

- p_X and p_A can be estimated from the data

Double binomial model

Independence assumption: $p_{A|X} = p_A = p_{A|\neg X}$

TWO INFINITE URNS:



Double binomial model

Probability of red sweet apples:

$$P(N_{XA}|fr(X), p_A) = \binom{fr(X)}{N_{XA}} p_A^{N_{XA}} (1 - p_A)^{fr(X) - N_{XA}}$$

Probability of green sweet apples:

$$P(N_{\neg XA}|fr(\neg X), p_A) = \binom{fr(\neg X)}{N_{\neg XA}} p_A^{N_{\neg XA}} (1 - p_A)^{fr(\neg X) - N_{\neg XA}}$$

Double binomial model

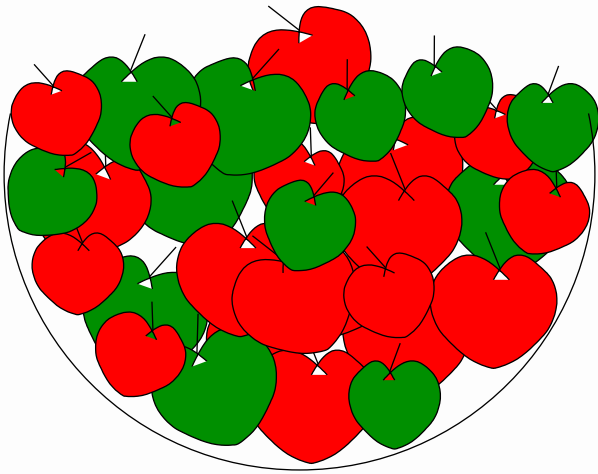
T_i is defined by variables N_{XA} and $N_{\neg XA}$.

$$P(N_{XA}, N_{\neg XA} | n, fr(X), fr(\neg X), p_A) = \binom{fr(X)}{N_{XA}} \binom{fr(\neg X)}{N_{\neg XA}} p_A^{N_A} (1 - p_A)^{n - N_A}$$

$$p = \sum_{T_i \geq T_0} P(N_{XA}, N_{\neg XA} | n, fr(X), fr(\neg X), p_A)$$

Hypergeometric model (Fisher's exact test)

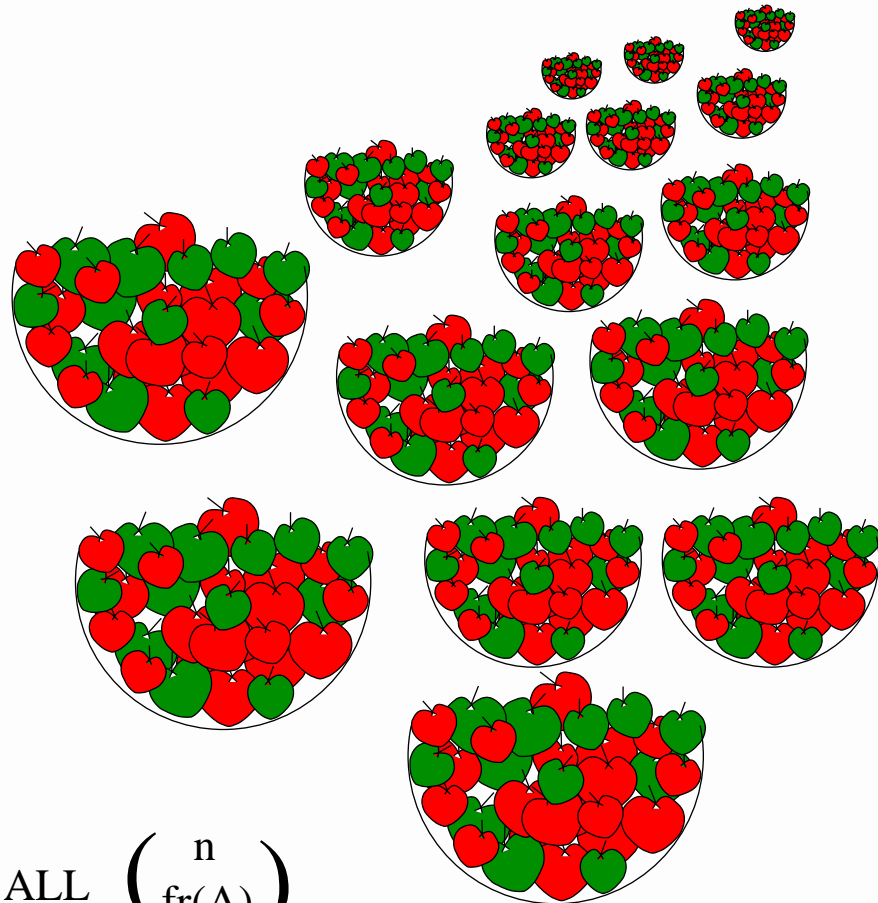
How many other similar urns have
at least as strong dependency as ours?



OUR URN n apples

$\text{fr}(A)$ sweet + $\text{fr}(\neg A)$ bitter

$\text{fr}(X)$ red + $\text{fr}(\neg X)$ green



ALL $\binom{n}{\text{fr}(A)}$

SIMILAR URNS

Like in a full permutation test

		X						$\neg X$			
		1	2	3	4	5	6	7	8	9	10
urn2	urn1	A	A	A	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$
		A	A	$\neg A$	A	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$
		A	A	$\neg A$	$\neg A$	A	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$
		•						•			
		•						•			
		•						•			
urn120		$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	$\neg A$	A	A	A

$n=10$

$\text{fr}(X)=6$

$\text{fr}(A)=3$

Hypergeometric model (Fisher's exact test)

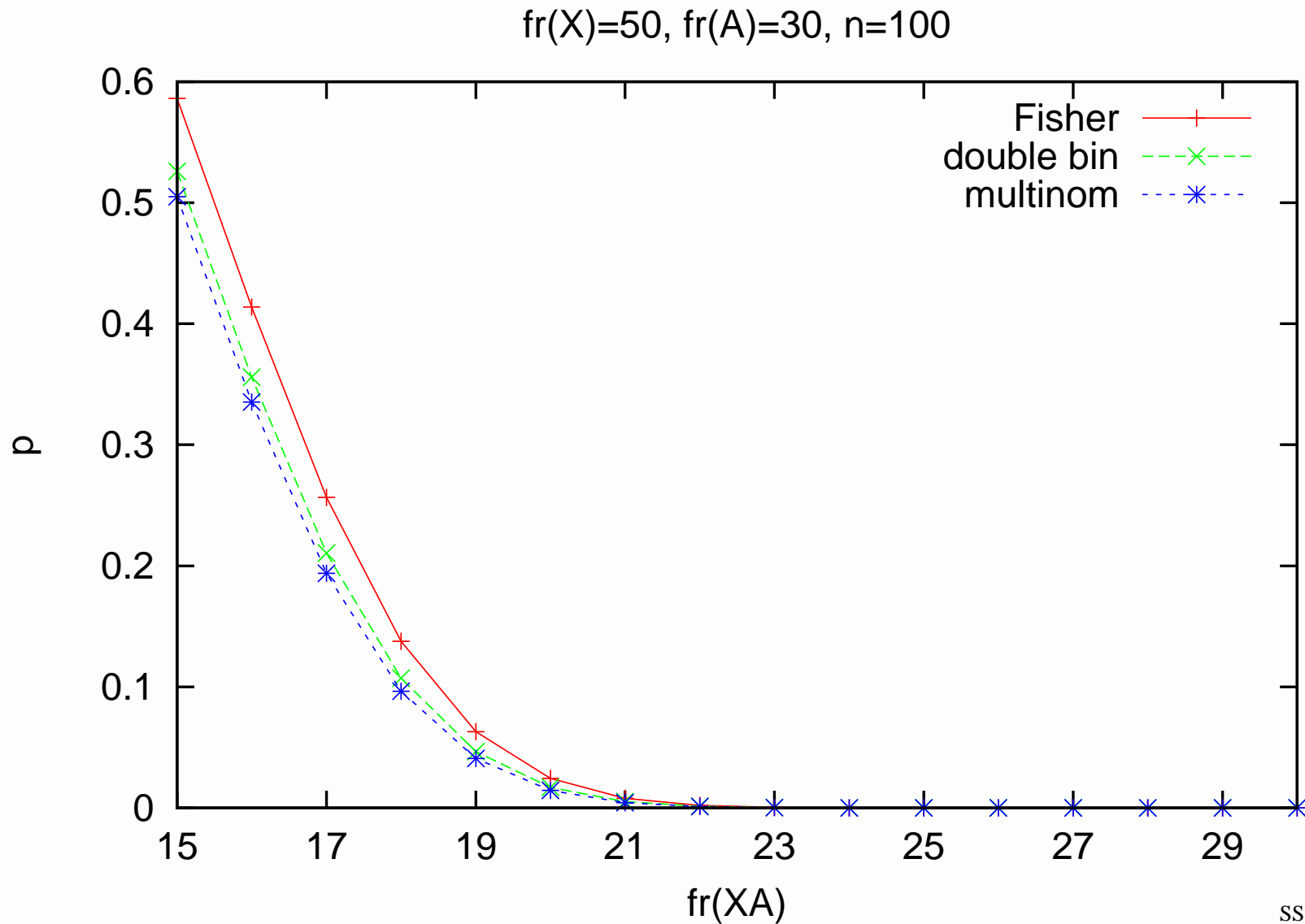
The number of all possible similar urns (fixed $N = n$, $N_X = fr(X)$ and $N_A = fr(A)$) is

$$\sum_{i=0}^{fr(A)} \binom{fr(X)}{i} \binom{fr(\neg X)}{fr(A) - i} = \binom{n}{fr(A)}$$

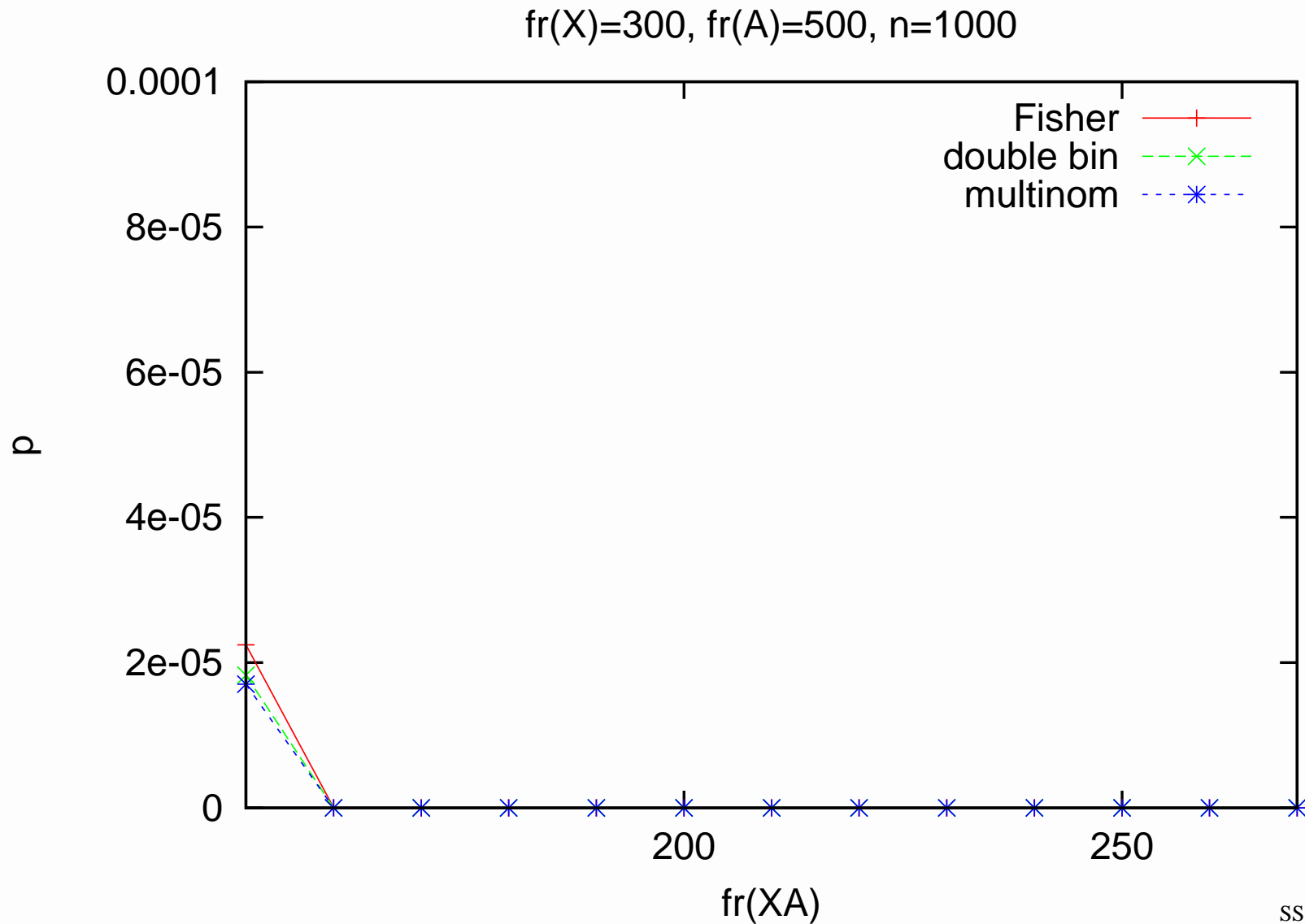
Now $(T_i \geq T_0) \equiv (N_{XA} \geq fr(XA))$. Easy!

$$p_F = \sum_{i=0}^{\infty} \frac{\binom{fr(X)}{fr(XA)+i} \binom{fr(\neg X)}{fr(\neg X \neg A)+i}}{\binom{n}{fr(A)}}$$

Example: Comparison of p -values



Example: Comparison of p -values



Example: Comparison of p -values

fr_{XA}	multi-nomial	double binomial	Fisher (hyperg.)
180	1.7e-05	1.8e-05	2.2e-05
200	2.3e-12	2.2e-12	3.0e-12
220	1.4e-22	7.3e-23	1.1e-22
240	2.9e-36	3.0e-37	4.4e-37
260	1.5e-53	4.2e-56	3.5e-56
280	1.3e-74	2.9e-80	1.6e-81
300	9.3e-100	3.5e-111	2.5e-119

Asymptotic measures

Idea: p -values are estimated indirectly

1. Select some “nicely behaving” measure M
 - e.g. M follows **asymptotically** the normal or the χ^2 distribution
2. Estimate $P(M \geq val)$, where $M = val$ in our data
 - Easy! (look at statistical tables)
 - But the accuracy can be poor

The χ^2 -measure

$$\begin{aligned}\chi^2 &= \sum_{i=0}^1 \sum_{j=0}^1 \frac{n(P(X = i, A = j) - P(X = i)P(A = j))^2}{P(X = i)P(A = j)} \\ &= \frac{n(P(X, A) - P(X)P(A))^2}{P(X)P(\neg X)P(A)P(\neg A)} = \frac{n\delta^2}{P(X)P(\neg X)P(A)P(\neg A)}\end{aligned}$$

- very sensitive to underlying assumptions!
- all $P(X = i)P(A = j)$ should be sufficiently large
- the corresponding hypergeometric distribution shouldn't be too skewed

Mutual information

$MI =$

$$\log \frac{P(XA)^{P(XA)} P(X\neg A)^{P(X\neg A)} P(\neg XA)^{P(\neg XA)} P(\neg X\neg A)^{P(\neg X\neg A)}}{P(X)^{P(X)} P(\neg X)^{P(\neg X)} P(A)^{P(A)} P(\neg A)^{P(\neg A)}}$$

- $2n \cdot MI = \log$ likelihood ratio
- follows asymptotically the χ^2 -distribution
- usually gives more reliable results than the χ^2 -measure

Comparison: Sampling models for variable-based dependencies

- Multinomial: impractical but useful for theoretical results
- Double binomial: **not exchangeable**
 $p(X \rightarrow A) \neq p(A \rightarrow X)$ (in general)
- Hypergeometric (Fisher's exact test): recommended, enables efficient search, reliable results
- Asymptotic: often sensitive to underlying assumptions
 - χ^2 very sensitive, not recommended
 - MI reliable, enables efficient search, approximates p_F

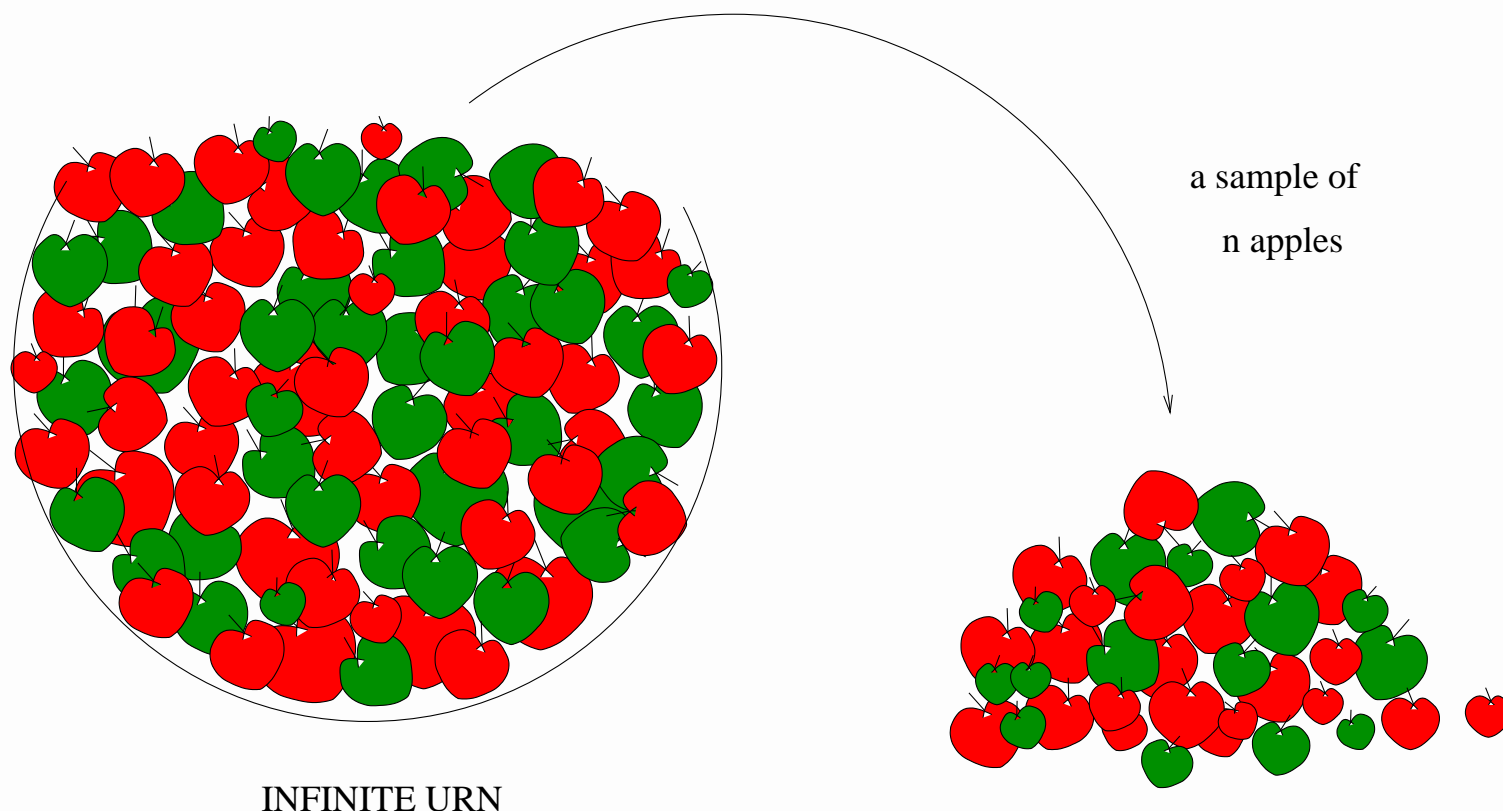
Sampling models for value-based dependencies

Main choices:

1. Classical sampling models but with a different extremeness relation
 - use lift γ to define a stronger dependency
 - Multinomial and Double binomial: can differ much from var-based
 - Hypergeometric: leads to Fisher's exact test, again!
2. Binomial models + corresponding asymptotic measures

Binomial model 1 (classical binomial test)

Probability of sweet red apples is $p_{XA} = p_X p_A$. If a random sample of n apples is taken, what is the probability to get $fr(XA)$ sweet red apples and $n - fr(XA)$ green or bitter apples?



Binomial model 1 (classical binomial test)

Probability of getting exactly N_{XA} sweet red apples and $n - N_{XA}$ green or bitter apples is

$$p(N_{XA}|n, p_{XA}) = \binom{n}{N_{XA}} (p_{XA})^{N_{XA}} (1 - p_{XA})^{n - N_{XA}}$$

$$p(N_{XA} \geq fr(XA)|n, p_{XA}) = \sum_{i=fr(XA)}^n \binom{n}{i} (p_{XA})^i (1 - p_{XA})^{n-i}$$

(or $i = fr(XA), \dots, \min\{fr(X), fr(A)\}$)

- Use estimate $p_{XA} = P(X)P(A)$
- Note: N_X and N_A unfixed

Corresponding asymptotic measure

z-score:

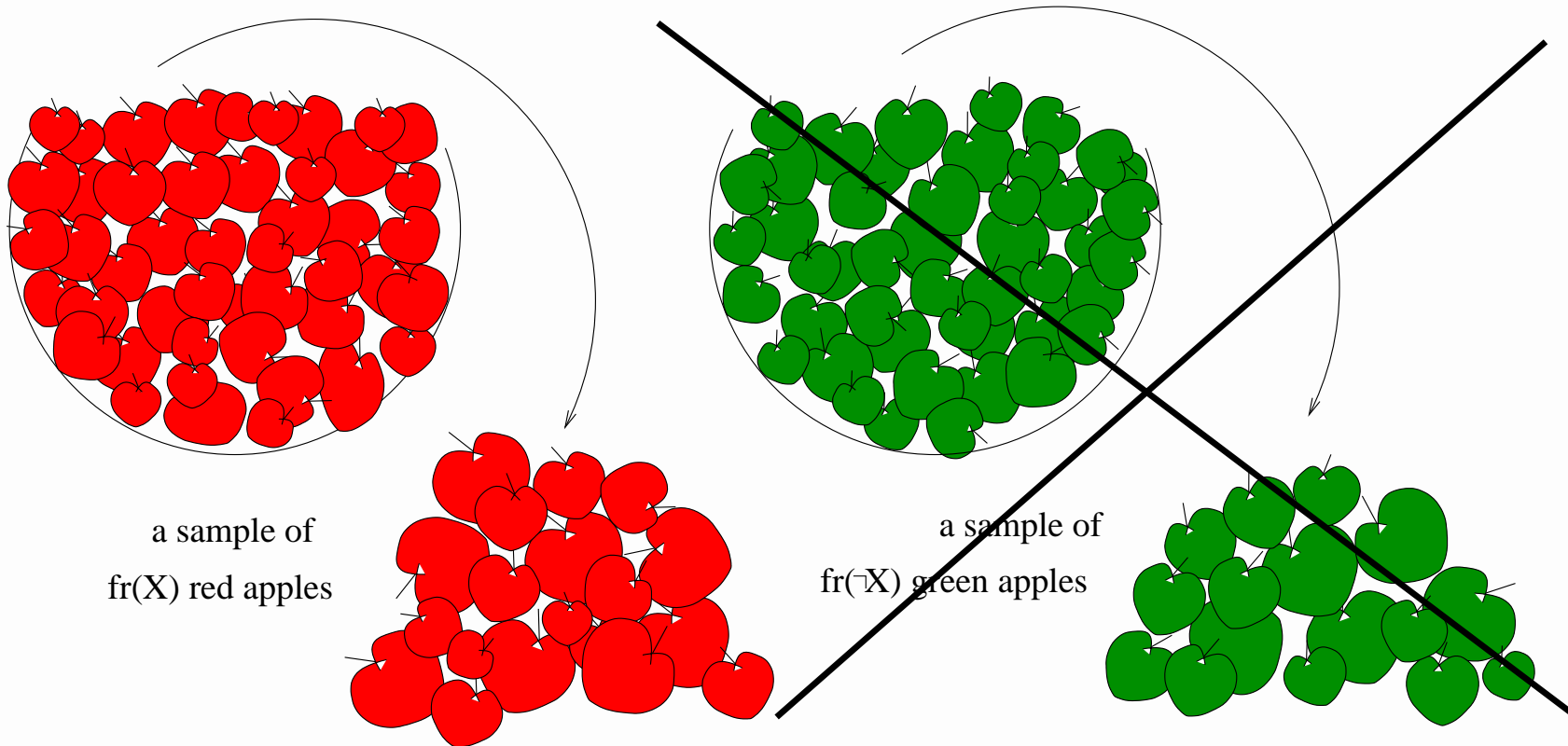
$$\begin{aligned} z_1(X \rightarrow A) &= \frac{fr(X, A) - \mu}{\sigma} = \frac{fr(X, A) - nP(X)P(A)}{\sqrt{nP(X)P(A)(1 - P(X)P(A))}} \\ &= \frac{\sqrt{n}\delta(X, A)}{\sqrt{P(X)P(A)(1 - P(X)P(A))}} = \frac{\sqrt{nP(XA)}(\gamma(X, A) - 1)}{\sqrt{\gamma(X, A) - P(X, A)}}. \end{aligned}$$

- follows asymptotically the normal distribution

Binomial model 2 (suggested in DM)

Like the double binomial model, but forget the other urn!

CONSIDER ONE FROM TWO INFINITE URNS:



Binomial model 2

$$p(N_{XA} \geq fr(XA) | fr(X), P(A)) = \sum_{i=fr(XA)}^{fr(X)} \binom{fr(X)}{i} P(A)^i P(\neg A)^{fr(X)-i}$$

Corresponding z -score:

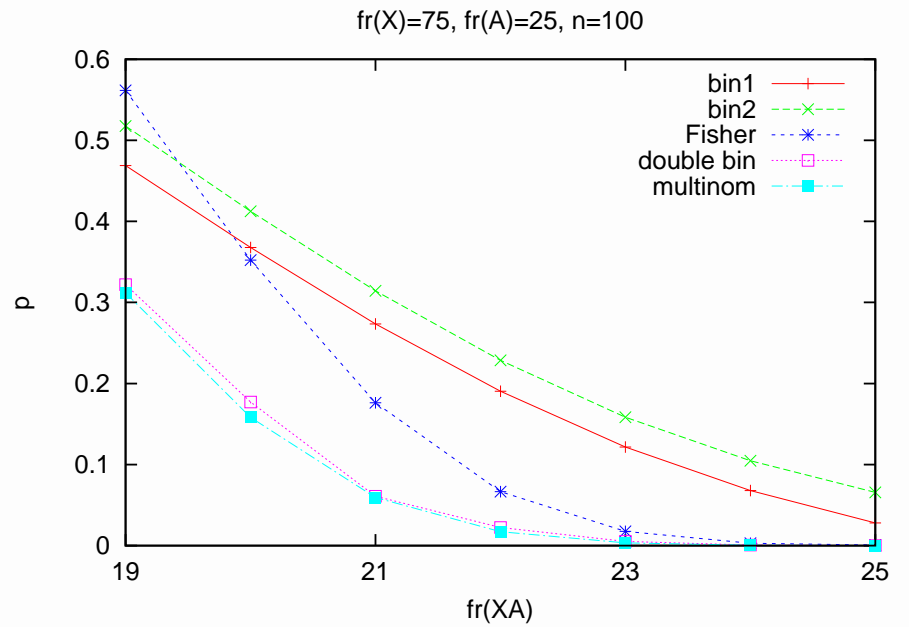
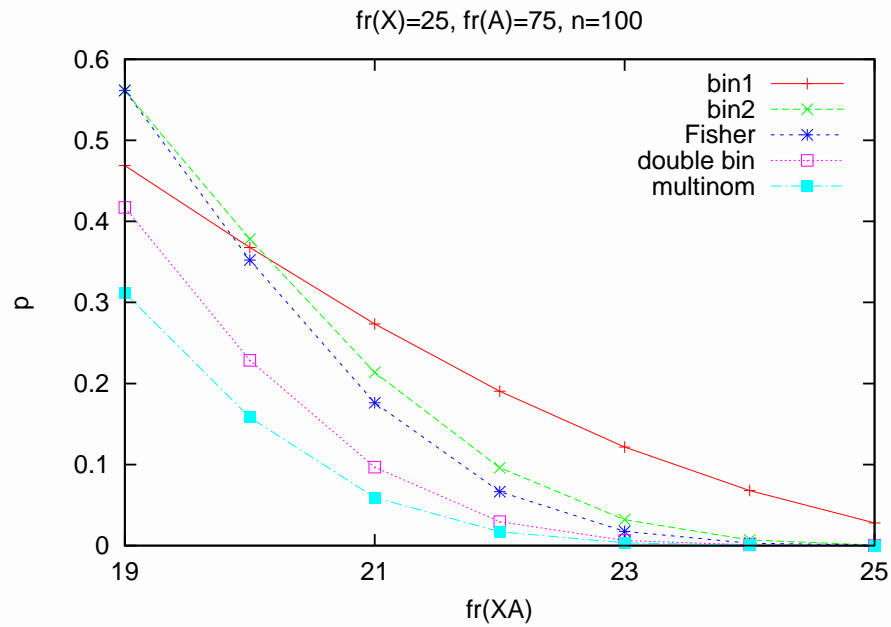
$$\begin{aligned} z_2 &= \frac{fr(XA) - \mu}{\sigma} = \frac{fr(XA) - fr(X)P(A)}{\sqrt{fr(X)P(A)P(\neg A)}} \\ &= \frac{\sqrt{n}\delta(X, A)}{\sqrt{P(X)P(A)P(\neg A)}} = \frac{\sqrt{fr(X)}(P(A|X) - P(A))}{\sqrt{P(A)P(\neg A)}} \end{aligned}$$

J-measure

\approx one urn version of *MI*

$$J = P(XA) \log \frac{P(XA)}{P(X)P(A)} + P(X\neg A) \log \frac{P(X\neg A)}{P(X)P(\neg A)}$$

Example: Comparison of p -values



Comparison: Sampling models for value-based dependencies

- Multinomial, Hypergeometric, classical Binomial + its z -score: $p(X \rightarrow A) = P(A \rightarrow X)$
- Double binomial, alternative Binomial + its z -score: $p(X \rightarrow A) \neq P(A \rightarrow X)$ (in general)
- The alternative Binomial, its z -score and J can disagree with the other measures (only the X -urn vs. whole data)
- z -score easy to integrate into search, but may be unreliable for infrequent patterns \rightarrow (classical) Binomial test in post-pruning improves quality!

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3.3 Multiple testing problem

The more patterns we test, the more spurious patterns we are likely to accept.

- If threshold $\alpha = 0.05$, there is 5% probability that a spurious dependency passes the test.
- If we test 10 000 rules, we are likely to accept 500 spurious rules!

Solutions to Multiple testing problem

1. **Direct adjustment approach:** adjust α (stricter thresholds)
 - easiest to integrate into the search
2. **Holdout approach:** Save part of the data for testing → Webb
3. **Randomization test approaches:** Estimate the overall significance of all discoveries or adjust the individual p -values empirically
→ e.g. Gionis et al., Hanhijärvi et al.

Contingency table for m significance tests

	spurious rule H_0 true	genuine rule H_1 true	All
declared significant	V false positives	S true positives	R
declared insignificant	U true negatives	T false negatives	$m - R$
All	m_0	$m - m_0$	m

Direct adjustment: Two approaches

(i) Control **familywise error rate** = probability of accepting at least one false discovery

$$FWER = P(V \geq 1)$$

(ii) Control **false discovery rate** = expected proportion of false discoveries

$$FDR = E \left[\frac{V}{R} \right]$$

	spurious rule	genuine rule	All
decl. sign.	V	S	R
decl. insign	U	T	$m - R$
All	m_0	$m - m_0$	m

(i) Control familywise error rate FWER

Decide $\alpha^* = FWER$ and calculate a new stricter threshold α .

- If tests are mutually independent: $\alpha^* = 1 - (1 - \alpha)^m$
 \Rightarrow Šidák correction: $\alpha = 1 - (1 - \alpha^*)^{\frac{1}{m}}$
- If they are not independent: $\alpha^* \leq m \cdot \alpha$
 \Rightarrow **Bonferroni correction**: $\alpha = \frac{\alpha^*}{m}$
- conservative (may lose genuine discoveries)
- How to estimate m ?
 - may be explicit and implicit testing during search
- **Holm-Bonferroni** method more powerful
 - but less suitable for the search (all p -values should be known, first)

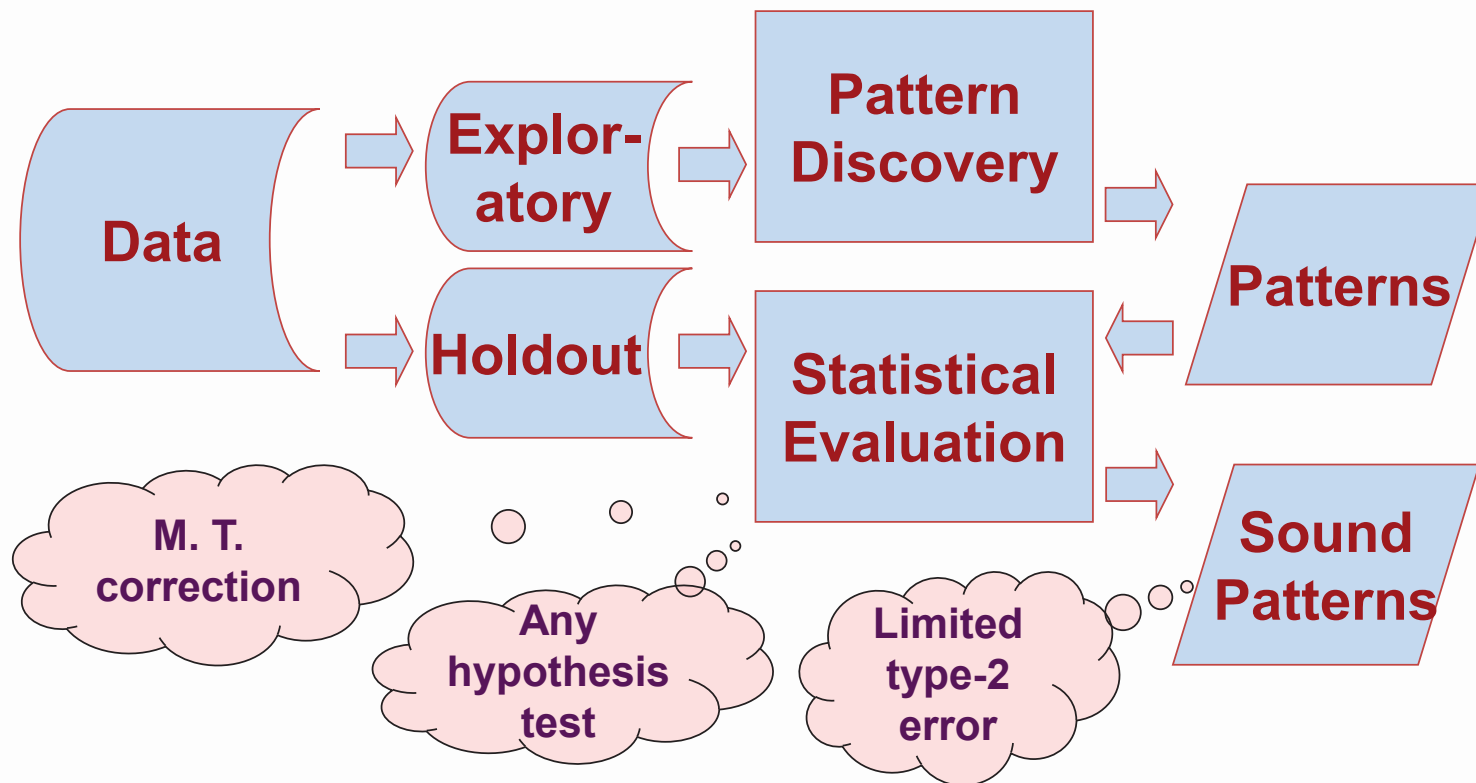
(ii) Control false discovery rate FDR

Benjamini–Hochberg–Yekutieli procedure

1. Decide $q = FDR$
2. Order patterns r_i by their p -values
Result r_1, \dots, r_m such that $p_1 \leq \dots \leq p_m$
3. Search the largest k such that $p_k \leq \frac{k \cdot q}{m \cdot c(m)}$
 - if tests mutually independent or positively dependent, $c(m) = 1$
 - otherwise $c(m) = \sum_{i=1}^m \frac{1}{i} \approx \ln(m) + 0.58$
4. Save patterns r_1, \dots, r_k (as significant) and reject r_{k+1}, \dots, r_m

Hold-out approach

Powerful because m is quite small!



Randomization test approaches

1. Estimate the overall significance of discoveries at once
 - e.g. What is the probability to find K_0 dependency rules whose strength is at least \min_M ?
 - Empirical p -value

$$p_{emp} = \frac{|\{d_i \mid K_i \geq K_0\}| + 1}{b + 1}$$

d_0 original set

d_1, \dots, d_b random sets

K_1, \dots, K_b numbers of discovered patterns from set d_i

→ Gionis et al.

Randomization test approaches (cont.)

2. Use randomization tests to correct individual p -values
 - e.g., How many sets contained better rules than $X \rightarrow A$?

$$p' = \frac{|\{d_i | (S_i \neq \emptyset) \wedge (\min p(Y \rightarrow B | d_i) \leq p(X \rightarrow A | d_0))\}|}{b + 1},$$

d_0 original set

d_1, \dots, d_b random sets

S_i =set of patterns returned from set d_i

→ Hanhijärvi

Randomization test approaches

- + dependencies between patterns not a problem → more powerful control over *FWER*
- + one can impose extra constraints (e.g. that a certain pattern holds with a given frequency and confidence)
- most techniques assume *subset pivotality* \approx the complete hypothesis and all subsets of true null hypotheses have the same distribution of the measure statistic

Remember also points mentioned in the single hypothesis testing

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4. Redundancy and significance of improvement

When $X \rightarrow A$ is redundant with respect to $Y \rightarrow A$ ($Y \subsetneq X$)? Improves it significantly?

Examples of redundant dependency rules:

- *smoking, coffee* \rightarrow *atherosclerosis*
coffee has no effect on *smoking* \rightarrow *atherosclerosis*
- *high cholesterol, sports* \rightarrow *atherosclerosis*
sports makes the dependency only weaker
- *male, male pattern baldness* \rightarrow *atherosclerosis*
adding *male* hardly any significant improvement

Redundancy and significance of improvement

- Value-based: $X \rightarrow A$ is **productive** if $P(A|X) > P(A|Y)$ for all $Y \subsetneq X$
- Variable-based: $X \rightarrow A$ is **redundant** if there is $Y \subsetneq X$ such that $M(Y \rightarrow A)$ is better than $M(X \rightarrow A)$ with the **given goodness measure M**
 $\Leftrightarrow X \rightarrow A$ is **non-redundant** if for all $Y \subsetneq X$ $M(X \rightarrow A)$ is better than $M(Y \rightarrow A)$
- When the improvement is significant?

Value-based: Significance of productivity

Hypergeometric model:

$$p(YQ \rightarrow A | Y \rightarrow A) = \frac{\sum_i \binom{fr(YQ)}{fr(YQA)+i} \binom{fr(Y \neg Q)}{fr(Y \neg QA)-i}}{\binom{fr(Y)}{fr(YA)}}$$

\approx probability of the observed or a stronger conditional dependency $Q \rightarrow A$, given Y , in a **value-based** model.

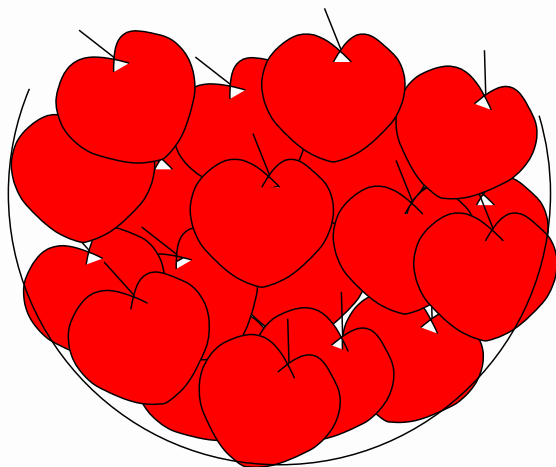
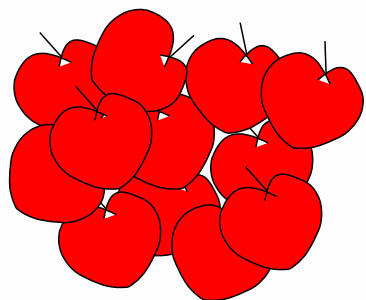
- also asymptotic measures (χ^2 , MI)

Apple problem: value-based

$$p(YQ \rightarrow A | Y \rightarrow A) = 0.0029$$

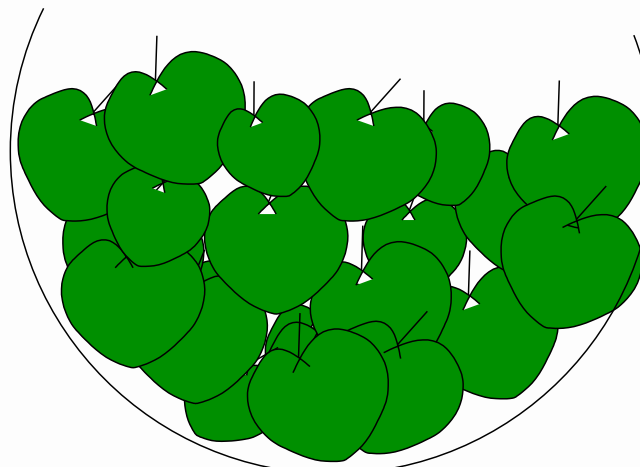
$Y=\text{red}, Q=\text{large}$

20 small
red apples
(15 sweet)



Basket 1

40 large red apples
(all sweet)

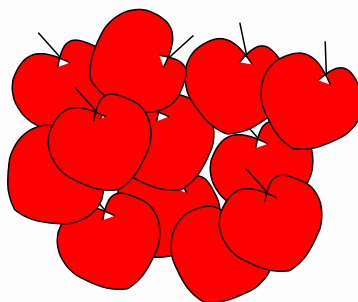


Basket 2

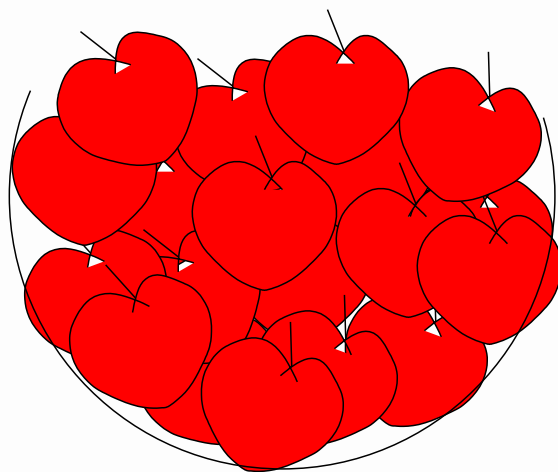
40 green apples
(all bitter)

Apple problem: variable-based?

$$p(\neg Y \rightarrow \neg A | \neg(YQ) \rightarrow \neg A) = 2.9e - 10 \ll 0.0029$$

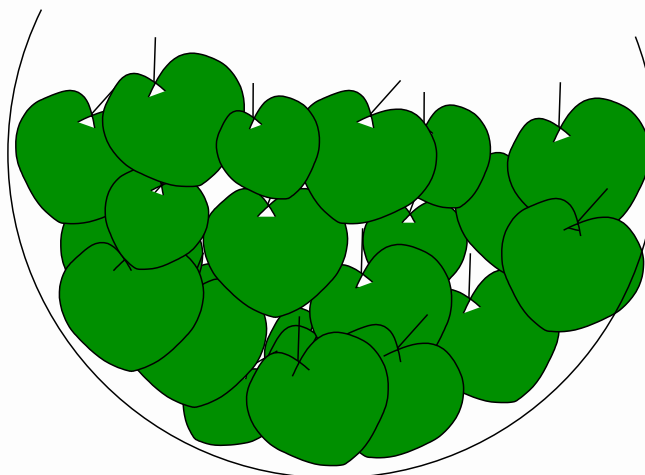


20 small
red apples
(15 sweet)



Basket 1

40 large red apples
(all sweet)



Basket 2

40 green apples
(all bitter)

Observation

$$\frac{p(\neg Y \rightarrow \neg A | \neg(YQ) \rightarrow \neg A)}{p(YQ \rightarrow A | Y \rightarrow A)} \approx \frac{p_F(Y \rightarrow A)}{p_F(YQ \rightarrow A)}$$

Thesis: Comparing productivity of $YQ \rightarrow A$ and $\neg Y \rightarrow \neg A \equiv$ redundancy test with $M = p_F$!

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5. Search strategies

1. Search for the strongest rules (with γ , δ etc.) that pass the significance test for productivity
→ MagnumOpus (Webb 2005)
2. Search for the most significant non-redundant rules (with Fisher's p etc.)
→ Kingfisher (Hämäläinen 2012)
3. Search for frequent sets, construct association rules, prune with statistical measures, and filter non-redundant rules??
 - No way!
 - closed sets? → redundancy problem
 - their minimal generators?

Main problem: non-monotonicity of statistical dependence

- $AB \rightarrow C$ can express a significant dependency even if A and C as well as B and C mutually independent
- In the worst case, the only significant dependency involves all attributes $A_1 \dots A_k$ (e.g. $A_1 \dots A_{k-1} \rightarrow A_k$)

⇒ 1) A greedy heuristic does not work!

⇒ 2) Studying only simplest dependency rules does not reveal everything!

ABCA1-R219K \rightarrow \neg alzheimer

ABCA1-R219K, female \rightarrow alzheimer

End of Part I

Questions?

