Statistical Methods in Particle Physics

1. Basic Concepts

Heidelberg University, WS 2020/21

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1.1 Introduction

Contents

- 1. Basics concepts
 - Probability
 - Mean, median, mode
 - Covariance and correlation
- 2. Probability distributions
- 3. Uncertainty
 - Statistical and systematic uncertainties
 - Propagation of uncertainties
 - Combination of uncorrelated measurements
- 4. Monte Carlo and numerical methods
 - Generation of random numbers
 - Monte Carlo integration
 - Applications in HE
- 5. Maximum likelihood estimation
 - Basics: consistency, bias, efficiency
 - Maximum likelihood method

- 6. Least squares
- 7. Goodness-of-fit and hypothesis testing
- 8. Confidence limits and intervals
 - Neyman construction
 - Feldman-Cousins confidence intervals
- 9. Machine learning
 - General Overview: machine learning, deep learning and all that
 - Neural Networks
 - Boosted Decision trees
- 10. Unfolding

"Bayes vs. frequentist"

Learning goals and required knowledge

This course is a natural follow-up to PEP4 for **Bachelor students** interested in Particle Physics. **Master students** are invited to attend this lecture in parallel or after the Particle Physics course.

Learning goals

- Get to know and apply the toolbox of statistical methods used in particle physics
- Understand error bars and confidence limits as reported in publications
- Solid understanding of maximum likelihood and least squares fits
- From measurement to message: which conclusion can you draw from your data (and which not)?
- Learn to apply machine learning methods

Required knowledge

- Basic understanding of experimental particle physics (as taught in the bachelor's course)
- Basic knowledge of python is helpful

Practical information (I)

- Website
 - https://uebungen.physik.uni-heidelberg.de/vorlesung/20202/1225
- Lecture
 - Flipped/inverted class room!
 - Links to slides and videos provided before Thursday meeting
 - Contact time on Thursdays:
 - Via Zoom
 - Questions / discussion, questions can be sent beforehand,
 e.g. through rocket.chat [room: "ws20-smipp"]) or email
 - Quizzes
 - Typical **no comprehensive repetition** of the contents of the lecture videos!
 - Exact time for Thursday meeting flexible, for example:
 - Thursdays, 16:00-17:00: time to study slides / videos
 - Thursdays, 17:00-17:30: Zoom-Meeting: discussion / quizzes
 - First Thursday meeting (5 Nov 2020) starts at 16:15

Practical information (II)

Tutorials

- Mondays, 16:00 17:45
- Zoom
- Weekly problem sheets, to be handed in on Thursday before 12:00
- See next slide for detailed schedule

Exam

- There will be a written exam at the end of the semester
- Refers to contents of lectures and exercises
- 60% of the points of the homework sheets required to be eligible to write the exam
- Date to be fixed

Schedule

Week	Tutorial Monday	Lecture Thursday	Exercise Hand in (12:00)	e Sheets Hand out (after L.)	
45: 2.11. – 8.11.	Intro, Python basic	Lecture 01		Sheet 01	
46: 9.11. – 15.11.	online exercises, Python adv.	Lecture 02	Sheet 01	Sheet 02	
47: 16.11. – 22.11.	Sheet 01	Lecture 03	Sheet 02	Sheet 03	
48: 23.11. – 29.11.	Sheet 02	Lecture 04	Sheet 03	Sheet 04	
49: 30.11. – 6.12.	Sheet 03	Lecture 05	Sheet 04	Sheet 05	
50: 7.12. – 13.12.	Sheet 04	Lecture 06	Sheet 05	Sheet 06	
51: 14.12 – 20.12.	Sheet 05	Lecture 07	Sheet 06	Sheet 07	
Xmas holidays: 3 weeks					
2: 11.1. – 17.1.	Sheet 06	Lecture 08	Sheet 07	Sheet 08	
3: 18.1. – 24.1.	Sheet 07	Lecture 09	Sheet 08	Sheet 09	
4: 25.1. – 31.1.	Sheet 08	Lecture 10	Sheet 09	Sheet 10	
5: 1.2. – 7.1.	Sheet 09	Lecture 11	Sheet 10		
6: 8.1 14.2.	Sheet 10	Lecture 12			
7: 15.1. – 21.1.			Study Week		
8: 22.1. – 28.1.	Exam week (date to be confirmed)				

Useful books

- G. Cowan, Statistical Data Analysis
- L. Lista, Statistical Methods for Data Analysis in Particle Physics
- Behnke, Kroeninger, Schott, Schoerner-Sadenius: Data Analysis in High Energy Physics: A Practical Guide to Statistical Methods
- R. Barlow, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences
- Bohm, Zech, Introduction to Statistics and Data Analysis for Physicist [available online]
- Blobel, Lohrmann: Statistische Methoden der Datenanalyse (in German), [free ebook]
- L. Lyons:

Statistics for Nuclear and Particle Physicists (Cambridge University Press)

- F. James, Statistical Methods in Experimental physics
- W. Metzger, Statistical Methods in Data Analysis [available online]

Further Material

- Glen Cowan: http://www.pp.rhul.ac.uk/~cowan/stat_course.html
- Scott Oser: http://www.phas.ubc.ca/~oser/p509/
- Terascale Statistics School: <u>https://indico.desy.de/indico/event/25594/other-view?view=standard</u>
- Particle Data Group reviews on Probability and Statistics
 - https://pdg.lbl.gov/2020/reviews/rpp2020-rev-probability.pdf
 - https://pdg.lbl.gov/2020/reviews/rpp2020-rev-statistics.pdf

Why bother with statistical methods?



Statistics: Draw reliable conclusions from data

In case of doubt: just get more data ...

Yes, but not always easy ...

A heavy Higgs boson? Peak disappeared with more

data ... [<u>link]</u>

Presentations by CMS and ATLAS, December 2015: https://indico.cern.ch/event/442432/

How knowledge is created?

Guess theory/model

- usually mathematical
- self-consistent
- simple explanations, few arbitrary parameters
- testable predictions

Perform experiment

- reject / modify theory in case of disagreement with data
- if theory requires too many adjustments it becomes unattractive

The advance of scientific knowledge is an evolutionary process



Karl Popper (1902–1994)

source: Wikipedia

Statistical methods are an important part of this process

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A look at other research fields

"Why Most Published Research Findings Are False":

Main thesis: large number, if not the majority, of published medical research papers contain results that cannot be replicated.

Reproducibility crisis:

Affects the social sciences and life sciences most severely (in particular psychology)



is characteristic of the field and ca

or searches for only one or a few

true relationships among thousands

and millions of hypotheses that may

bility of a relationship

vary a lot depending on whether the field targets highly likely relationships

Why Most Published Research Findings Are False ohn P. A. Ioannid

blished research findings are sometimes refuted by subsequent evidence, with ensuing confusion and disappointment, Refutation and controversy is seen across the range of esearch designs, from clinical trials and traditional epidemiological studies [1-3] to the most modern molecular research [4,5]. There is increasing concern that in modern research, fals

factors that influence this problem and some corollaries thereof. Modeling the Framework for False

Positive Findings Several methodologists have

As has been shown previou

robability that a research finding

is indeed true depends on the prior

obability of it being true (before

doing the study), the statistical power

ointed out [9-11] that the high be postulated. Let us also consider rate of nonzeplication flack of for computational simplicity. confirmation) of research discoveries circumscribed fields where either these is only one true relationship (among is a consequence of the convenient, many that can be hypothesized) or yet ill-founded strategy of claiming conclusive research findings solely on the power is similar to find any of the the basis of a single study assessed by several existing true relationships. The pre-study pr formal statistical significance, typically being true is R/(R + 1). The probabili for a p-value less than 0.05. Research of a study finding a true relationship is not most appropriately represented and summarized by p-values, but, reflects the power $1 - \beta$ (one minus unfortunately, there is a widespread the Type II error rate). The probability notion that medical research articles of claiming a relationship when none truly exists reflects the Type I error It can be proven that rate, o. Assuming that crelationships are being probed in the field, the most claimed research expected values of the 2 × 2 table are findings are false. given in Table 1. After a research

finding has been claimed based on achieving formal statistical significance. should be interpreted based only on pvalues. Research findings are defined the post-study probability that it is true is the positive predictive value, PPV. here as any relationship reaching The PPV is also the corr formal statistical significance, e.g. robability of what Wacholder et al effective interventions, informative have called the false positive report oredictors, risk factors, or association probability [10]. According to the 2 × 2 table, one gets PPV = $(1 - \beta)R/(R)$ 'Negative" research is also very useful. Negative" is actually a misnomer, and βR + α). A research finding is thus the ministerpretation is widespread. However, here we will target relationships that investigators claim exist, rather than null findings.

als, the

Citation: Journich JPA (2005) Why urch findings are false PLoS Med 2(8) e924 Copyright: 0 2005 John P.A. Isannida, This is

Sources of uncertainty

- Underlying theory (quantum mechanics) is probabilistic
 - true randomness
- Limited knowledge about the measurement process
 - present even without quantum mechanics

We quantify uncertainty using probability

Mathematical definition of probability

Let A be an event. Then probability is a number obeying three conditions, the *Kolmogorov axioms*:

1. $P(A) \ge 0$ (non-negative real number)



Kolmogorov, 1933

- 2. P(S) = 1, where S is the set of all A, the sample space
- 3. $P(A \cup B) = P(A) + P(B)$ for any A, B which are exclusive, i.e., $A \cap B = 0$

From these axioms further properties can be derived, e.g.:

 $P(\bar{A}) = 1 - P(A)$ $P(\emptyset) = 0$ if $A \subset B$ then $P(A) \le P(B)$ $P(A \cup B) = P(A) + P(B) - P(A \cap B)$



But what does P mean?

Interpretations of probability

https://plato.stanford.edu/entries/probability-interpret/

Classical

- Assign equal probabilities based on symmetry of the problem, e.g., rolling dice: P(6) = 1/6
- difficult to generalize

Frequentist

Let A, B, ... be outcomes of an repeatable experiment:

$$P(A) = \lim_{n \to \infty} \frac{\text{times outcome is } A}{n}$$

- Bayesian (subjective probability)
 - ► A, B, ... are hypotheses (statements that are true or false)

P(A) =degree of believe that A is true

Criticisms of the probability interpretations

Criticisms of the frequency interpretation

- ▶ $n \rightarrow \infty$ can never be achieved in practice. When is *n* large enough?
- P is not an intrinsic property of A, it depends on the how the ensemble of possible outcomes was constructed
 - Example: P(patient is treated in hospital | positive Corona test) is different wether or not one knows the age of the person
- We want to talk about the probability of events that are not repeatable
 - Example 1: P(it will rain tomorrow), but there is only one tomorrow
 - Example 2: P(Universe started with a Big Bang), but only one universe
- Criticisms of the subjective Bayesian interpretation
 - "Subjective" estimates have no place in science
 - How to quantify the prior state of our knowledge upon which we base our probability estimate?

Fun with probabilities

Monty Hall problem ("Ziegenproblem")

Suppose you're on a game show, and you're given the choice of three doors: Behind one door is a car; behind the others, goats. You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat. He then says to you, "Do you want to pick door No. 2?" Is it to your advantage to switch your choice?



Standard assumptions

- > The host must always open a door that was not picked by the contestant
- The host must always open a door to reveal a goat and never the car.
- The host must always offer the chance to switch between the originally chosen door and the remaining closed door.

Under these assumptions you should switch your choice!

Conditional probability and independent events

For two events A and B, the conditional probability is defined as

$$P(A|B) = rac{P(A \cap B)}{P(B)}$$

Example: rolling dice: $P(n < 3 | n \text{ even}) = \frac{P((n < 3) \cap n \text{ even})}{P(n \text{ even})} = \frac{1/6}{1/2} = 1/3$

Events A and B independent $\iff P(A \cap B) = P(A) \cdot P(B)$

An event A is independent of B if P(A|B) = P(A)

Bayes' theorem

Definition of conditional probability:



$$P(A|B) = \frac{P(A \cap B)}{P(B)} \quad \text{and} \quad P(B|A) = \frac{P(B \cap A)}{P(A)}$$
$$P(A \cap B) = P(B \cap A) \quad \rightarrow \quad P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

[doubtful whether the portrait actually shows Bayes]



First published (posthumously) by the Reverend Thomas Bayes (1702–1761)

First modern formulation by Pierre-Simon Laplace in 1812

Accepted by everyone if probabilities are not Bayesian probabilities

Example of using Bayes' theorem: Test for a rare disease

Base probability (for anyone)P(D) = 0.001to have a disease D:P(no D) = 0.999

Consider a test for the disease: result is positive or negative (+ or –):

"sensitivity"
$$\longrightarrow P(+|D) = 0.98$$
 $P(+|no D) = 0.03$
 $P(-|D) = 0.02$ "specificity" $\longrightarrow P(-|no D) = 0.97$

Suppose your result is +. How worried should you be?

$$P(D|+) = \frac{P(+|D)P(D)}{P(+)} = \frac{P(+|D)P(D)}{P(+|D)P(D) + P(+|D)P(D)}$$
$$= \frac{0.98 \times 0.001}{0.98 \times 0.001 + 0.03 \times 0.999} = 0.032$$

Probability for you to have the disease is 3.2%, i.e., you're probably ok.

Remark: false positives **not** a relevant issue in statistics of Corona cases (in case of a positive result usually double checks are made resulting in very high specificity)

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Bayesian inference: Degree of believe in a theory given a certain set of data (I)



Addresses question: "What should I believe?"

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Bayesian inference: Degree of believe in a theory given a certain set of data (II)

For a continuous parameter λ :

$$P_{\text{posterior}}(\lambda|m) = rac{f(m|\lambda)P_{\text{prior}}(\lambda)}{f_1(m)}$$

- λ : true value of a parameter of nature
- m: measurement

$$f_1(m) = \int f(m|\lambda')P(\lambda') d\lambda'$$

Problems with Bayesian inference

What functional form to chose for $P_{\text{prior}}(\lambda)$?

Uninformed prior: flat? In which variable, e.g., in λ , λ^2 , $1/\lambda$, $\ln \lambda$?

Bayesian reply

Choice of prior usually unimportant after a few experiments

Jaynes' robot: Priors are uniquely determined by your state of knowledge. Thus scientists with the same background knowledge construct the same priors.

Example of a posterior distribution

GW190814: Gravitational waves from the coalescence of a 23 solar mass Black Hole with a 2.6 solar mass compact object



LIGO Scientific Collaboration and Virgo Collaboration:

The Astrophysical Journal Letters, 896:L44 (20pp), 2020 June 20

Note:

Sampling from a multi-parameter posterior distribution typically involves Markov chain Monte Carlo (MCMC)

Are you a Frequentist or a Bayesian?

Suppose mass of a particle is measured with Gaussian resolution σ and the result ist reported as

 $m \pm \sigma$

Bayesian

 $P(m|m_{ ext{true}}) \propto e^{-(m-m_{ ext{true}})^2/(2\sigma^2)}$ flat prior for $m_{ ext{true}}$ $P(m_{ ext{true}}|m) \propto e^{-(m-m_{ ext{true}})^2/(2\sigma^2)}$

Frequentist

This is a statement about the interval $[m-\sigma, m+\sigma]$. For a large number of hypothetically repeated experiments the interval would contain the true value in 68% of the cases. In the frequentist approach, a probabilistic statement about the true value is nonsense (the true value is what it is).

"Bayesians address the questions everyone is interested in by using assumptions that no one believes. Frequentist use impeccable logic to deal with an issue that is of no interest to anyone." – Louis Lyons

Bayesian inference: Jeffreys' prior

How to model complete ignorance about the value of a parameter θ ?

- Uniform distribution in θ , exp θ , In θ , 1/ θ , ...?
- Example: Lifetime τ of a particle, uniform distribution in τ or particle's width $\Gamma = 1/\tau$?

Jeffreys' prior (non-informative prior) for a model $L(\vec{x}|\vec{\theta})$ of the measurement:

$$\pi(\vec{\theta}) \propto \sqrt{I(\vec{\theta})} \qquad I(\vec{\theta}) = \det \left[\left\langle \frac{\partial \ln L(\vec{x}|\vec{\theta})}{\partial \theta_i} \frac{\partial \ln L(\vec{x}|\vec{\theta})}{\partial \theta_j} \right\rangle \right]$$

$$\int \det(\vec{x}) \det(\vec{x}) determinant) = \det(\vec{x}) dt(\vec{x}) dt(\vec{x})$$

Examples:

PDF parameter	Jeffreys' prior	
Poissonian mean µ	p(μ) ∝ 1/√μ	
Gaussian mean µ	p(µ) ∝ 1	

Jeffreys' prior: Example

Exponential distribution:

$$L(t \mid \tau) = \frac{1}{\tau} e^{-t/\tau}$$

Jeffreys' prior:
$$\pi(\tau) \propto \sqrt{I(\tau)} = \sqrt{\mathsf{E}\left[\left(\frac{d}{d\tau}\ln L(t \mid \tau)\right)^2\right]}$$

$$\frac{d}{d\tau} \ln L(t|\tau) = -\frac{1}{\tau} + \frac{t}{\tau^2}$$

$$E\left[\left(\frac{t}{\tau^2} - \frac{1}{\tau}\right)^2\right] = E\left[\left(\frac{t-\tau}{\tau^2}\right)^2\right] = \frac{1}{\tau^4}V[t] = \frac{\tau^2}{\tau^4} = \frac{1}{\tau^2}$$

$$\rightsquigarrow \quad \pi(\tau) \propto \frac{1}{\tau} \qquad \text{(prior distribution)}$$

[based on L. Lyons]

	Bayesian	Frequentist
Meaning of probability	degree of belief	frequentist definition
Probability of parameters	yes	anathema
Needs prior	yes	no
Unphysical / empty intervals	excluded by prior	can occur
Final statement	posterior probability distribution	parameter values, hypothesis test (<i>p</i> -value)
Systematics	Integrate over nuisance parameter	Various methods, e.g., profile likelihood, hard
Combination of measurements	can be hard (prior)	ok

Bayesian versus Frequentism



https://xkcd.com/1132/

1.2 Describing the Data

Random variables and probability density functions

Random variable:

- Variable whose possible values are numerical outcomes of a random phenomenon
- Can be discrete or continuous

Probability density function (pdf) of a continuous variable:

probability density function

$$P(x \text{ found in } [x, x + dx]) = f(x) dx$$

Normalization: $\int_{-\infty}^{\infty} f(x) dx = 1$

"x must be somewhere"

Histograms

Histogram:

 representation of the frequencies of the numerical outcome of a random phenomenon

pdf = histogram for

- infinite data sample
- zero bin width
- normalized to unit area

 $f(x) = \frac{N(x)}{n\Delta x}$

n = total number of entries

 $\Delta x = \text{bin width}$



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Mean, Median, and Mode

~ /

Mean of a data sample
$$\frac{1}{N} \sum_{i=1}^{N} \overline{x}_{i}^{i} = \frac{1}{N} \sum_{i=1}^{N} x_{i}^{i}$$

Mean of a pdf:

$$\mu \equiv \langle x \rangle \equiv \int x P(x) dx$$

= $\mu \equiv \langle x \rangle \equiv \int dx P(x) x$
= expectation value $E[x]$

Median:

point with 50% probability above and 50% probability below

Mode:

the most likely value



Variance and standard deviation

Variance of a distribution: $V(x) = \int dx P(x)(x-\mu)^2 = E[(x-\mu)^2]$

$$V(x) = \int dx P(x)x^2 - 2\mu \underbrace{\int dx P(x)x + \mu^2 \int dx P(x) = \langle x^2 \rangle - \mu^2 = \langle x^2 \rangle - \langle x \rangle^2}_{=\mu}$$

Sample variance:

$$V(x) = \frac{1}{N} \sum_{i} (x_i - \bar{x})^2 = \overline{x^2} - \bar{x}^2$$

This formula underestimates the variance of underlying distribution as it uses the mean calculated from data!

Use this if you have to estimate the mean from data (*unbiased sample variance*):

Use this if you know the true mean
$$\mu$$
:

$$\hat{V}(x) = \frac{1}{N-1} \sum_{i} (x_i - \bar{x})^2$$

Standard deviation: $\sigma = \sqrt{V(x)}$

$$V(x) = \frac{1}{N} \sum_{i} (x_i - \mu)^2$$

Multivariate distributions

Outcome of experiment characterized by a vector ($x_1, ..., x_n$)

$$P(A \cap B) = f(x, y) \, dx dy$$
joint pdf

Normalization:

$$(A \iint B) \int \overline{\mathcal{T}}(x_1, \dots, x_n) dx dy = 1$$

Sometimes we want only the pdf of one component:

 $f_{x}(x) = \int f(x, y) \, dy \qquad \text{"marginal pdf"} \qquad x$ = projection of joint pdf onto individual axes $\int \cdots \int f(x_{1}, \dots, x_{n}) dx_{1} \cdots dx_{n} = \mathbf{1}_{\text{"s | 1. Basic Concepts 34}}$



Marginal pdf = projections



х

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10

Covariance and correlation

• Covariance
$$(\mu_x := \langle x \rangle, \mu_y := \langle y \rangle)$$
:

$$\operatorname{cov}[x, y] = E[(x - \mu_x)(y - \mu_y)]$$

Correlation coefficient (dimensionless):

$$\rho_{xy} = \frac{\text{cov}[x, y]}{\sigma_x \sigma_y} \qquad f_x(x) = \int dy \, f(x, y)$$

x, y independent, i.e., $f(x, y) = f_x(x) \cdot f_y(y)$: $f_y(y) = \int dx \, f(x, y)$

$$E[(x - \mu_x)(y - \mu_y)] = \int dx \int dy (x - \mu_x)(y - \mu_y)f(x, y)$$

= $\int (x - \mu_x)f_x(x) dx \int (y - \mu_y)f_y(y) dy = 0$
 $\rightarrow \operatorname{cov}[x, y] = 0$ (N.B. converse not always true)

Correlation coefficient



 $\operatorname{cov}[x, y] = E[(x - \mu_x)(y - \mu_y)]$

Never trust summary statistics alone; always visualize your data

https://www.autodeskresearch.com/publications/samestats



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Linear combinations of random variables

Consider two random variables with known covariance cov(x, y):

$$\langle x + y \rangle = \langle x \rangle + \langle y \rangle$$

$$\langle ax \rangle = a \langle x \rangle$$

$$V[ax] = a^2 V[x]$$

$$\operatorname{cov}(x, x) = V[x]$$

$$V[x + y] = V[x] + V[y] + 2\operatorname{cov}(x, y)$$

Example of more detailed calculation:

$$V[x + y] = E[(x + y - \mu_x - \mu_y)^2] = E[(x - \mu_x + y - \mu_y)^2]$$

= $E[(x - \mu_x)^2 + (y - \mu_y)^2 + 2(x - \mu_x)(y - \mu_y)]$
= $E[(x - \mu_x)^2] + E[(y - \mu_y)^2] + 2E[(x - \mu_x)(y - \mu_y)]$
= $V[x] + V[y] + 2\text{cov}(x, y)$

Higher moments



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Correlation \neq Causation

Examples of illogically inferring causation from correlation

https://en.wikipedia.org/wiki/Correlation_does_not_imply_causation

Example 1 ("reverse causality"):

- > The faster windmills are observed to rotate, the more wind is observed to be.
- Therefore wind is caused by the rotation of windmills.

Example 2 ("third factor C causes both A and B"):

- Sleeping with one's shoes on is strongly correlated with waking up with a headache.
- Therefore, sleeping with one's shoes on causes headache.



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What makes nobel prize winners?



Correlation coefficient: 0.791

Improved cognitive function associated with a regular intake of flavonoids???

Probably not ...

F. Messerli, 2012, New England Journal of Medicine, 2012

Correlation \neq Causation



PERMANENT LINK TO THIS COMIC: HTTP://XKCD.COM/552/

IMAGE URL (FOR HOTLINKING/EMBEDDING): HTTP://IMGS.XKCD.COM/COMICS/CORRELATION.PNG