Reproducible Research Wieso? Weshalb? Warum? Aber... Und Wie?

Manuel J. A. Eugster

Institut für Statistik Ludwig-Maximiliams-Universität München

Herbstworkshop, Ruhr-Universität Bochum, 2011

Joint work with Friedrich Leisch and Torsten Hothorn: *Executable papers for the R community: The R² platform for reproducible research.* Procedia Computer Science, 4:618–626, 2011. Proceedings of the International Conference on Computational Science, ICCS 2011. (Leisch et al., 2011)

Joint work with Anne-Laure Boulesteix:

Seminar: Reproduzierbarkeit. Institut für Statistik, Ludwig-Maximilans-Universität München. Winter term 2011/2012.

(*) Parts of this talk are based on Hothorn (2010) and Boulesteix (2010/2011).

THE VIEWS EXPRESSED IN THIS TALK DO NOT NECESSARILY REPRESENT THE VIEWS OF MY COLLABORATORS!

Reproducible research in computational science

Computational science or scientific computing is "the analysis of mathematical models implemented on computers" (Wikipedia, 2011a).

Reproducible research is the ability to independently recompute—i.e., to verify—findings (and to conduct alternative analyses, Peng et al., 2006).

Reproducible research in computational science

Computational science or scientific computing is "the analysis of mathematical models implemented on computers" Wikipedia, 2011a). "Cornerstone of the scientific method!" Reproducible research Scientific community: ernative recomputeanalyses, I

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QVÆSTIO VIII.

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Clearbout's principle:

"An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures."

(*) Buckheit and Donoho (1995) and de Leeuw (2001)

"Publish data and source code!"

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Under the hood—truly interdisciplinary field:

Philosophy of science: scientific method, contribution to knowledgeLaw: licensing for scientific innovationForensics: reproducibility of publicationsComputer science: consequences of heterogeneous technology

Implementation: tools and workflows for practical realization

Wieso? Weshalb? Warum?

Local and global improvements of publishing source code and data

Local improvements

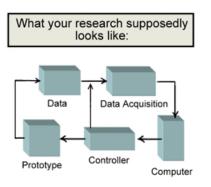


Figure 1. Experimental Diagram

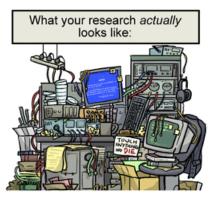


Figure 2. Experimental Mess

Global improvements

"We reproduced two analyzes in principle and six partially or with some discrepancies; ten could not be reproduced. The main reason for failure to reproduce was data unavailability, and discrepancies were mostly due to incomplete data annotation or specification of data processing and analysis."

(*) Ioannidis et al. (2009) on microarray gene expression analysis

THE CONTINES

Archive Article

Please enjoy this article from The Times & The Sunday Times archives.

From The Sunday Times

January 18, 2009

Wealthy men give women more orgasms

Jonathan Leake, Science and Environment Editor

Scientists have found that the pleasure women get from making love is directly linked to the size of their partner's bank balance.

They found that the wealthier a man is, the more frequently his partner has orgasms.

"Women's orgasm frequency increases with the income of their partner," said Dr Thomas Pollet, the Newcastle University psychologist behind the research.

(*) Nettle and Pollet (2009), and Herberich et al. (2010)

Nettle and Pollet (2009):

"Partner wealth predicts self-reported orgasm frequency in a sample of Chinese women".

The study is based on the freely available Chinese Health and Family Life Survey.

The main conclusion is drawn from a proportional odds model linking the self-reported orgasm frequency of women with male partners to sociodemographic and wealth variables of the couple.

Reproducing Nettle and Pollet (2009):

The paper is actually reproducible because

- the data are publically available,
- the data preprocessing is well-described in the manuscript, and
- the software used to fit the model and perform AIC-based model selection is cited (SPSS).

However, Esther Herberich and Torsten Hothorn failed to reproduce the analysis in R.

It turned out that SPSS 15.0 did not exclude a model-specific constant in the multinomial log-likelihood before comparing models differing in the covariates.

Herberich, Hothorn, Nettle, and Pollet (2010):

When calculating the AIC in a correct manner, the women's education is most strongly (positively) related to the response.

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When calculating the AIC in a correct manner, the women's education is most strongly (positively) related to the response.



ORGASMUS-STUDIE

Kluge Frauen kommen öfter

Klischee vom geilen Dummerchen haben Münchner Uni-Forscher widerlegt





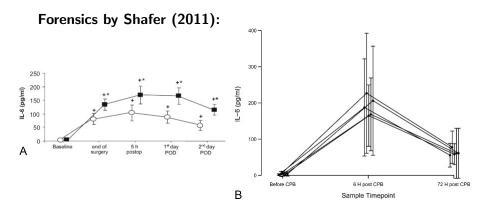
100 Pine Street, Suite 230, San Francisco, CA 94111 Phone: (415) 777-2750, Fax: (415) 777-2803

Steven L. Shafer, MD Editor-in-Chief

February 25, 2011

To our readers:

In 2009 Dr. Joachim Boldt published a manuscript in *Anesthesia & Analgesia* comparing albumin and hydroxyethyl starch priming cardiopulmonary bypass.¹ The study was retracted in December 2010 for lack of IRB approval.² A subsequent investigation by Klinikum Ludwigshafen determined that the study was fabricated.³



Three readers contacted the journal to question the small standard deviations of the interleukin IL-6 concentrations reported by Boldt (A). For comparison, B shows a similar study.

Forensics F	Table 1. Findings from LÄK-	RLP, October 25, 2010]
	Statement in article	Finding by LÄK-RLP	
250 = 200	Fifty consecutive patients undergoing elective coronary artery bypass grafting were studied after approval of the IRB.	For the respective study, there does not exist an approval by the respective IRB.	
(m 200 - 150 - 9 - 1100 - 50 -	And after receiving individual written informed consent.	For the respective study, there does not exist written informed consent.	
A Baseline end of surgery	The patients were prospectively randomized into one of the two groups by a computergenerated list and sealed envelopes.	For the respective study, there does not exist a prospective randomization process into two groups by a computer- generated list and sealed envelopes.	PB 72 H past CPB
Three reade deviations c (A). For co	A questionnaire was sent to the patients' primary physicians to receive information on patients' serum creatinine, renal failure requiring renal replacement therapy, and mortality approximately 60 days after hospital discharge.	For the respective study, there does not exist a written questionnaire sent to the patients' primary physicians approximately 60 days after hospital discharge.	all standard d by Boldt
	LÄK-RLP = Landesärztekammer Rheinlar	nd-Pfalz.	

Reality check "CSDA, Volume 56, Issue 3":

Number of 23 papers with simulation studies and/or examples giving direct access to data or code (0.5 if code either for simulation or example):

Simulation	Example	Data	Code
21	19	6.5	2.5

(*) For numbers on *Bioinformatics* see Hothorn and Leisch (2011).

Aber...

Discussion on publishing source code and data

• "A precise description does it as well!"

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A trivial example:

"A multivariate logistic regression model was built based on the predictors sex, age, and tumor localisation and the response variable 'relapse yes/no'. A forward selection was applied with entry threshold = 0.05."

• "A precise description does it as well!"

A trivial example:

"A multivariate logistic regression model was built based on the predictors sex, age, and tumor localisation and the response variable 'relapse yes/no'. A forward selection was applied with entry threshold = 0.05."

- How was the coding of sex and localisation?
- How did they handle missing values?
- How did they compute the *p*-value for the forward selection procedure? Wald? LR?

^(*) See, for example, Donoho (2010)

- "My code is crap."
- "With the next Software update, it doesn't work anymore."
- "No one will spend hours to check my code."
- "People will find errors."
- "Statistical analysis is only a small part of the scientific approach."

- "My code is crap."
- "With the next Software update, it doesn't work anymore."
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- "People will find errors."
- "Statistical analysis is only a small part of the scientific approach."

Probably true for all points; however, not really an excuse to do unreproducible statistical analysis. It is always better to have a code than no code at all.

(*) See, for example, Barnes (2010)

• "Replication is the important thing."

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Drummond (2009):

"[...] replicability is not reproducibility. Replicability requires changes; reproducibility avoids them."

True, but verifying the findings based on the same data is the minimum standard and the basis for more complex verification.

 $(\ensuremath{^*})$ Note that terms are changed to match with the remaining publications

• "I don't have the authorization to publish the source code and the data."

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Is this then "the game" of scientific research anymore? Or industrial research?

• "But it's my intellectual property!"

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Stodden (2009) defines a Reproducible Research Standard:

Source code: GNU GPL or (modified) BSD license Media: Creative commons attribution license (CC BY) Data: Science Commons Database Protocol

(*) See Free Software Foundation, Creative Commons, Science Commons

• "You need to know the substantive context."

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Keiding (2010a) and Keiding (2010b):

"The statistician needs to understand how data were generated and selected in order to produce relevant analyses."

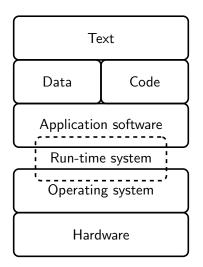
"[...], there at least has to be sufficient information to make it realistic for another interdisciplinary group of researchers to understand the substantive context and the strengths and weaknesses of the data."

"Availability of naked datasets may well be counterproductive."

• "I used a Mac..."

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Reproducibility in the view of heterogeneous technology:



The pitfalls of verifying floating-point computations:

"An important factor throughout the discussion is that it is not the hardware platform that matters in itself, but its combination with the software context, including the compiler, libraries, and possible run-time environment."

(*) Monniaux (2008)

The dot or scalar product:

1

$$a = (a_1, a_2, \dots, a_n)$$

$$b = (b_1, b_2, \dots, b_n)'$$

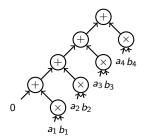
$$a \cdot b = \sum_{i=1}^n = a_1 \times b_1 + a_2 \times b_2 + \dots + a_n \times b_b$$

 λI

We suppose (in an arbitrary mathematical software) that a function dotprod(a, b) returns the correct mathematical dot product.

(*) Example by Whitehead and Fit-Florea (2011)

Serial method:



t = 0

for i from 1 to 4 :

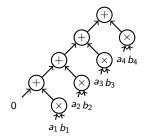
$$p = \operatorname{rn}(a_i \times b_i)$$

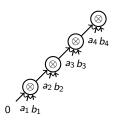
 $t = \operatorname{rn}(t + p)$

return t

Serial method:

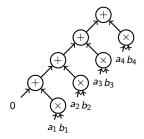
FMA method:



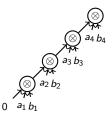


t = 0for *i* from 1 to 4 : $p = rn(a_i \times b_i)$ t = rn(t + p)return *t* t = 0
for *i* from 1 to 4 :
 $t = rn(a_i \times b_i + t)$
return *t*

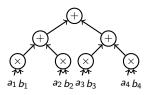
Serial method:



t = 0for *i* from 1 to 4 : $p = rn(a_i \times b_i)$ t = rn(t + p)return *t*



t = 0for *i* from 1 to 4 : $t = rn(a_i \times b_i + t)$ return *t* Parallel method:



 $p_1 = \operatorname{rn}(a_1 \times b_1)$ $p_2 = \operatorname{rn}(a_2 \times b_2)$ $p_3 = \operatorname{rn}(a_3 \times b_3)$ $p_4 = \operatorname{rn}(a_4 \times b_4)$ $s_l = \operatorname{rn}(p_1 + p_2)$ $s_r = \operatorname{rn}(p_3 + p_4)$ $t = \operatorname{rn}(s_l + s_r)$

return t

Serial method: FMA method: Parallel method: a4 b4 a4 b4 $a_3 b_3$ a4 b4 0 Method Result float value b_1) 0.0559587528435... 0x3D65350158... exact b₂) serial 0.0559588074 0x3D653510 b3) t =FMA 0.0559587515 0x3D653501 b4) for i parallel 0.0559587478 0x3D653500 $p_2)$ р p4) t $t = \operatorname{rn}(s_l + s_r)$ return t

return t

• "It requires so much time."

• "It requires so much time."

Yes! And motivation, patience, good organization, etc.

• "It requires so much time."

"How to be a Highly Cited Author in the Mathematical Sciences" by Donoho (2002):

"I am a statistician, so when ISI contacted me with the news that I was a 'Highly Cited Author' [...] I looked at my list of 10 highly cited papers [...]"

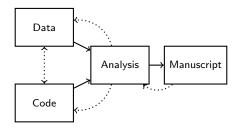
"In our most-cited papers, we developed methodology for wavelet-based noise removal which was implemented in MATLAB [...] was available for free download over the Internet [...]"

Wie?

Warning: my attempt to make my research reproducible



 $(\ensuremath{^*})$ Image from Volkswagen Commercial Vehicles: Choose the right tool 1



Local:

- 1. Programming environment
- **2.** Document preparation system (literate programming)
- 3. Version control

(*) See, for example, Koenker and Zeileis (2009)

Global:

- 1. Mainstream & Long-Term Software
- 2. Distribution system
- **3.** (Open)

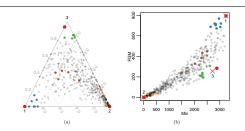


Figure 2: (a) Visualization of the α coefficients using a ternary plot and (b) the data set in case of the k = 3 archetypes solution. The red dots are the archetypes' nearest players; dots colored with blue, orange, and green are players where Archetype 1, 2, and 3 contribute more than 0.8.

problem (Formula 1) define how much each archetype contributes to the approximation of each individual observation (as convex combination). This allows the assignment of the observations to their nearest archetypes and, consequently, the identification of the most archetypal observation(s). Figure 2 shows the corresponding ternary plot of the α coefficients for the above k = 3 archetypes solution. The three players (red points) nearest to the respective archetypes (red crosses) are:

	Name	Team	Role	Min	FGM	$\alpha_{.1}$	$\alpha_{.2}$	$\alpha_{.3}$
Archetype 1	Kevin Durant	OKL	SF	3241	794	1.00	0.00	0.00
Archetype 2	Dwayne Jones	PHO	C	7	0	0.00	1.00	0.00
Archetype 3	Jason Kidd	DAL	\mathbf{PG}	2883	284	0.06	0.00	0.94

Archetype 1 and 3 have well-defined nearest observations; Archetype 2, on the contrary, has a set of nearest observations and the concrete player identification should be considered as a "random" selection from the set of similar players.

We have identified Archetype 1 as the "good" archetype in this data setting—on this account. Kevin Durant can be considered as the best scorer. To find other good scorers.

Programming environment

"The programming language should support the user in turning theory into software that reflects how we think about the underlying method conceptually."

"To assure reproducibility and reusability by other authors, the structural features of a language should facilitate (and not suppress) the ability to build on innovations of prior authors."

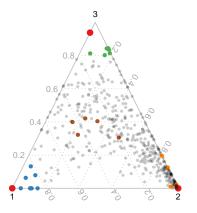
(*) Koenker and Zeileis (2009)

The R Project for Statistical Computing:

R is 'GNU S', a freely available language and environment for statistical computing and graphics which provides a wide variety of statistical and graphical techniques, and is highly extensible.

CRAN with 3420 add-on packages, daily checked.

(*) R Development Core Team (2011)



> library("RColorBrewer")
> library("vcd")
> col_pal <- brewer.pal(7, "Set1")
> ternaryplot(coef(a3, "alphas"),
+ col = col_pal, [...])

Document preparation system Literate programming

Knuth (1986) proposed in *Literate Programming* the combination of a programming language and a documentation language:

from "instructing a computer what to do" to "explaining a human beeing what we want a computer to do"

Literate programming enables to interleave code and documentation chunks: weave-ing creates the manuscript, tangle-ing the source code.

Sweave: R & LaTeX (Leisch, 2002) odfWeave: R & OpenOffice (Kuhn, 2010) StatWeave: R, SAS, Stata, ... & LaTeX, OpenOffice (Lenth, 2011) Matweave: Matlab, Octave & LaTeX (Lawrence, 2011) α coefficients for the above k = 3 archetypes solution. The three players (red points) nearest to the respective archetypes (red crosses) are:

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Archetype 1 and 3 have well-defined nearest observations; Archetype 2, on the con-

archeplayers.Rnw:

The three players (red points) nearest to the respective archetypes (red crosses) are: \begin{center}

```
<<results=tex>>=
## Archetypal players:
atypes <- apply(coef(a3, "alphas"), 2, which.max)</pre>
atypes_coef <- coef(a3, "alphas")[atypes, ]</pre>
colnames(atypes_coef) <- sprintf("$\\alpha_{\\cdot%s}$", 1:3)</pre>
atypes_dat <- dat[atypes, ]</pre>
atypes_dat <- cbind(atypes_dat, atypes_coef)</pre>
rownames(atypes_dat) <- sprintf("Archetype %s", 1:3)</pre>
print(xtable(atypes_dat), floating = FALSE,
      sanitize.colnames.function = identity)
0
```

```
\end{center}
Archetype~1 and 3 have well-defined nearest observations;
```

Sweave("archeplayers.Rnw") \Rightarrow archeplayers.tex:

The three players (red points) nearest to the respective archetypes (red crosses) are: \begin{center}

```
% latex table generated in R 2.13.1 by xtable 1.5-6 package
% Tue Sep 13 10:27:53 2011
\begin{tabular}{rlllrrrrr}
 \hline
 & Name & Team & Role & Min & FGM & $\alpha_{\cdot1}$ & $\alpha_{\cdot
 \hline
 Archetype 1 & Kevin Durant & OKL & SF & 3241 & 794 & 1.00 & 0.00 & 0.
  Archetype 2 & Dwayne Jones & PHO & C & 7 & 0 & 0.00 & 1.00 & 0.00
  Archetype 3 & Jason Kidd & DAL & PG & 2883 & 284 & 0.06 & 0.00 & 0.94
 \hline
\end{tabular}
\end{center}
Archetype~1 and 3 have well-defined nearest observations;
```

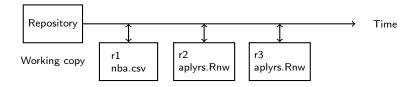
Stangle("archeplayers.Rnw") \Rightarrow archeplayers.R:

```
## Archetypal players:
atypes <- apply(coef(a3, "alphas"), 2, which.max)
atypes_coef <- coef(a3, "alphas")[atypes, ]
colnames(atypes_coef) <- sprintf("$\\alpha_{\\cdot%s}$", 1:3)
atypes_dat <- dat[atypes, ]
atypes_dat <- cbind(atypes_dat, atypes_coef)</pre>
```

```
rownames(atypes_dat) <- sprintf("Archetype %s", 1:3)
```

Version control

Version control is the management of changes to data, programs, documents, and other information stored as computer files. Well-known systems are Subversion and Git.



(*) See Subversion and Git

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Trans	actions									ې 🖶	월 🔻 🕈 🗗
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Distribution system

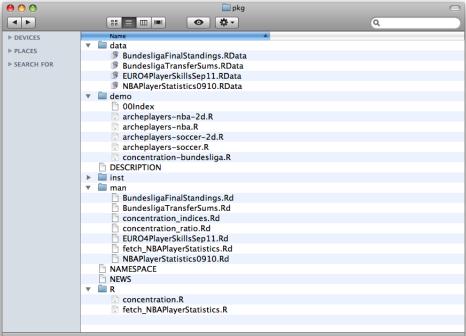
Manuscripts are published in a standardized way—publish source code, data, etc. using a standardized distribution system as well.

R add-on packages and CRAN:

Packages provide a mechanism for loading optional code, data, and attached documentation as needed.

Is is a standardized directory hierarchy with some mandatory files. A series of checks are available to ensure the technical correctness.

CRAN publishes daily checked packages.



27 items, 126.23 GB available

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archetypes (using the α coefficients). The two examples—basketball and soccer—shows that this is an appropriate approach; the estimated archetypal athletes definitely are consistent with the general opinion.

Computational details

All computations and graphics have been done using the statistical software R 2.13.1 [R Development Core Team, 2011], the archetypes package [Eugster, 2010], and the Sports-Analytics package [Eugster, 2011]. R itself and all packages used are freely available under the terms of the General Public License from the Comprehensive R Archive Network at http://CRAN.R-project.org/.

Data sets and source codes for replicating our analyses are available in the SportsAnalytics package. An individual analysis is executed via (replace *** with nba-2d, nba and soccer):

```
R> demo("archeplayers-***", package = "SportsAnalytics")
```

The source code file for a demo is accessible via:

```
R> edit(file = system.file("demo", "archeplayers-***.R",
+ package = "SportsAnalytics"))
```

References

Christian Bauckhage and Christian Thurau. Making archetypal analysis practical. In

(*) Page 14 of Archetypal Athletes, Eugster (2011)



SportsAnalytics: Infrastructure for Sports Analytics

The aim of this package is to provide infrastructure for sports analysis. Anyway, currently it is a selection of data sets, functions to fetch sports data, examples, and demos – with the ambition to develop bit by bit a set of classes to represent general concepts of sports analysis.

	Version:	0.1						
	Depends:	methods, stats						
	Suggests:	archetypes						
	Published:	2011-10-12						
	Author:	Manuel J. A. Eugster						
	Maintainer:	Manuel J. A. Eugster <manuel.eugster at="" stat.uni-muenchen.de=""></manuel.eugster>						
	License:	<u>GPL (≥ 2)</u>						
	URL:	http://soccer.r-forge.r-project.org/						
	CRAN checks: SportsAnalytics results							
	Downloads:							
Package source:		SportsAnalytics 0.1.tar.gz						
MacOS V hinaru		r Sports Analytics 0.1 tez						

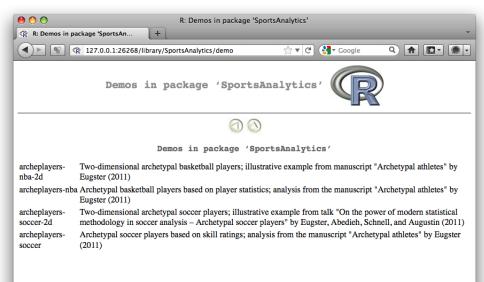
MacOS X binary: <u>SportsAnalytics 0.1.tgz</u> Windows binary: <u>SportsAnalytics 0.1.zip</u>

Reference manual: SportsAnalytics.pdf

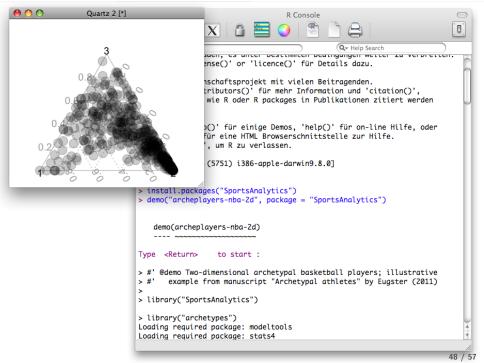
News/ChangeLog: NEWS













Also!

Start doing reproducible research because ...

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- **4.** A second execution of the analyses on the authors' computers is not "reproducibility". Analyses must be reproducible on an unbiased open platform.

Lawrence (2010):

- It's about habits, not rules.
- It's about good practice: like spell checking.
- It's about courtesy to other researchers.
- It's about keeping track of collaborators work.
- It's about making research reproducible.
- It's something you should all be doing.

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Images

page 6: Page 85 of Diophantus' Arithmetica (with problem II.VIII); via http://en.wikipedia.org/wiki/Fermat%27s_Last_Theorem

page 12: PHD Comics: Reserach Diagram/Research Reality; http://www.phdcomics.com/comics.php?f=961

page 49: Volkswagen Commercial Vehicles: Choose the right tool, 1; via http://adsoftheworld.com/media/print/volkswagen_commercial_vehicles_choose_the_right_tool_1

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