Karlsruher Institut für Technologie

Geodatenanalyse I: Monte Carlo Methoden

Kathrin Menberg

Stundenplan

	08:30 – 12:30 Uhr	13:30 – 17:30 Uhr
Montag	Tag 1 / Block 1	Tag 1 / Block 2
Dienstag	Tag 2 / Block 1	Tag 2 / Block 2
Mittwoch	Tag 3 / Block 1	**Tag 3 / Block 2**
Donnerstag	Tag 4 / Block 1	Tag 4 / Block 2
Freitag	Tag 5 / Block 1	Tag 5 / Block 2

- **2.7 Monte Carlo Methoden**
- 2.8 Grundlagen der Sensitivitätsanalyse
- 2.9 Fortgeschrittene Sensitivitätsanalyse

Lernziele Block 2.7

Am Ende der Stunde werden die Teilnehmer :

- … mit dem Prinzip von Unsicherheiten und statistischen Zufallsexperimenten vertraut sein.
- … einen Überblick über Methoden für (Pseudo-) Zufallsexperimente haben.
- … einfache Monte Carlo Simulationen in Python durchführen und auswerten können.

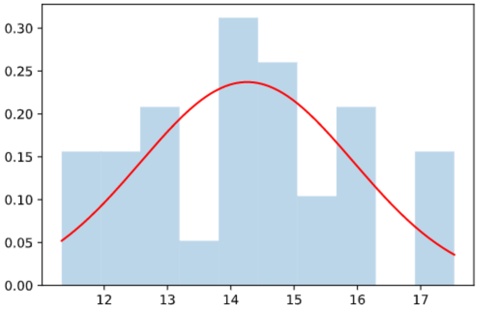
Unsicherheiten

„*Nothing is certain, but our ignorance*." (unbekannt)

- Welche „Unsicherheiten" fallen Euch in Bezug auf Geodatenanalyse ein?

Arten von Unsicherheit

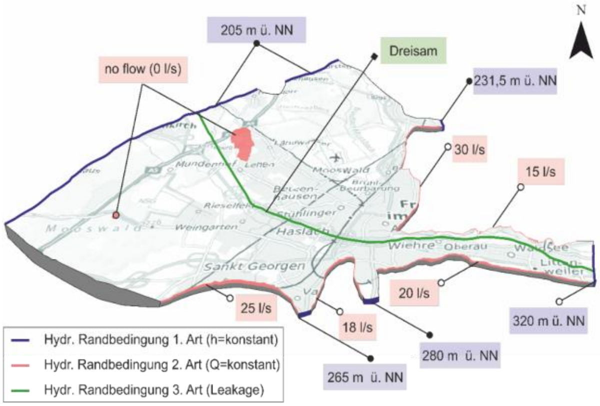
- Aleatorisch (aleatoric)
  - statistische Unsicherheit
  - Unbestimmbare Größen, die in wiederholten Experimenten variieren
  - Komplexe Prozesse, die nicht erfassbar sind
  - usw.



- Epistemisch (epistemic)
  - Systematische Unsicherheit
  - Größen, die in Experimenten nicht gemessen wurden.
  - Vereinfachungen in numerischen Modellen
  - Usw.

Quellen von Unsicherheiten

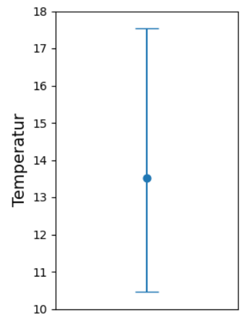
- Daten, Parameter
  - Messfehler, Messgenauigkeit
  - Szenarien
- Modelle
  - Annahmen (Randbedingungen usw.)
  - Vernachlässigte Prozesse
  - Auflösung, bzw. Diskretisierung
  - Numerische Fehler, Approximation
- Modellierer
  - Bedienungsfehler, Eingabefehler
- und viele mehr…

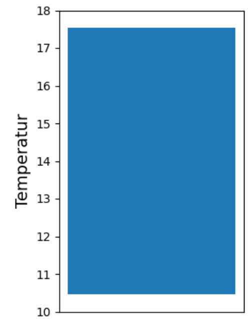


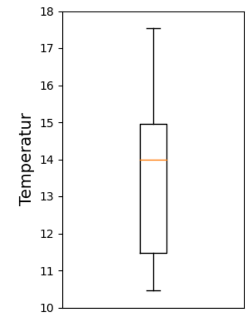
Ohmer et al. (2021)

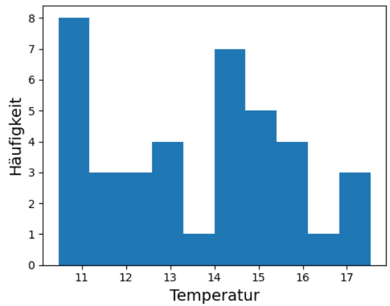
Visualisierung von Unsicherheiten

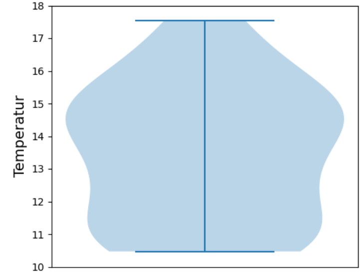
- Fehlerbalken
- Balkendiagramme
- Histogramme
- Boxplots
- Violinen Diagramme
- Schwarmplot
- u.v.m.

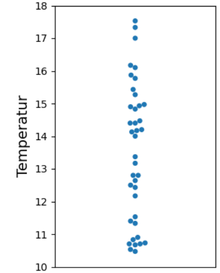








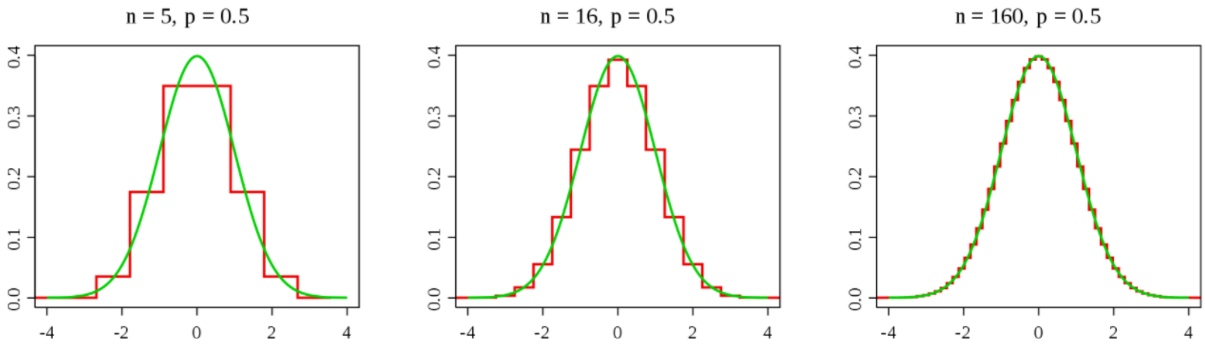




Zentraler Grenzwertsatz

- engl. central limit theorem
- Für $n \to \infty$ nähert sich die empirische Verteilungsfunktion $Z_n$der Standardnormalverteilung $\Phi(z)$
  - Konvergenz gegen $\Phi(z)$

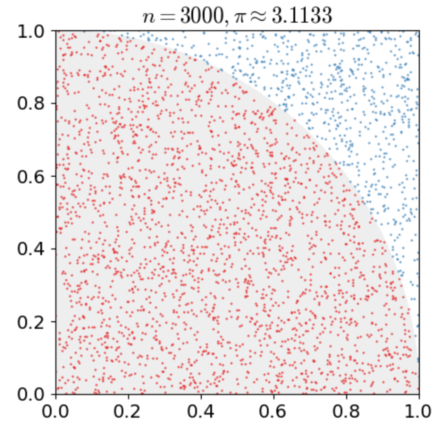
$$\lim_{n \to \infty} P(Z_n \leq z) = \Phi(z)$$



www.wikipedia.org

Monte Carlo Simulation

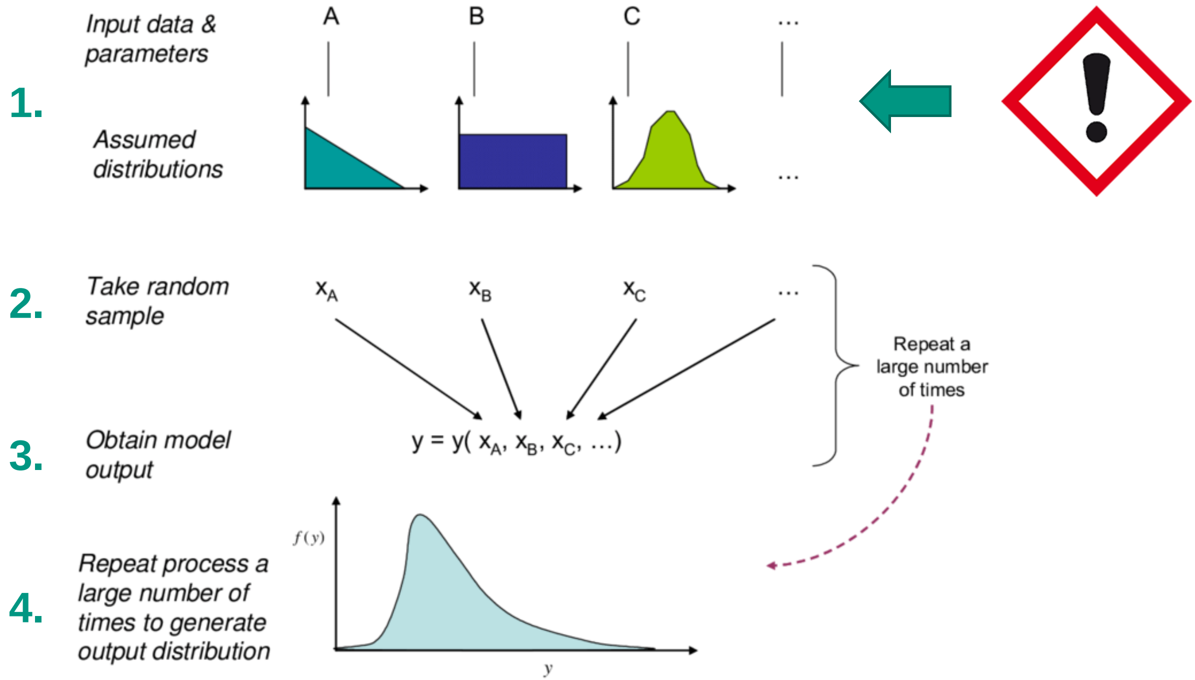
- Ziele (Beispiele)
  - Approximation von irrationalen Zahlen
  - Verteilungseigenschaften von Zufallsvariablen
  - Nachbildung komplexer Prozesse (z.B. Wetter- und Klimaphänomene)



www.wikipedia.org

- Prinzip:
  1. mögliche Inputs definieren
  2. zufällige Inputs anhand einer Wahrscheinlichkeitsfunktion generieren
  3. <u>deterministische</u> Berechnung mit den Inputs durchführen
  4. Ergebnisse zusammenfassen

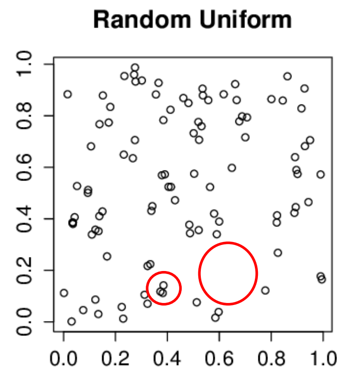
Monte Carlo Simulation



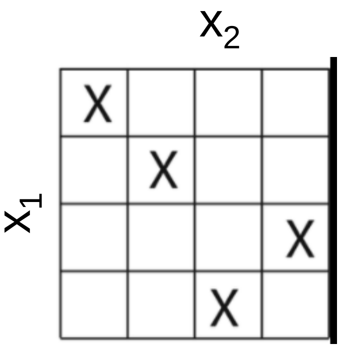
Henderson & Bui 2005

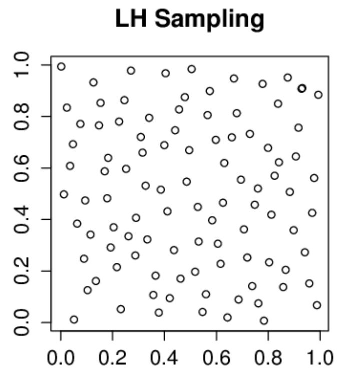
Generieren von Zufallswerten

- einfache Zufallswerte (random values)
  - z.B. in Python über numpy.random



- „near-random“ Zufallswerte
  - Latin Hypercube sampling
  - Orthogonal sampling
  - Sobol Sequenzen
  - …

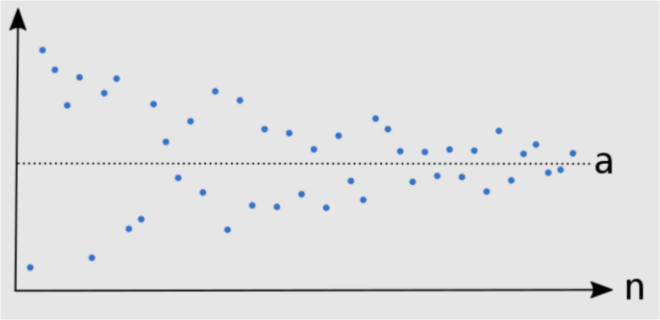




www.wikipedia.org

Wie groß muss *n* sein?

- Konvergenz gegen unbekanntes $\Phi(z)$
- 1. Option: *n* richtig hoch ansetzen (z.B. 10^7)
  - lange Rechenlaufzeiten!
- 2. Option: *n* schrittweise erhöhen und Ergebnisse beobachten



www.wikipedia.org

Übung 2.7: Monte-Carlo Methoden

- Bestimmung der Unsicherheit von biologischen Abbauraten in einem kontaminierten Aquifer
  - Monte Carlo Simulation für das analytische Modell in Eq. (6):

$$\lambda = \frac{\Delta\delta^{13}C \cdot k_f \cdot i}{\varepsilon \cdot s \cdot n_e}$$

  - Angaben zu Parametern in Tab. 1
  - Brunnen G10m – G30u
- Aufgaben in Jupyter Notebook: geodatenanalyse_1-2-7

Journal of Contaminant Hydrology 238 (2021) 103757

Contents lists available at ScienceDirect

Journal of Contaminant Hydrology

journal homepage: www.elsevier.com/locate/jconhyd

Quantifying biodegradation rate constants of o-xylene by combining compound-specific isotope analysis and groundwater dating

Andreas Würth [a], Kathrin Menberg [a], Peter Martus [b], Jürgen Sültenfuß [c], Philipp Blum [a,*]

[a] Karlsruhe Institute of Technology (KIT), Institute for Applied Geosciences (AGW), Kaiserstraße 12, 76131 Karlsruhe, Germany
[b] AECOM Deutschland GmbH, Siemensstraße 10, 63263 Neu-Isenburg, Germany
[c] University of Bremen, Institute of Environmental Physics, Otto-Hahn-Allee, 28359 Bremen, Germany

ARTICLE INFO

Keywords:
Coal tar
Compound-specific isotope analysis (CSIA)
^3H-^3He-dating
Hydraulic conductivity
Biodegradation

ABSTRACT

The objective of this study is to estimate hydraulic conductivities and biodegradation rate constants in a coal-tar contaminated aquifer by compound-specific isotope analysis (CSIA) and tracer-based (^3H–^3He) groundwater dating (TGD). In two observation wells downgradient from the contaminant source in situ biodegradation of o-xylene, toluene and naphthalene under sulfate-reducing redox conditions could be demonstrated using CSIA. Median biodegradation rate constants for o-xylene ranging between 0.08 and 0.22 a^{-1} were estimated. By using tracer-based groundwater dating in these two wells, hydraulic conductivities could be also estimated, which are in a similar range as k-values derived from sieve analysis, a pumping test and a calibrated groundwater flow model. These results clearly demonstrate the applicability of tracer-based groundwater dating for the determination of in situ hydraulic conductivities in aquifers without pumping contaminated groundwater. Finally, a sensitivity analysis is performed using a Monte Carlo simulation. These results indicate high sensitivities of the assumed effective porosity for the estimation of the hydraulic conductivity and the selected isotope enrichment factor for the biodegradation rate constant, respectively. Conversely, the outcome also evidently demonstrates the main limitations of the novel combined isotope approach for a successful implementation of monitored natural attenuation (MNA) at such field sites.

1. Introduction

The contamination of the subsurface due to leaking point sources from industrial plants is a widespread issue and often requires extensive long term monitoring and remediation (Schwarzenbach et al., 2010). A common example for such incidences is the release of coal tar and creosote constituents into the subsurface. Most of the latter occur as dense non-aqueous phase liquids (DNAPL). Once they enter the subsurface, these liquids typically seep through unsaturated and saturated zones of the aquifer until reaching a natural barrier, such as impermeable or low-permeable soils or geological layers, where they tend to accumulate and migrate in groundwater flow direction (e.g. D'Affonseca et al., 2008a). When it comes to monitoring and remediation, biodegradation is often considered as an appropriate remediation strategy in the form of monitored natural attenuation (MNA) at such sites (e.g. Blum et al., 2007, 2011; Martus and Schaal, 2010). The qualitative and quantitative proof of biodegradation is crucial for a successful implementation of MNA (e.g. Rügner et al., 2006).

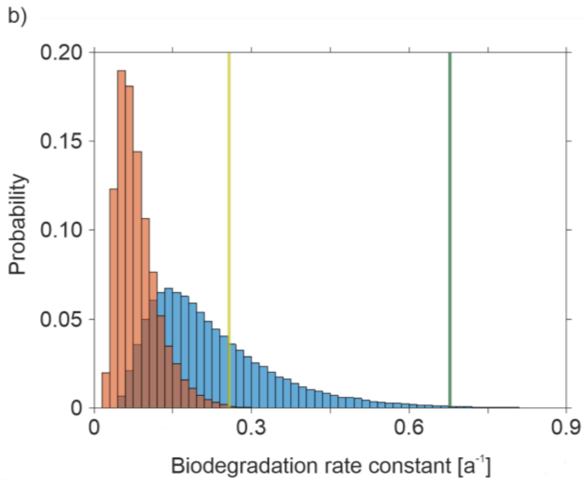
During the last decades stable compound-specific isotope analysis (CSIA) has been established as the major method for assessing the occurrence of biodegradation in contaminated aquifers (e.g. Sturchio et al., 1998; Hunkeler et al., 1999a; Sherwood Lollar and Slater, 2001; Richnow et al., 2003a, 2003b; Griebler et al., 2004). It uses the fact that (bio-)chemical reactions degrading organic contaminants are accompanied by isotope fractionation according to the kinetic isotope effect (Elsner, 2010). A large number of studies exist showing the potential of CSIA. Thus, one can assess the fate of organic pollutants (Meckenstock et al., 2004; Braeckevelt et al., 2012), differentiate between multiple source zones (Hunkeler et al., 2004), or reveal transformation mechanisms and pathways via multi isotope analysis (Elsner et al., 2005). However, the concept of CSIA also have some challenges and limitations: It struggles when concentrations of organic contaminants are low and therefore only tap the full potential at highly polluted field sites (Schmidt et al., 2004). Furthermore, field applicability suffers from factors that potentially influence observable isotope shifts, namely limited bioavailability (Braeckevelt et al., 2012), and physical processes,

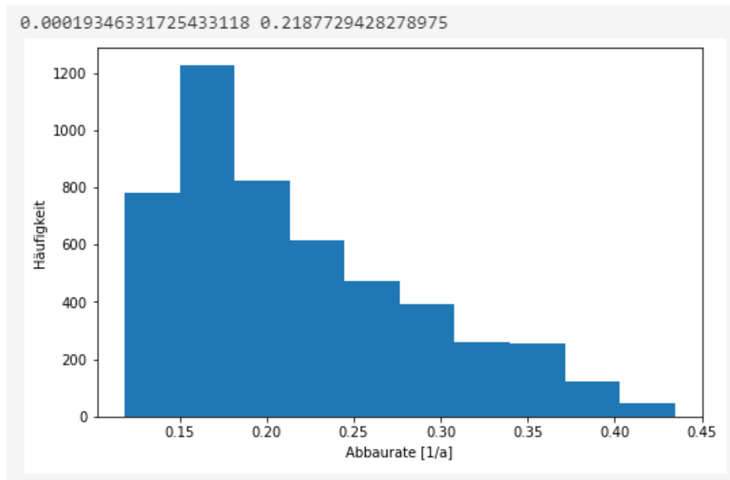
* Corresponding author.
E-mail address: blum@kit.edu (P. Blum).

https://doi.org/10.1016/j.jconhyd.2020.103757
Received 5 June 2020; Received in revised form 26 October 2020; Accepted 12 December 2020
Available online 5 January 2021

Aufgabenbesprechung

- Monte Carlo Simulation (Würth et al. 2021, Abb. 3)





Literatur

- Bättig (2017): Angewandte Datenanalyse, 2. Aufl., Springer Spektrum
- Gelman et al. (2014): Bayesian Data Analysis, 2nd Ed., CRC Press
- Würth et al. (2021): Quantifying biodegradation rate constants of o-xylene by combining compound-specific isotope analysis and groundwater dating. Journal of Contaminant Hydrology, 238, 103757


thank you
danke
謝謝
teşekkür ederim
gracias
спасибо
dank je
tapadh leat
bedankt
dziękuję
hvala
mauruuru
mochchakkeram
go raibh maith agat
obrigado
sukriya
kop khun krap
sagolun
arigatō
takk
dakujem
grazie
terima kasih
мерси
merci
감사합니다
ありがとう
ευχαριστώ
Баярлалаа
рахмат
хвала
blagodaram
mersi
tack
paldies
asante
chnorakaloutioun
gracies
sulpay
taiku
tanemirt
rahmet
diolch
dhanyavadagalu
shukriya
xiexie
trugarez
mamnun
enkosi
nandri
kiitos
dankie
faafetai lava
vinaka
matondo
misaotra
barka
spas
najis tuke
mesi
sabed
dekuji