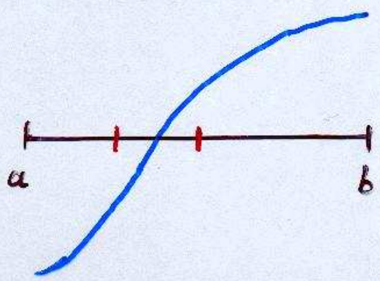
Verfahren zur Nullstellenbestimmung

1.) Bisektion

Bekannt: eine Nullstelle im Intervall $[a,b]$

(Vorzeichenwechsel)

Intervallschachtelung:



Konvergenz: $\varepsilon = (b-a) \cdot \left(\frac{1}{2}\right)^n$

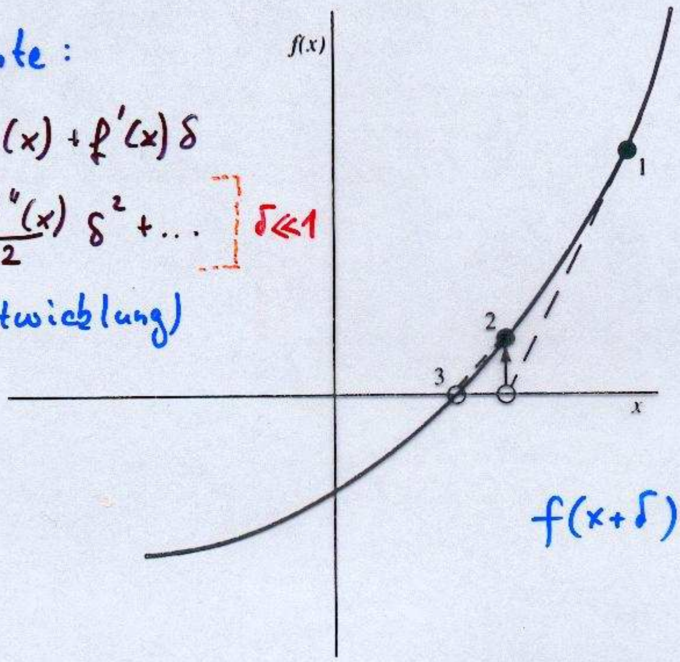
$$\varepsilon_{i+1} = \frac{1}{2} \varepsilon_i = \frac{1}{2} \varepsilon_i^1$$ lineare Konvergenz

$$\varepsilon_i = (b-a) \cdot \left(\frac{1}{2}\right)^i$$

Tangente statt Sekante:

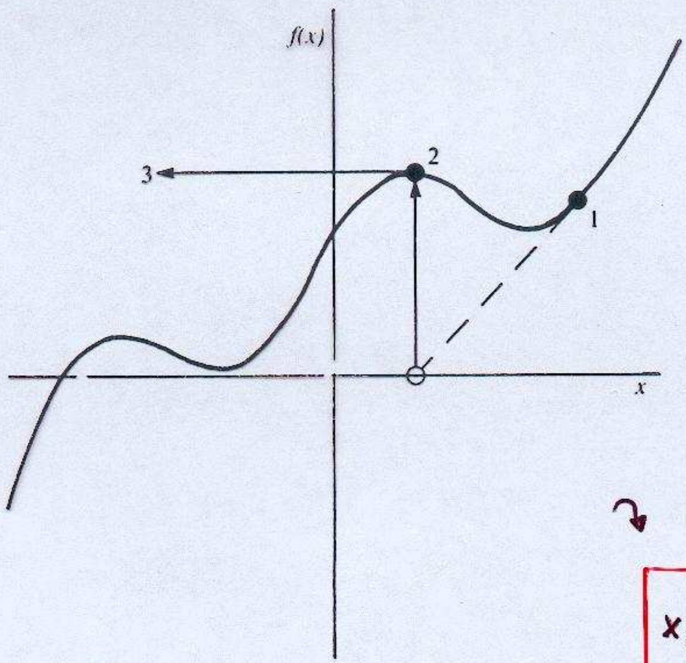
$$f(x+\delta) = f(x) + f'(x)\,\delta + \frac{f''(x)}{2}\,\delta^2 + \dots \qquad \delta \ll 1$$

(Taylor-Entwicklung)



$$f(x+\delta) = 0 \iff \delta = -\frac{f(x)}{f'(x)}$$

Figure 9.4.1. Newton's method extrapolates the local derivative to find the next estimate of the root. In this example it works well and converges quadratically.



Nullstelle der Tangente:

$$f(x+\delta) = f(x) + f'(x)\,\delta = 0$$

$$\curvearrowright \ \delta = -\frac{f(x)}{f'(x)}$$

$$\boxed{x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}}$$

Figure 9.4.2. Unfortunate case where Newton's method encounters a local extremum and shoots off to outer space. Here bracketing bounds, as in RTSAFE, would save the day.

Konvergenzbedingungen fürs Newtonverfahren:

x_0 : wahre Nullstelle

$$\underbrace{x_{i+1} - x_0}_{\varepsilon_{i+1}} = \underbrace{x_i - x_0}_{\varepsilon_i} - \frac{f(x_i)}{f'(x_i)}$$

Taylorentwicklung:

$$f(x_i) = f(x_0 + \varepsilon_i) = f(x_0) + \varepsilon_i f'(x_0) + \frac{\varepsilon_i^2}{2} f''(x_0)$$

$$\varepsilon_{i+1} = \varepsilon_i - \frac{f(x_0) + \varepsilon_i f'(x_0) + \varepsilon_i^2 f''(x_0)/2}{f'(x_i)}$$

$$f'(x_i) \approx f'(x_0)$$

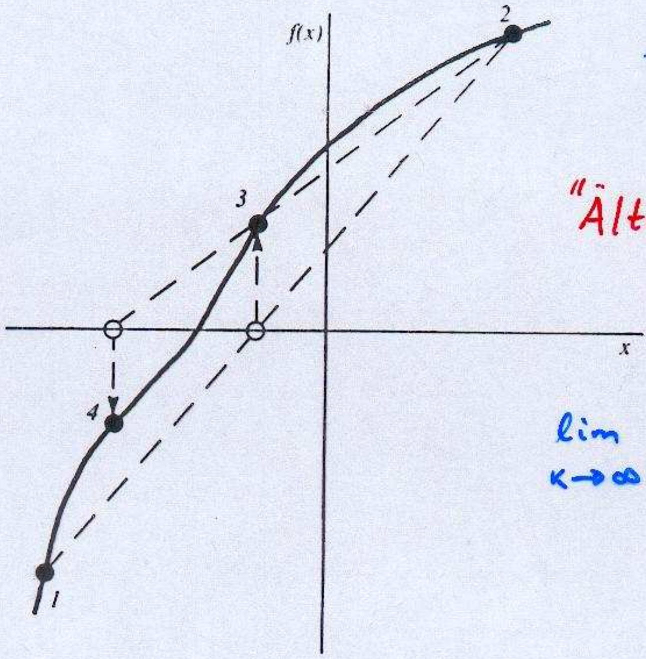
$$\varepsilon_{i+1} = \varepsilon_i - \frac{0}{f'(x_i)} - \varepsilon_i \underbrace{\frac{f'(x_0)}{f'(x_i)}}_{\approx 1} - \varepsilon_i^2 \frac{f''(x_0)}{2f'(x_i)}$$

$$\varepsilon_{i+1} = -\varepsilon_i^2 \frac{f''(x_0)}{2f'(x_0)} = \varepsilon_i^2 \cdot c$$ quadratische Konv.

relative Genauigkeit: $r_i = \frac{\varepsilon_i}{x_0}$

$$r_{i+1} = \frac{\varepsilon_{i+1}}{x_0} = \frac{r_i^2 x_0^2 \cdot c}{x_0} = -r_i^2 \cdot x_0 \frac{f''(x_0)}{2f'(x_0)}$$

Konvergenzbedingung: $\left| x_0 \frac{f''(x_0)}{2f'(x_0)} \right| < 1$

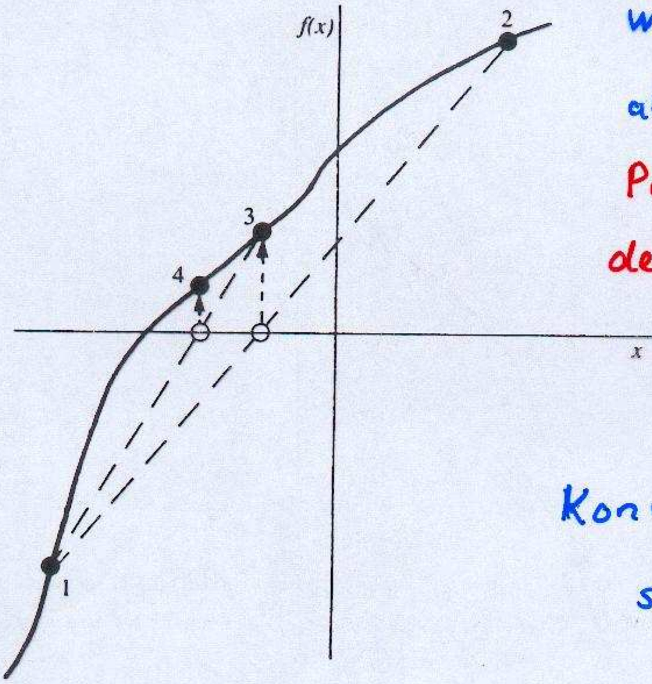


Sekanten-verfahren:

„Ältesten" Punkt verwerfen

$$\lim_{k\to\infty} \varepsilon_{k+1} \approx c \cdot |\varepsilon_k|^{1.618}$$

Figure 9.2.1. Secant method. Extrapolation or interpolation lines (dashed) are drawn through the two most recently evaluated points, whether or not they bracket the function. The points are numbered in the order that they are used.



Regula falsi

wie Sekantenverf.

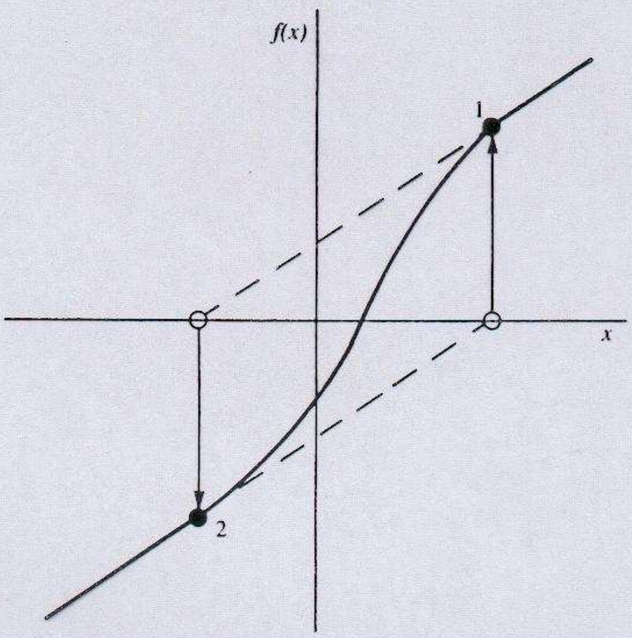
aber:

Punkt verwerfen, der die Nullstelle NICHT einschließt.

Konvergenz: langsamer sicherer

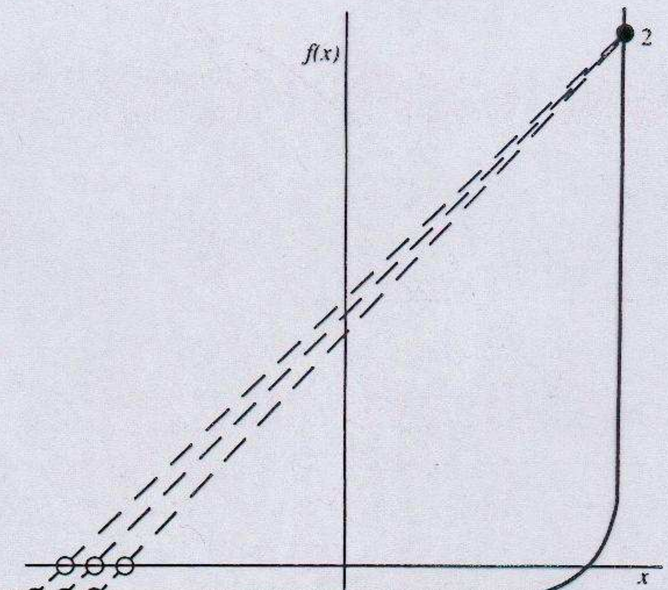
Figure 9.2.2. False position method. Interpolation lines (dashed) are drawn through the most recent points *that bracket the root.* In this example, point 1 thus remains "active" for many steps. False position converges less rapidly than the secant method, but it is more certain.

Problemfälle:



Newton

Figure 9.4.3. Unfortunate case where Newton's method enters a nonconvergent cycle. This behavior is often encountered when the function f is obtained, in whole or in part, by table interpolation. With a better initial guess, the method would have succeeded.



Sekanten verfahren

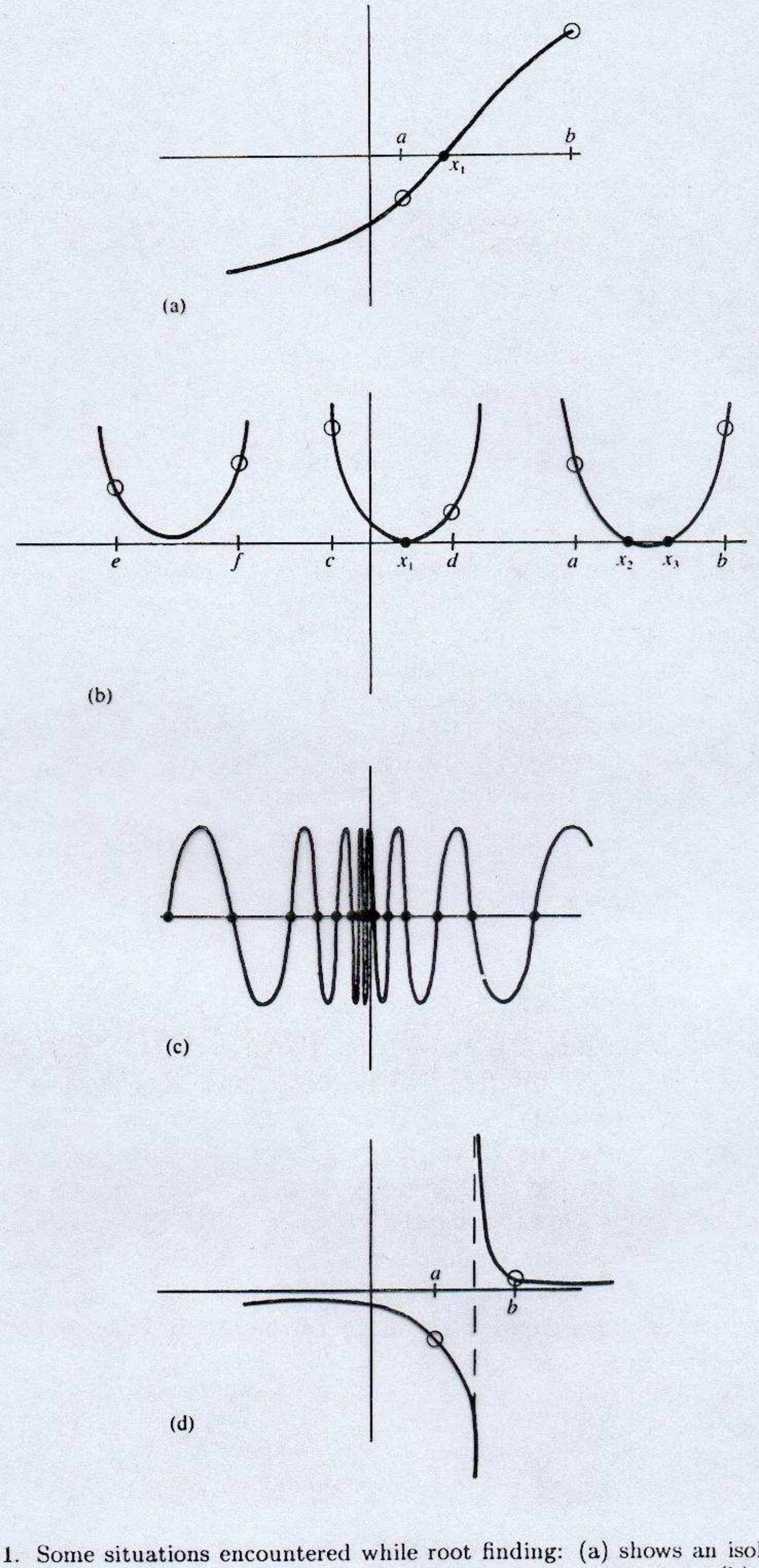


Figure 9.1.1. Some situations encountered while root finding: (a) shows an isolated root x_1 bracketed by two points a and b at which the function has opposite signs; (b) illustrates that there is not necessarily a sign change in the function near a double root (in fact, there is not necessarily a root!); (c) is a pathological function with many roots; in (d) the function has opposite signs at points a and b, but the points bracket a singularity, not a root.

Fixpunkt - Verfahren

Umformung: $f(x) = 0 \rightarrow x = \phi(x)$ NICHT eindeutig:

z.B.: $f(x) = \exp(-x) - \frac{0.1}{1+x} = 0$

a) $1 + x = 0.1 \cdot \exp(x)$

$$x = \underbrace{0.1 \exp(x) - 1}$$

$\phi_1(x)$, $\phi_1'(x) = 0.1 \exp(x)$

$x_1 = 4$: $\phi_1'(4) = 5.5$ (>1)

b) $\exp(x) = \frac{1+x}{0.1} = 10(1+x)$

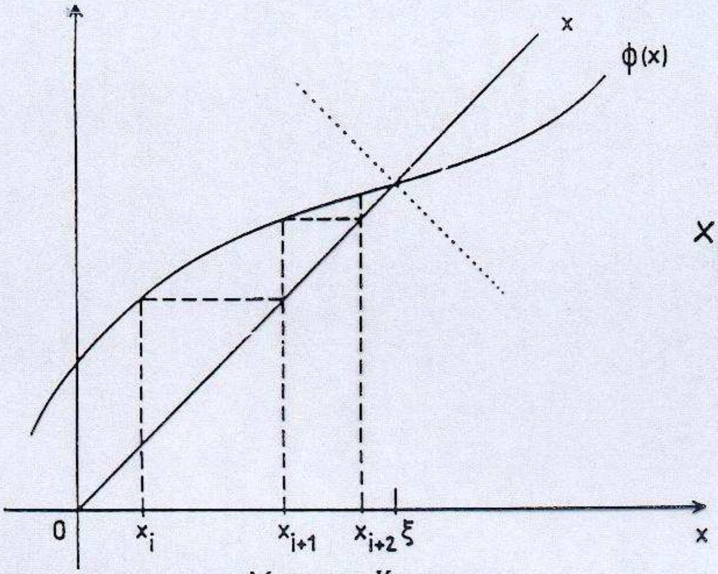
$$x = \underbrace{\ln(10(1+x))}$$

$\phi_2(x)$, $\phi_2'(x) = \frac{10}{10(1+x)} = \frac{1}{1+x}$

$x_1 = 4$: $\phi_2'(4) = \frac{1}{1+4} = 0.2$ (<1)

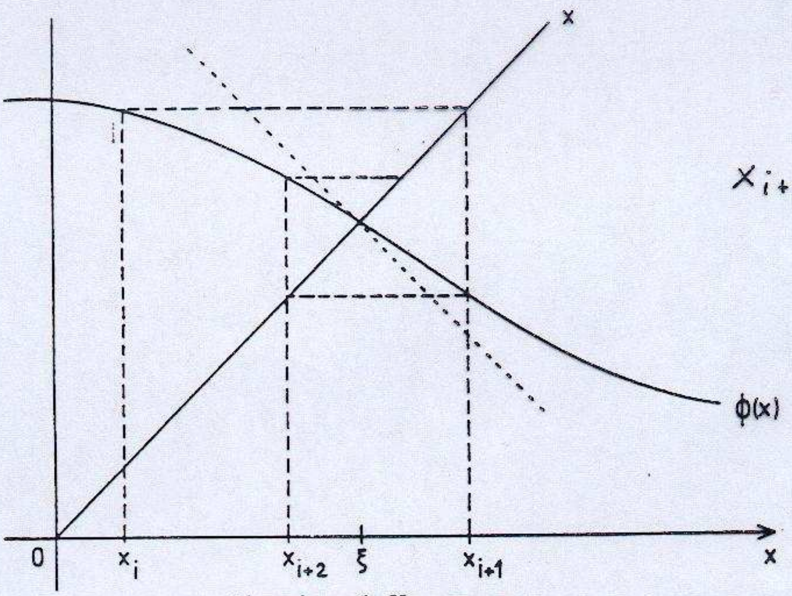
Fixpunktverfahren
(einfache Iteration)

$x = \phi(x)$



Monotone Konvergenz

$x_{i+1} = \phi(x_i)$



Alternierende Konvergenz

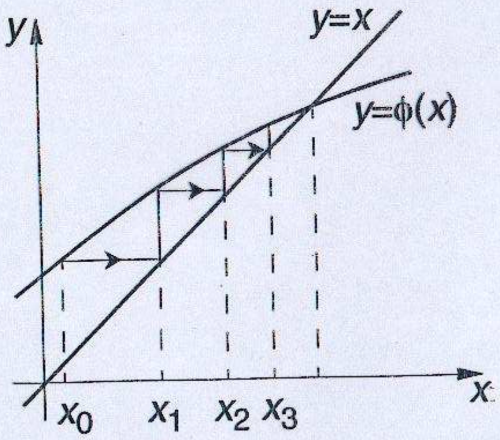
$x_{i+1} = \phi(x_i)$

Konvergenzbed.: Kontrahierde Abbildung:

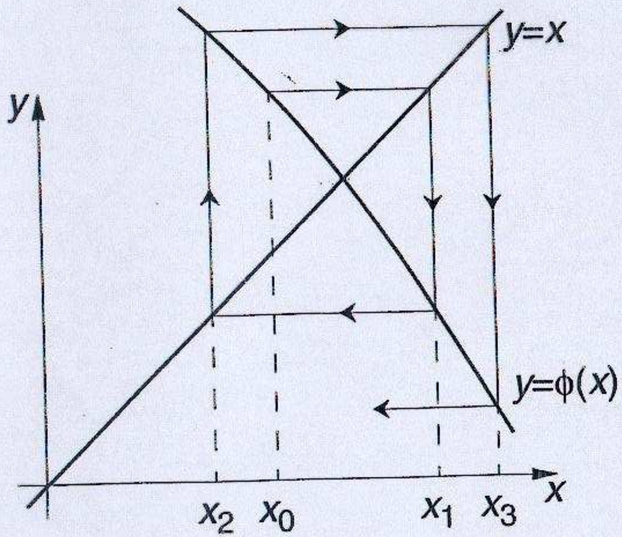
$|\phi'(x)| < 1$

Iteration

$$f(x)=0 \Leftrightarrow x=\phi(x) \qquad\qquad x_{n+1}=\phi(x_n)$$



Konvergenz



Divergenz

$|\phi'(x)| > 1$

$\rightarrow$ Divergenz

Der Iterationsprozeß konvergiert, wenn $|\phi'(x)| \leq k < 1$.

$|\phi'(x)| \leq k$ in einer Umgebung der Wurzel a $\Rightarrow |x_{n+1}-a| \leq \dfrac{k}{1-k}\,|x_{n+1}-x_n|$.

LUDWIGS-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

— SEKTION PHYSIK —

Joachim Puls · Sigmund Stintzing

Numerik für Physiker

Sebastian Bauer, Stephan Maciej, Benjamin Rieff

Wintersemester 2002/2003

Numerical Recipes
in FORTRAN
The Art of Scientific Computing
Second Edition

William H. Press

Harvard-Smithsonian Center for Astrophysics

Saul A. Teukolsky

Department of Physics, Cornell University

William T. Vetterling

Polaroid Corporation

Brian P. Flannery

EXXON Research and Engineering Company

CAMBRIDGE
UNIVERSITY PRESS