

# Numerische Verfahren

## ■ Numerische Auswertung symbolischer Ergebnisse

### ■ Numerische Auswertung von Ausdrücken

```
ClearAll["Global`*"]
```

```
N[Sin[ $\frac{\pi}{4}$ ]]
```

```
0.707107
```

```
N[Sin[ $\frac{\pi}{4}$ ], 60]
```

```
0.707106781186547524400844362104849039284835937688474036588340
```

Ist das Argument numerischer Natur und trägt der verarbeitende Funktionsbezeichner das Attribut **NumericFunction**, so wird beim Auswerten eine numerische Näherungsroutine aufgerufen. Da die Auswertung der **FullForm** `Sin[Times[Pi, Power[4., -1]]]` von innen nach außen stets einen numerischen Wert als Argument für den nächsten Funktionsaufruf liefert, wird letztlich ein numerischer Wert zurückgegeben.

```
Sin[ $\frac{\pi}{4.}$ ]
```

```
0.707107
```

Hier die Bestätigung, dass alle beteiligten Funktionen das Attribut **NumericFunction** tragen.

```
MemberQ[Attributes[#], NumericFunction] & /@ {Sin, Times, Power}
```

```
{True, True, True}
```

```
N[ $\sqrt{2}$ ] N[ $\sqrt{8}$ ] - 4
```

```
8.88178 × 10-16
```

```
% // Chop
```

```
0
```

```
 $\sqrt{2} \sqrt{8} - 4$ 
```

```
0
```

## Rechengenauigkeit

```
ClearAll["Global`*"]
```

```
$MachinePrecision
```

```
15.9546
```

Rechnungen werden standardmäßig mit Maschinengenauigkeit ausgeführt. **Precision** gibt in diesem Fall den symbolischen Wert **MachinePrecision** zurück, der numerisch (mit **N**) zu einem Zahlenwert ausgewertet wird, der auch in der Systemkonstanten **\$MachinePrecision** gespeichert ist. In früheren Versionen war dieser Wert ganzzahlig.

```
 $\sqrt{2.}$ 
```

```
1.41421
```

```
% // Precision
```

```
MachinePrecision
```

```
% // N
```

```
15.9546
```

```
 $\sqrt{2.^{30}}$ 
```

```
1.414213562373095048801688724210
```

```
% // Precision
```

```
30.301
```

```
 $a_1 = 0.3; b = \frac{1}{10};$ 
```

```
 $c_1 = N[a_1^b, 40]$ 
```

```
0.886568
```

```
Precision /@ {a1, b, c1}
```

```
{MachinePrecision, ∞, MachinePrecision}
```

```
0.325
```

```
0.300000000000000000000000000000
```

```
a2 = 0.300000000000000000000000000000;
```

```
c2 = N[a2b, 40]
```

```
0.8865681505652133345154271
```

```
u = Precision /@ {a2, b, c2}
```

```
{24.4771, ∞, 25.4771}
```

```

MachineNumberQ /@ {a1, a2, c1, c2}

{True, False, True, False}

a3 = N[π2, 30]
b3 = N[π, 35]2

9.86960440108935861883449099988

9.869604401089358618834490999876151

a3 // InputForm

9.86960440108935861883449099987615113532`30.

Precision[12 345.1234567890123456789]
Accuracy[12 345.1234567890123456789]

23.0915

19.

c3 = a3 - b3

0. × 10-30

Precision /@ {a3, b3, c3}

{30., 34.699, 0.}

```

Ungenaue Eingaben an wenig signifikanter Stelle haben auf die Ergebnisgenauigkeit geringen Einfluss, so dass sich in einem solchen Fall die Genauigkeit auch vergrößern kann.

```

105 + c2

100 000.8865681505652133345154271

% // Precision

30.5294

```

## ■ Näherungswerte in exakte Werte verwandeln

```

ClearAll["Global`*"]

u =  $\frac{5.}{17}$ 
Rationalize[u]

0.294118

 $\frac{5}{17}$ 

```

Diese beiden Rechnungen sehen zwar gleich aus, sind es aber nicht!

```
u1 = 3.14159
Rationalize[u1]

3.14159


$$\frac{314159}{100000}$$


u2 = N[ $\pi$ ]
Rationalize[u2]

3.14159

3.14159

InputForm /@ {u1, u2}

{3.14159, 3.141592653589793}
```

Die Umwandlung kann man erzwingen, indem als Präzision 0 angegeben wird.

```
Rationalize[u2, 0.007]
% - N[ $\pi$ , 20]


$$\frac{22}{7}$$


0.0012644892673496187

Rationalize[u2, 0]
% - N[ $\pi$ , 25]


$$\frac{245850922}{78256779}$$


 $-7.8179366 \times 10^{-17}$ 

Rationalize[N[ $\pi$ , 40], 0]
% - N[ $\pi$ , 50]


$$\frac{262452630335382199398}{83541266890691994833}$$


 $1.011863227 \times 10^{-40}$ 
```

## ■ Gleichungen numerisch lösen

### ■ Solve und NSolve

```
ClearAll["Global`*"]
```



```
red = Reduce[sys, {x, y}, Backsubstitution -> True]
```

```
(x == 0 && y == 1) || (x == 1 && y == 0) ||  

(x == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 1], {0, 1, 0, 0}] &&  

  y == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 1], {0, 1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 2], {0, 1, 0, 0}] &&  

  y == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 2], {0, 1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 3], {0, 1, 0, 0}] &&  

  y == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 3], {0, 1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 4], {0, 1, 0, 0}] &&  

  y == AlgebraicNumber[Root[-1 + #1^3 + #1^4 &, 4], {0, 1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 1],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 1], {-2, -2, -1, -1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 2],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 2], {-2, -2, -1, -1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 3],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 3], {-2, -2, -1, -1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 4],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 4], {-2, -2, -1, -1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 5],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 5], {-2, -2, -1, -1, 0, 0}]) ||  

(x == AlgebraicNumber[Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 6],  

  {0, 1, 0, 0, 0, 0}] && y == AlgebraicNumber[  

  Root[3 + 5 #1 + 6 #1^2 + 6 #1^3 + 4 #1^4 + 2 #1^5 + #1^6 &, 6], {-2, -2, -1, -1, 0, 0}])
```

```

sol = {red // N // ToRules}

{{x → 0., y → 1.}, {x → 1., y → 0.}, {x → -1.38028, y → -1.38028},
 {x → 0.819173, y → 0.819173}, {x → -0.219447 - 0.914474 i, y → -0.219447 - 0.914474 i},
 {x → -0.219447 + 0.914474 i, y → -0.219447 + 0.914474 i},
 {x → -1.04414 - 0.390425 i, y → -0.188646 + 1.18298 i},
 {x → -1.04414 + 0.390425 i, y → -0.188646 - 1.18298 i},
 {x → -0.188646 - 1.18298 i, y → -1.04414 + 0.390425 i},
 {x → -0.188646 + 1.18298 i, y → -1.04414 - 0.390425 i},
 {x → 0.232786 - 1.27599 i, y → 0.232786 + 1.27599 i},
 {x → 0.232786 + 1.27599 i, y → 0.232786 - 1.27599 i}}

Eliminate[sys, y]

3 x3 + 2 x4 + x5 - 3 x6 - 7 x7 - 5 x8 - 2 x9 + x10 + 4 x11 + 3 x12 + 2 x13 + x14 == 0

f = FactorList[First[%]]

{{1, 1}, {-1 + x, 1}, {x, 3}, {-1 + x3 + x4, 1}, {3 + 5 x + 6 x2 + 6 x3 + 4 x4 + 2 x5 + x6, 1}}

GroebnerBasis[Prepend[sys, f[[5, 1]] == 0], {y, x}]

{3 + 5 x + 6 x2 + 6 x3 + 4 x4 + 2 x5 + x6, 2 + 2 x + x2 + x3 + y}

sys /. sol

{{True, True}, {True, True}, {True, True}, {True, True},
 {False, False}, {False, False}, {True, False}, {True, False},
 {False, False}, {False, False}, {False, False}, {False, False}}

esys = First /@ sys

{x4 + y3, x3 + y4}

esys /. sol

{{1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1. - 2.22045 × 10-16 i, 1. - 2.22045 × 10-16 i},
 {1. + 2.22045 × 10-16 i, 1. + 2.22045 × 10-16 i}, {1. + 0. i, 1. + 4.44089 × 10-16 i},
 {1. + 0. i, 1. - 4.44089 × 10-16 i}, {1. - 2.22045 × 10-16 i, 1. + 2.22045 × 10-16 i},
 {1. + 2.22045 × 10-16 i, 1. - 2.22045 × 10-16 i},
 {1. - 2.22045 × 10-16 i, 1. + 1.11022 × 10-15 i}, {1. + 2.22045 × 10-16 i, 1. - 1.11022 × 10-15 i}}

```

**NSolve** liefert dasselbe Ergebnis wie **Solve[sys,vars]/N**, jedoch deutlich schneller und in einer anderen Reihenfolge.

```

(nsol = NSolve[sys, {x, y}];) // Timing

{0.09, Null}

nsol // Length
nsol // Union // Length

16

12

```

```
sys /. nsol
```

```
{{False, False}, {False, False}, {False, False}, {False, False}, {False, False},
{False, False}, {True, True}, {True, True}, {True, True}, {True, True}, {True, True},
{True, True}, {False, False}, {False, False}, {False, False}, {False, False}, {True, True}}
```

```
esys /. nsol
```

```
{{1. - 3.55271 × 10-15 i, 1. + 5.55112 × 10-15 i},
{1. + 3.55271 × 10-15 i, 1. - 5.55112 × 10-15 i}, {1. + 5.77316 × 10-15 i, 1. - 4.21885 × 10-15 i},
{1. - 5.77316 × 10-15 i, 1. + 4.21885 × 10-15 i}, {1. - 1.39888 × 10-14 i, 1. + 1.9984 × 10-15 i},
{1. + 1.39888 × 10-14 i, 1. - 1.9984 × 10-15 i}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.},
{1., 1.}, {1., 1.}, {1., 1.}, {1. + 5.77316 × 10-15 i, 1. + 6.88338 × 10-15 i},
{1. - 5.77316 × 10-15 i, 1. - 6.88338 × 10-15 i}, {1., 1.}}
```

```
% // Chop
```

```
{{1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.},
{1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}, {1., 1.}}
```

```
red = Reduce[sys, {x, y}, Reals]
```

```
(x == 0 && y == 1) || (x == 1 && y == 0) ||
```

```
(x == AlgebraicNumber[Root[-1 + #13 + #14 &, 1], {0, 1, 0, 0}] &&
```

```
y == AlgebraicNumber[Root[-1 + #13 + #14 &, 1], {0, 1, 0, 0}]) ||
```

```
(x == AlgebraicNumber[Root[-1 + #13 + #14 &, 2], {0, 1, 0, 0}] &&
```

```
y == AlgebraicNumber[Root[-1 + #13 + #14 &, 2], {0, 1, 0, 0}])
```

```
{red // N // ToRules}
```

```
{{x → 0., y → 1.}, {x → 1., y → 0.},
{x → -1.38028, y → -1.38028}, {x → 0.819173, y → 0.819173}}
```

```
Select[nsol // Union, (x /. #) ∈ Reals &]
```

```
{{x → -1.38028, y → -1.38028}, {x → 0., y → 1.},
{x → 0.819173, y → 0.819173}, {x → 1., y → 0.}}
```

## ■ Nullstellenbestimmung mit FindRoot

Essentiell transzendente Gleichungen lassen sich mit den Kommandos **Solve**, **NSolve** oder **Reduce** nicht bearbeiten.

```
g1 = Log[1 + x] + Log[3 + x] + x;
```



```
Solve[g1 == 5, x]
```

```
Solve::tdep :
```

The equations appear to involve the variables to be solved for in an essentially non-algebraic way.

```
Solve[x + Log[1 + x] + Log[3 + x] == 5, x]
```

```
Reduce[g1 == 5, x]
```

```
Reduce::nsmet :
```

This system cannot be solved with the methods available to Reduce.

```
Reduce[x + Log[1 + x] + Log[3 + x] == 5, x]
```

```
NSolve[g1 == 5, x]
```

```
Solve::tdep :
```

The equations appear to involve the variables to be solved for in an essentially non-algebraic way.

```
NSolve[x + Log[1 + x] + Log[3 + x] == 5, x]
```

```
FindInstance[g1 == 5, x]
```

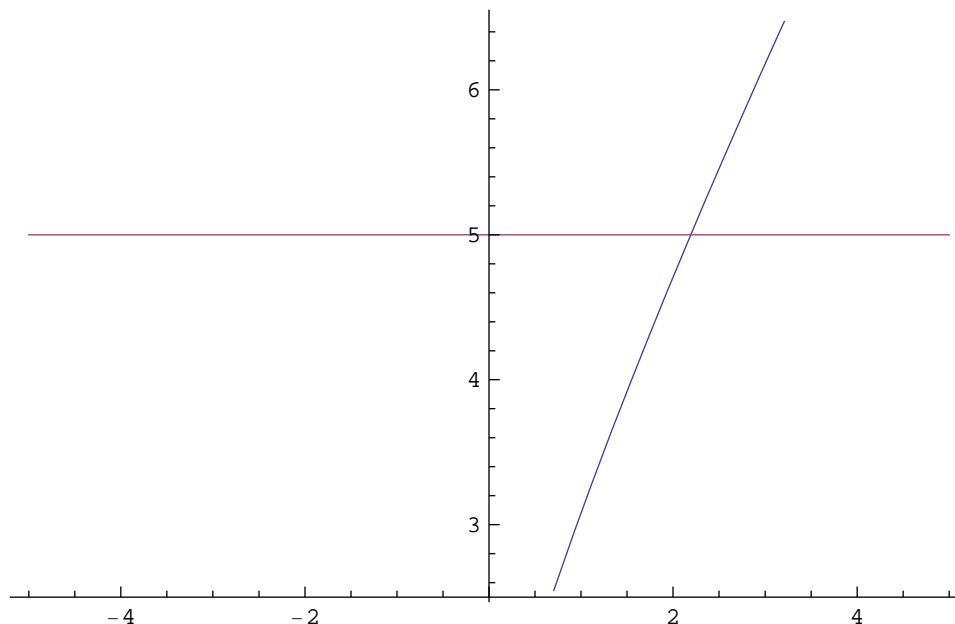
```
FindInstance::nsmet :
```

The methods available to FindInstance are insufficient to find the requested instances or prove they do not exist.

```
FindInstance[x + Log[1 + x] + Log[3 + x] == 5, x]
```

Der Plot zeigt, dass eine reelle Lösung von  $g1=5$  in der Nähe von  $x=2$  liegt.

```
Plot[{g1, 5}, {x, -5, 5}]
```



Diese kann mit **FindRoot** bestimmt werden.

```
FindRoot[g1 == 5, {x, 2}]
```

```
{x → 2.19215}
```

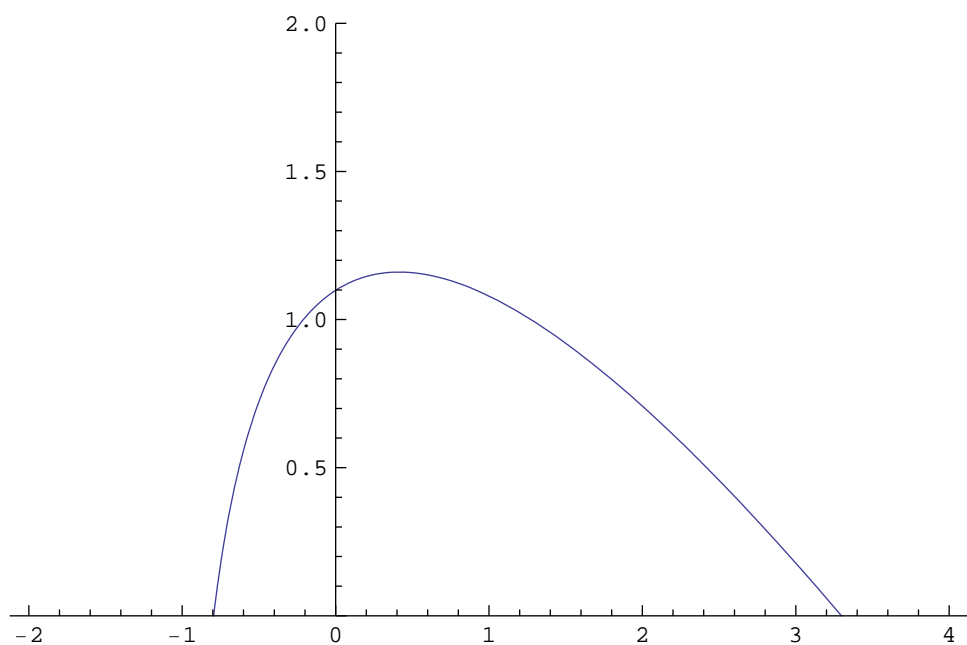
```
g1 /. %
```

```
5.
```

```
g2 = Log[1 + x] + Log[3 + x] - x
```

```
-x + Log[1 + x] + Log[3 + x]
```

```
Plot[g2, {x, -2, 4}, PlotRange -> {0, 2}]
```



```
FindRoot[g2 == 2, {x, -2}]
```

```
{x → -0.209427 + 1.66589 i}
```

```
FindRoot[g2 == 1, {x, -2}]
```

```
{x → 1.27428 - 2.32469 × 10-21 i}
```

```
FindRoot[g2 == 1, {x, 0}]
```

```
{x → -0.210511}
```

```
FindRoot[g2 == 2, {x, 0}]
```

```
FindRoot::nlnum:
```

```
The function value {Indeterminate} is not a list of numbers  
with dimensions {1} at {x} = {-1.}.
```

```
{x → 0.419252}
```

```
g2 /. %
```

```
1.1603
```

```
FindRoot[g2 == 2, {x, 0 + 0.001 I}]
```

```
{x → -0.209427 + 1.66589 i}
```

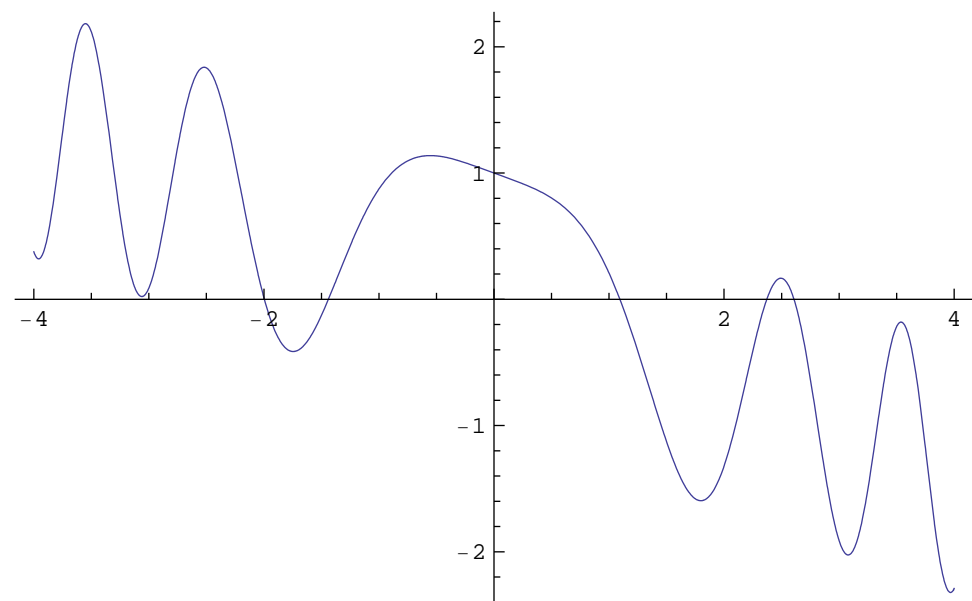
```
sys = {x2 + y2 == 10, xy == 2};
```

```
FindRoot[sys, {x, 1}, {y, 1}]
```

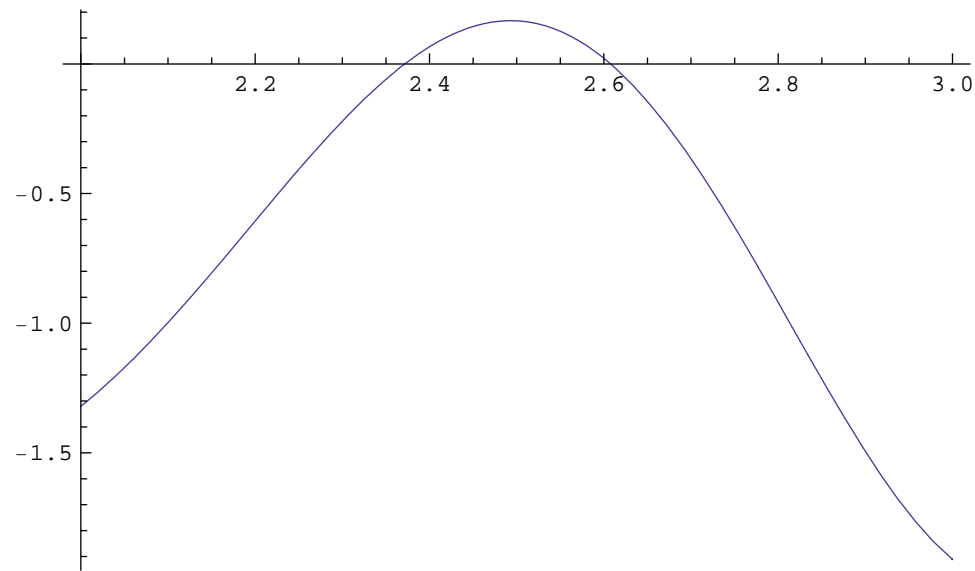
```
{x → 1.27043, y → 2.89586}
```

```
f := Cos[x2] -  $\frac{x}{3}$ ;
```

```
Plot[f, {x, -4, 4}]
```



`Plot[f, {x, 2, 3}]`



Nullstellenbestimmung mit dem Newtonverfahren.

`FindRoot[f == 0, {x, #}] & /@ {2.4, 2.6}`

`{{x -> 2.3715}, {x -> 2.60774}}`

Nullstellenbestimmung mit dem Sekantenverfahren. Hierfür muss  $f$  nicht symbolisch differenzierbar sein.

`FindRoot[f, {x, 2.4, 3}]`

`{x -> 2.60774}`

Problem: Die Nullstelle kann in einem Extremwert liegen.

`FindRoot[f^2 == 0, {x, 3}]`

`{x -> 2.60774}`

Analyse in der Nähe von  $x=3.5$ : Suche mit Startwert und Intervallbegrenzung

```
FindRoot[f, {x, 3.5, 3.3, 3.7}]
```

```
FindRoot::lstol :
```

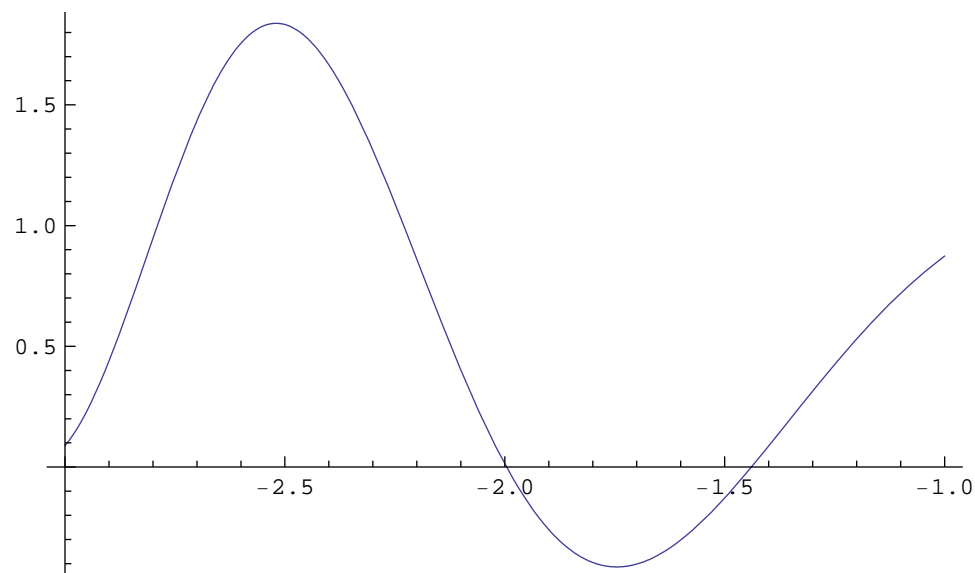
The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
{x → 3.53826}
```

```
FindMaximum[f, {x, 3.5}]
```

```
{-0.180528, {x → 3.53826}}
```

```
Plot[f, {x, -3, -1}]
```



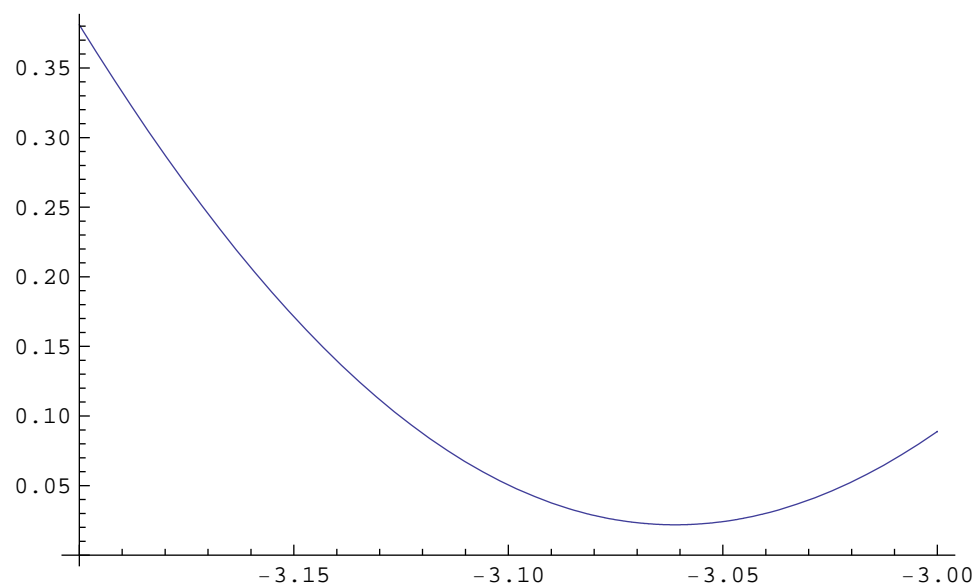
```
FindRoot[f == 0, {x, #}] & /@ {-2, -1.5}
```

```
{{x → -1.9961}, {x → -1.43914}}
```

```
Plot[f, {x, -4, -3}]
```



```
Plot[f, {x, -3.2, -3}]
```



```
FindRoot[f, {x, -3.0}]
```

```
FindRoot::lstol:
```

The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
{x → -3.0611}
```

```
FindRoot[f, {x, -3.1, -3.0}]

FindRoot::cvmit: Failed to converge to the
  requested accuracy or precision within 100 iterations.
{x -> -3.10075}

FindMinimum[f, {x, -3.0}]

{0.0218484, {x -> -3.0611}}
```

## ■ Numerische Integration

```
ClearAll["Global`*"]
```

Numerische Bestimmung definierter Integrale ist eine Möglichkeit, wenn keine Stammfunktion in Termini anderer Funktionen berechnet werden kann.

```
Integrate[Sin[x^2 + Cos[x]], {x, 0, 2}]


$$\int_0^2 \sin[x^2 + \cos[x]] \, dx$$


% // N

1.48203
```

Das Ergebnis von **Integrate**[f,{x,a,b}]/N und **NIntegrate**[f,{x,a,b}] ist dasselbe.

**NIntegrate** geht in einem solchen Fall aber schneller, weil der Aufwand zur Feststellung, dass es keine Stammfunktion in geschlossener Form gibt, nicht anfällt.

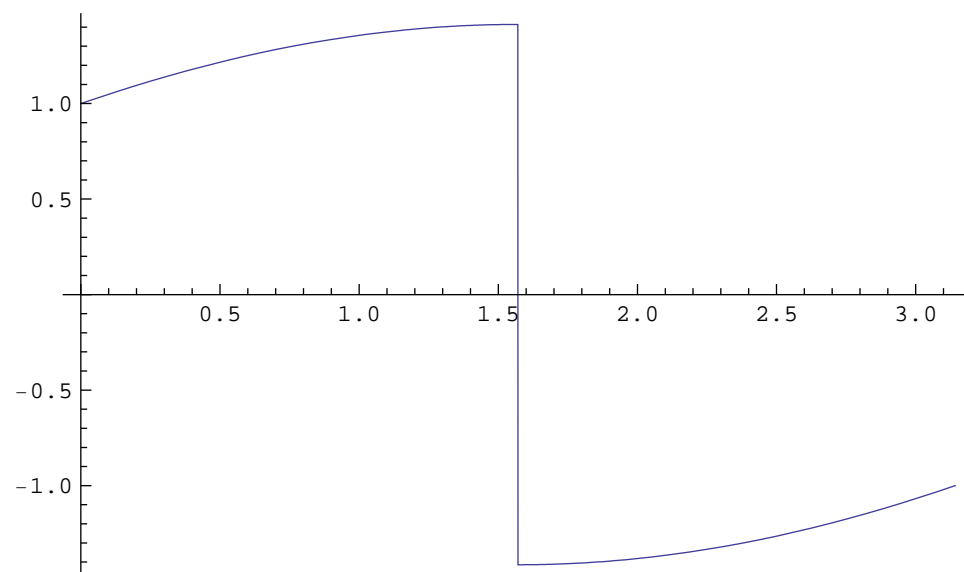
```
NIntegrate[Sin[x^2 + Cos[x]], {x, 0, 2}]

1.48203
```

Integration einer Funktion mit Sprungstelle im Integrationsintervall.

```
f =  $\frac{\cos[x]}{\sqrt{1 - \sin[x]}}$ ;
```

```
Plot[f, {x, 0,  $\pi$ }]
```



```
sf[x_] =  $\int f \, dx$  // Simplify
```

```
 $-2 \sqrt{1 - \sin[x]}$ 
```

```
 $\int_0^{\pi/2} f \, dx$ 
```

```
2
```

```
NIntegrate[f, {x, 0,  $\frac{\pi}{2}$ }]
```

```
2.
```

```
 $\int_0^{3\pi/4} f \, dx$ 
```

```
 $2 - \sqrt{4 - 2\sqrt{2}}$ 
```

```
% // N
```

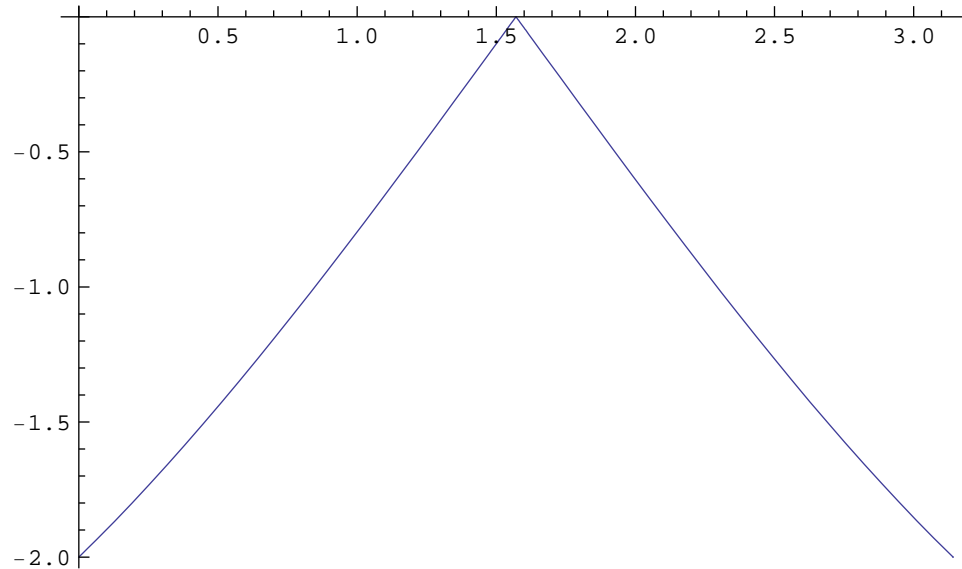
```
0.917608
```

```
sf[ $\frac{3\pi}{4}$ ] - sf[0] // Simplify
```

```
 $2 - \sqrt{4 - 2\sqrt{2}}$ 
```



```
Plot[sf[x], {x, 0,  $\pi$ }]
```



```
NIntegrate[f, {x, 0,  $\frac{3\pi}{4}$ }]
```

```
NIntegrate::slwcon:
```

Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

```
NIntegrate::ncvb:
```

NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in x near {x} = {1.5693}. NIntegrate obtained 0.9170805749970934` and 0.0008453999243025678` for the integral and error estimates.

```
0.917081
```

```
NIntegrate[f, {x, 0,  $\frac{3\pi}{4}$ }, MaxRecursion -> 20]
```

```
NIntegrate::slwcon:
```

Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

```
0.917607
```

```
NIntegrate[f, {x, 0,  $\frac{3\pi}{4}$ }, MaxRecursion -> 40, WorkingPrecision -> 20]
```

```
NIntegrate::slwcon:
```

Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

```
0.91760779972387813954
```

```
NIntegrate[f, {x, 0,  $\frac{\pi}{2}$ ,  $\frac{3\pi}{4}$ }]
```

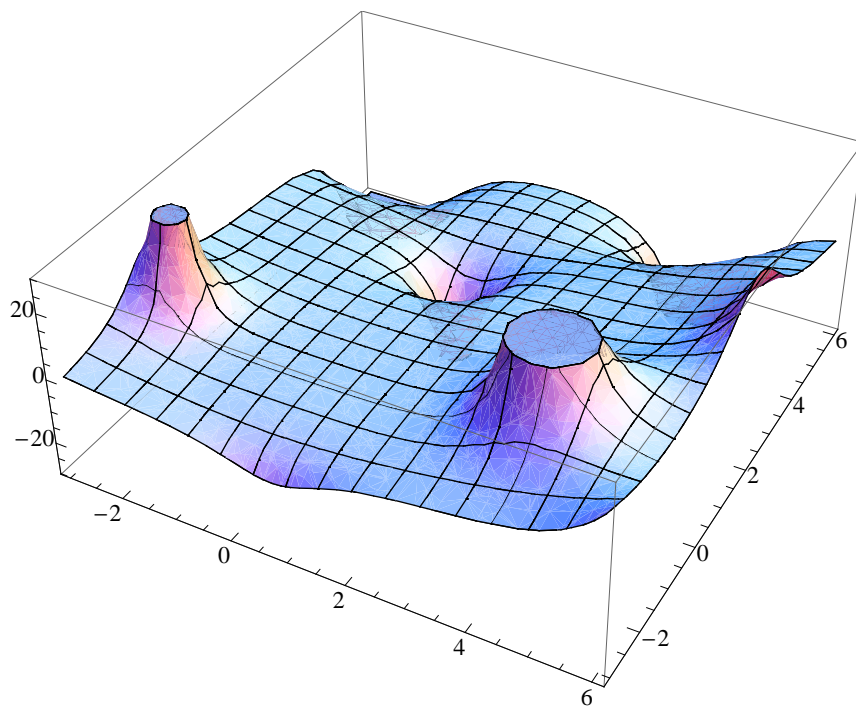
```
0.917608
```

Beispiel: Mehrdimensionales Integral

```
Clear[f]
```

```
f :=  $\frac{x^2 - y^2}{\cos[x + y] + \sin[x - y] + \frac{21}{10}};$ 
```

```
Plot3D[f, {x, -3, 6}, {y, -3, 6}]
```



**Integrate** kommt hier in vernünftiger Zeit gar nicht durch. Das Kommando ist deshalb auskommentiert.

```
(* (i=Integrate[f,{x,-3,6},{y,-3,6}];)//Timing *)
```

```

NIntegrate[f, {x, -3, 6}, {y, -3, 6}] // Timing

NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the
  following: singularity, value of the integration is 0,
  highly oscillatory integrand, or WorkingPrecision too small.

{1.38, -109.52}

NIntegrate[f, {x, -3, 6}, {y, -3, 6},
  WorkingPrecision -> 15] // Timing

NIntegrate::slwcon :
  Numerical integration converging too slowly; suspect one of the
  following: singularity, value of the integration is 0,
  highly oscillatory integrand, or WorkingPrecision too small.

{12.66, -109.519572644826}

%[[2]] // Precision

15.

```

## ■ Datenanalyse

### ■ Fit mit vorgegebenen Basisfunktionen

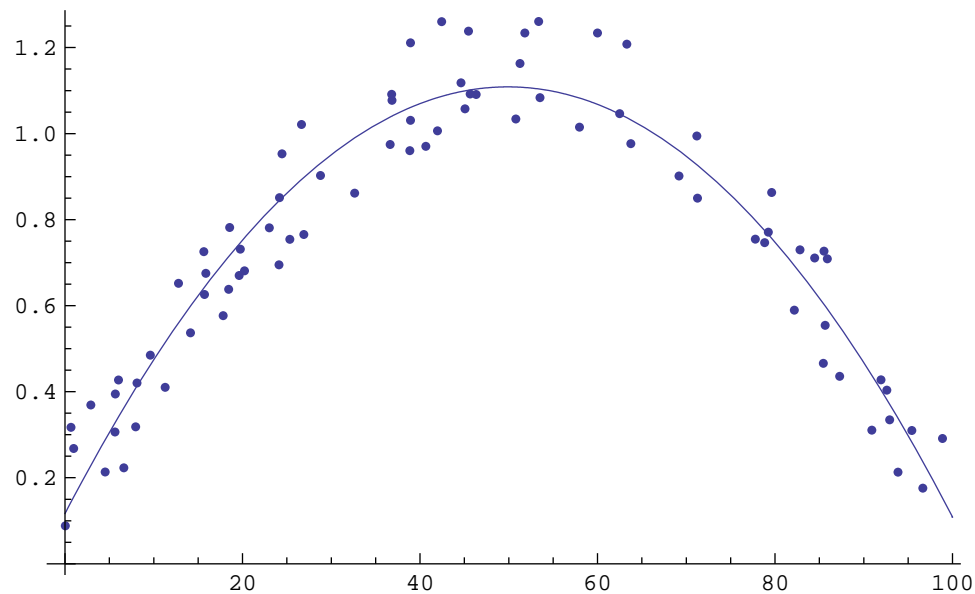
```

ClearAll["Global`*"]
list1 = Table[Random[Real, 100], {80}];
data = {#, Sin[ $\frac{\#}{100}$  Pi] + Random[Real, 0.3]} & /@ list1;
gr0 = ListPlot[data, PlotStyle -> PointSize[0.01]];

```

```
f1 = Fit[data, {1, x, x^2}, x]
gr1 = Plot[f1, {x, 0, 100}];
Show[{gr0, gr1}]
```

$0.116791 + 0.0397563 x - 0.000398392 x^2$



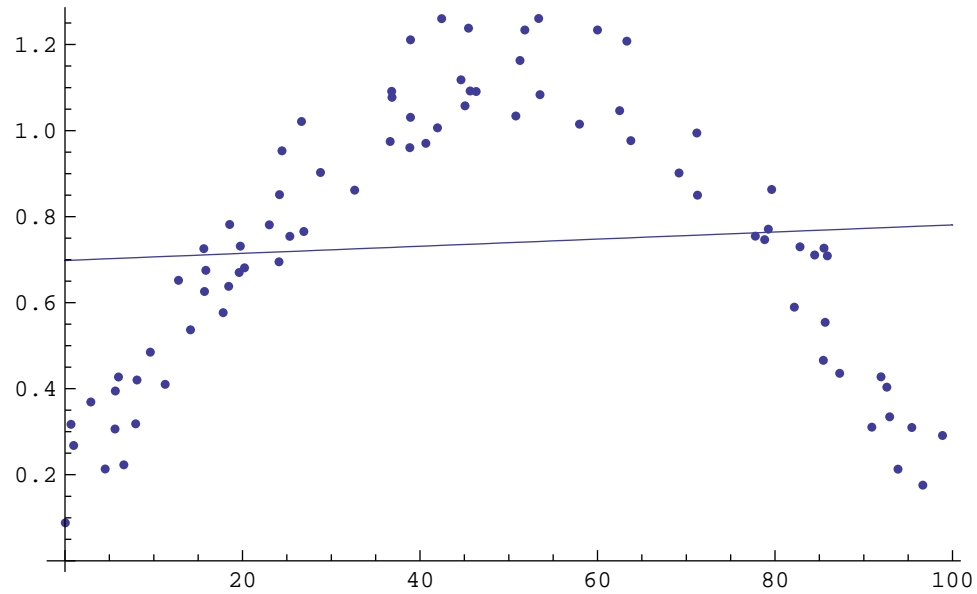
Dieselbe Aufgabe mit **FindFit**.

```
FindFit[data, f1a = a x^2 + b x + c, {a, b, c}, x];
f1a /. %
```

$0.116791 + 0.0397563 x - 0.000398392 x^2$

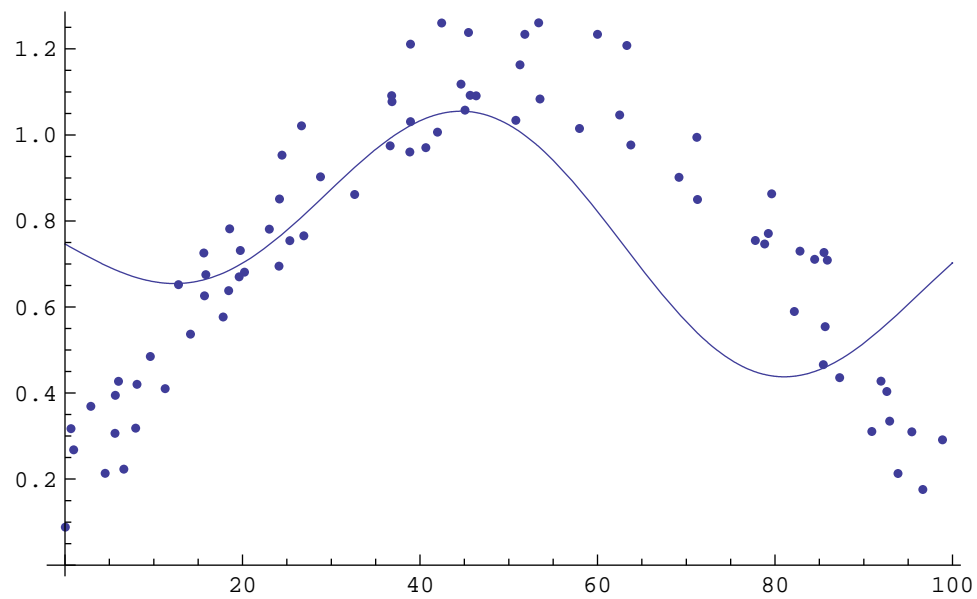
```
f2 = Fit[data, {1, x}, x]  
gr2 = Plot[f2, {x, 0, 100}];  
Show[{gr0, gr2}]
```

$0.698034 + 0.000827811 x$



```
f3 = Fit[data, {1, Sin[ $\frac{x}{10}$ ], Sin[ $\frac{x}{20}$ ]}, x]  
gr3 = Plot[f3, {x, 0, 100}];  
Show[{gr0, gr3}]
```

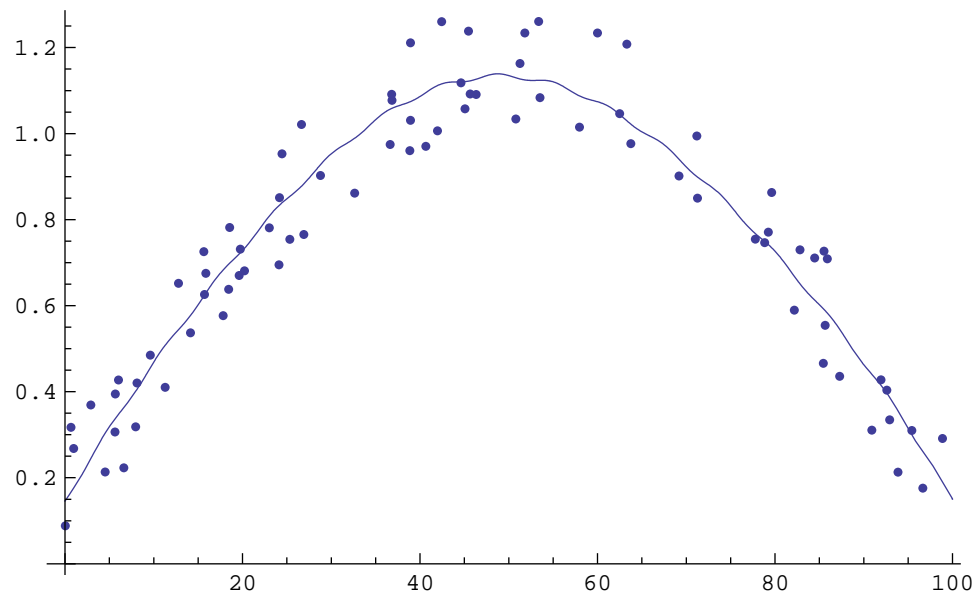
$0.74644 + 0.154888 \sin\left[\frac{x}{20}\right] - 0.192338 \sin\left[\frac{x}{10}\right]$



## ■ Regressionsanalyse (Regress)

```
f4 = Fit[data, {1, x, x^2, Sin[x], Sin[ $\frac{x}{10}$ ]}, x]
```

```
gr4 = Plot[f4, {x, 0, 100}];  
Show[{gr0, gr4}]
```

$$0.145863 + 0.0384732 x - 0.000386209 x^2 - 0.0307277 \sin\left[\frac{x}{10}\right] - 0.00510776 \sin[x]$$


Informationen über die Güte der Approximation liefert das Kommando **Regress** aus dem Paket **LinearRegression**. Standardmäßig wird die Parametertabelle ausgegeben, es gibt aber auch andere interessante Optionen.

```
Needs["LinearRegression`"]
```

```
Regress[data, {1, x, x^2, Sin[x], Sin[ $\frac{x}{10}$ ]}, x]
```

		Estimate	SE	TStat	PValue
{ParameterTable →	1	0.145863	0.0320593	4.54977	0.000020298
	x	0.0384732	0.00159762	24.0816	0.
	x <sup>2</sup>	-0.000386209	0.0000158051	-24.4357	1.87863 × 10 <sup>-37</sup> ,
	Sin[x]	-0.00510776	0.015009	-0.340313	0.734573
	Sin[ $\frac{x}{10}$ ]	-0.0307277	0.0174871	-1.75716	0.0829715
RSquared → 0.918915, AdjustedRSquared → 0.91459, EstimatedVariance → 0.00856012,					
ANOVATable →		DF	SumOfSq	MeanSq	FRatio
	Model	4	7.27571	1.81893	212.488
	Error	75	0.642009	0.00856012	0.
	Total	79	7.91772		

**RegressionReportValues[Regress]**

```
{AdjustedRSquared, ANOVATable, BestFit, BestFitParameters,
BestFitParametersDelta, CatcherMatrix, CoefficientOfVariation,
CookD, CorrelationMatrix, CovarianceMatrix, CovarianceMatrixDetRatio,
DurbinWatsonD, EigenstructureTable, EstimatedVariance, FitResiduals,
HatDiagonal, JackknifedVariance, MeanPredictionCITable, ParameterCITable,
ParameterConfidenceRegion, ParameterTable, PartialSumOfSquares, PredictedResponse,
PredictedResponseDelta, RSquared, SequentialSumOfSquares, SinglePredictionCITable,
StandardizedResiduals, StudentizedResiduals, SummaryReport, VarianceInflation}
```

■ **Nichtlineare Regression (FindFit)**

```
ClearAll["Global`*"]
data = Table[{x, 3 Sin[5 x] + Random[]}, {x, 0, 2 Pi, 0.01 Pi}];
f = a Sin[b x];
```

Nichtlineare Fits sind sehr von den Anfangswerten für die gewählten Parameter abhängig. Defaultstartwert für alle Parameter ist 1, was hier weit von den wirklichen Werten entfernt ist.

```
f1 = f /. FindFit[data, f, {a, b}, x]
```

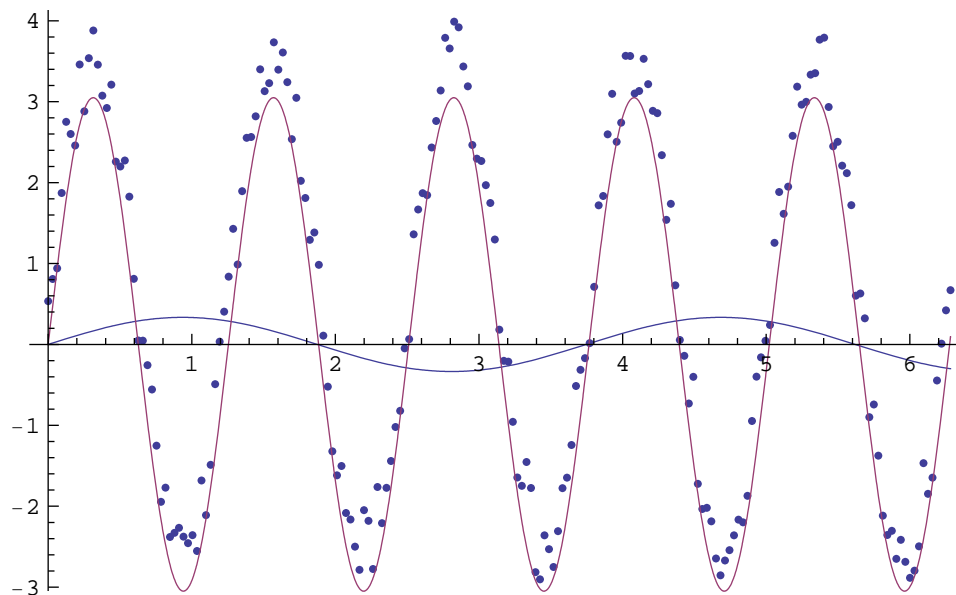
```
0.334611 Sin[1.67702 x]
```

Mit besseren Startwerten erhalten wir, trotz des hohen Rauschanteils in den Daten, einen sehr guten Fit.

```
f2 = f /. FindFit[data, f, {{a, 5}, {b, 5.2}}, x]
```

```
3.0494 Sin[5.00504 x]
```

```
Show[ ListPlot[data], Plot[{f1, f2}, {x, 0, 2 Pi}]]
```



```
data1 = Table[{x, 20 Sin[3 x] + 10 Exp[0.2 x] + 10 Random[]}, {x, 0, 2 Pi, 0.01 Pi}];
f = a Sin[b x] + c Exp[d x];
```

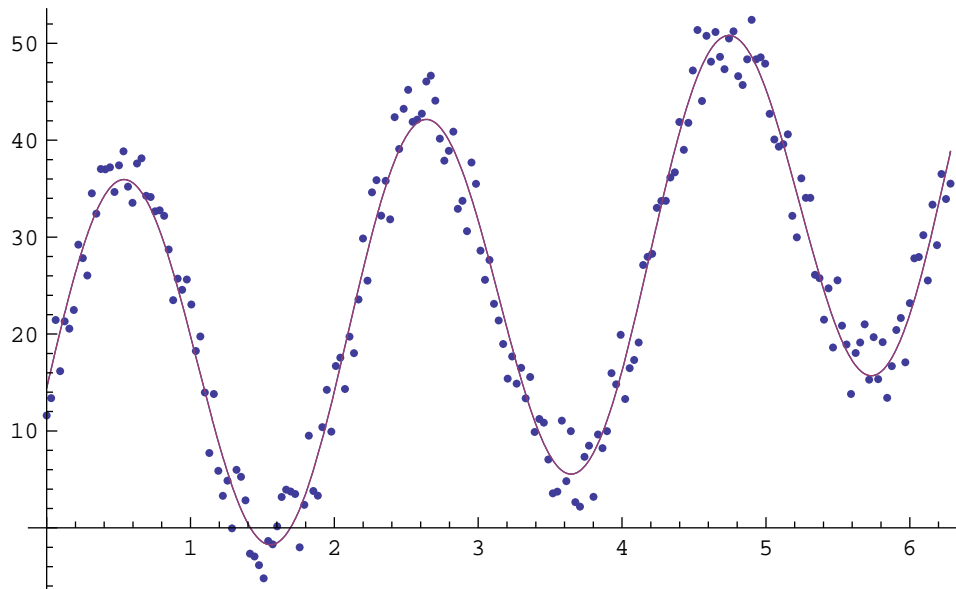
```
f1 = f /. FindFit[data1, f, {a, b, c, d}, x]

14.434 e0.15868 x + 20.2378 Sin[2.99776 x]

f2 = f /. FindFit[data1, f, {{a, 12.}, {b, 2.8}, {c, 7.}, {d, 0.3}}, x]

14.434 e0.15868 x + 20.2378 Sin[2.99776 x]

Show[ListPlot[data1], Plot[{f1, f2}, {x, 0, 2 Pi}]]
```



## ■ Zur Genauigkeit numerischer Rechnungen

### ■ PrecisionGoal, AccuracyGoal, WorkingPrecision

Normalerweise rechnet *Mathematica* mit Maschinengenauigkeit und verwendet dazu die schnelle interne Hardware-Arithmetik.

```
ClearAll["Global`*"]

sys = {x2 + y2 == 10, xy == 2};
sol = FindRoot[sys, {x, 1}, {y, 1}]
sol // Precision
% // N
sol // Accuracy

{x → 1.27043, y → 2.89586}

MachinePrecision

15.9546

15.4928
```



```

sol = FindRoot[sys , {x, 1}, {y, 1}, PrecisionGoal → 30]
% // Precision

{x → 1.27043, y → 2.89586}

MachinePrecision

sol = FindRoot[sys , {x, 1}, {y, 1}, WorkingPrecision → 20]
sol // Precision
sol // Accuracy

{x → 1.2704333456136053792, y → 2.8958589596789795152}

20.

19.5382

sol = FindRoot[sys , {x, 1}, {y, 1},
  WorkingPrecision → 20, AccuracyGoal → 4]
sol // Precision
sol // Accuracy

{x → 1.2704333456143941074, y → 2.8958589596788429836}

20.

19.5382

(First /@ sys) /. sol
% // Accuracy

{10.000000000001213301, 2.0000000000035303354}

18.699

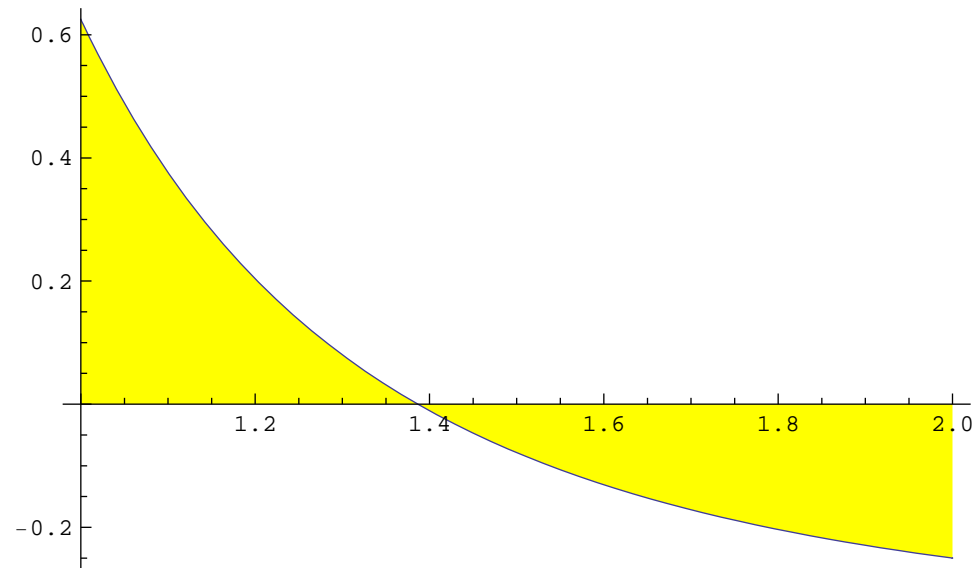
```

Bei schlecht konditionierten numerischen Problemen muss oft eine andere als die Standardeinstellung zwischen den verschiedenen Präzisionsparametern verwendet werden.

Im folgenden Beispiel lautet das exakte Ergebnis Null, so dass ein Näherungsverfahren mit Stellenauslöschung zu "kämpfen" hat. Dies ist klarerweise ein Wechselspiel zwischen **AccuracyGoal** – wieviele Stellen nach dem Komma garantiert werden sollen – und **WorkingPrecision** – auf wieviele Stellen genau dafür zu rechnen ist. **PrecisionGoal** – wieviele gültige Ziffern zu produzieren sind – kann dagegen keine Rolle spielen, da das (erwartete) Ergebnis ja gleich Null ist und folglich überhaupt keine gültigen Ziffern hat.

$$f = \frac{1}{x^3} - \frac{3}{8};$$

```
Plot[f, {x, 1, 2}, Filling -> Axis, FillingStyle -> Yellow]
```



$$\int_1^2 f \, dx$$

In der Standardeinstellung kommt das richtige Ergebnis heraus, aber die nötige Konvergenzgüte wird nicht erreicht.

```
NIntegrate[f, {x, 1, 2}]
% // Accuracy
```

```
NIntegrate::slwcon:
```

Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

```
NIntegrate::ncvb:
```

NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in x near {x} = {1.08009}. NIntegrate obtained  $-1.30104 \times 10^{-17}$  and  $1.7550522667109103 \times 10^{-17}$  for the integral and error estimates.

```
0. × 10-17
```

```
16.7557
```

Wird **AccuracyGoal** heruntergesetzt, so verschwinden die Warnungen. Arbeits- und Ergebnisgenauigkeit sind im Einklang; das Ergebnis hat geringere **Accuracy**.

```

NIntegrate[f, {x, 1, 2}, AccuracyGoal → 4]
% // Accuracy

0. × 10-7

6.12363

```

Dasselbe mit **PrecisionGoal** hat dagegen keinen Einfluss auf das Verhalten, selbst wenn die **WorkingPrecision** hochgesetzt wird.

```

NIntegrate[f, {x, 1, 2}, PrecisionGoal → 4]
% // Accuracy

NIntegrate::slwcon :
Numerical integration converging too slowly; suspect one of the
following: singularity, value of the integration is 0,
highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate::ncvb :
NIntegrate failed to converge to prescribed accuracy
after 9 recursive bisections in x near {x} =
{1.08009}. NIntegrate obtained  $-1.30104 \times 10^{-17}$  and
1.7550522667109103-17 for the integral and error estimates.

0. × 10-17

16.7557

```

```

NIntegrate[f, {x, 1, 2}, PrecisionGoal → 4, WorkingPrecision → 80]
% // Accuracy

NIntegrate::slwcon :
Numerical integration converging too slowly; suspect one of the
following: singularity, value of the integration is 0,
highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate::ncvb :
NIntegrate failed to converge to prescribed accuracy
after 9 recursive bisections in x near {x}
= {<<136>>}. NIntegrate obtained <<141>> and
<<141>> for the integral and error estimates.

2.1124470614182909034152702541059070869410917869662368343576064419684852049464831×
10-87

166.675

```

**AccuracyGoal** schon.

```

NIntegrate[f, {x, 1, 2}, AccuracyGoal → 30, WorkingPrecision → 40]
% // Accuracy

0. × 10-31

30.584

```

