Software Packages In Physics 1

Chapter 4

Numerical Computation

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4.1 Numerical Evaluation

The *accuracy* is the effective number of digits which appear to the right of a decimal point. To achieve full consistency in the treatment of numbers, precision and accuracy often have values that do not correspond to integer numbers of digits.

N[*expr*] gives the numerical value of expr.
N[*expr,n*] attempts to give a result with *n*-digit precision.
Accuracy [*x*] gives the effective number of digits to the right of the decimal point in the number *x*.
For exact numbers such as integers, Accuracy [*x*] is Infinity.
Precision [*x*] gives the effective number of digits of precision in the number *x*.
Precision [*x*] gives a measure of the relative uncertainty in the value of *x*.
Precision [*x*] is the total number of significant decimal digits in *x*.
Accuracy [*x*] is the number of significant decimal digits to the right of the decimal point in *x*.

Accuracy *is the difference between the mean of the measurements and the reference value (match between the measured and the true value).* Accuracy is the degree to which a digital database matches true or accepted values. Accuracy is an issue pertaining to the quality of data and the number of errors contained in a data set. *The accuracy is the degree to which a given quantity is correct and free from error.*

Precision *is the degree of reproducibility which refers to the level of measurement and exactness of description.* In many cases precision can be characterized in terms of the *standard deviation* of the measurements. The smaller the standard deviation, the higher is the precision.

```
? MachinePrecision
```

```
MachinePrecision is a symbol used to indicate machine-number precision. More...
```

```
{Map[Sin, {π / 3, π / 4, π / 5.}], Sin /@ {π / 3, π / 4, π / 5.}}
MachinePrecision // N
```

$$\left\{\left\{\frac{\sqrt{3}}{2}, \frac{1}{\sqrt{2}}, 0.587785\right\}, \left\{\frac{\sqrt{3}}{2}, \frac{1}{\sqrt{2}}, 0.587785\right\}\right\}$$

```
15.9546
```

```
x = {1.61, 21.618034, 321.618034};
$MachinePrecision - Log[10., Abs[x]]
{Map[Accuracy, x], Accuracy /@ x}
Precision /@ x
```

```
{15.7478, 14.6198, 13.4472}
```

```
{{15.7478, 14.6198, 13.4472}, {15.7478, 14.6198, 13.4472}}
```

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

```
{f = N[√2, 4], Precision[f], Precision[√2], Accuracy[f]}
```

```
{1.414, 4., ∞, 3.84949}
```

```
N[Pi^10]
{Precision[%], Accuracy[%]}
```

```
93648.
```

```
{MachinePrecision, 10.9831}
```

```
N[Pi^10, 30]
{Precision[%] // N, Accuracy[%]}
```

```
93648.047476083020973716690184 9
```

```
{30., 25.0285}
```

4.2 Equation Solving

4.2.1 Solve

Solve[*eqns, vars*] attempts to solve an equation or set of equations for the variables vars.
Solve[*eqns, vars*, *elims*] attempts to solve the equations for *vars*, eliminating the variables *elims*.
Equations are given in the form *lhs* == *rhs*.
Simultaneous equations can be combined either in a list or with &&.
Solve gives solutions in terms of rules of the form *x* →*sol*.

```
Clear[x]
Solve[x^3 + q/3 x + r/27 == 0, x]
```

$$\left\{\left\{x \to \frac{1}{3}\left(-\frac{2^{1/3}\,q}{\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}+\frac{\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}{2^{1/3}}\right)\right\},\right.$$

$$\left\{x \to \frac{\left(1+i\sqrt{3}\right)q}{3\,2^{2/3}\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}-\frac{\left(1-i\sqrt{3}\right)\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}{6\,2^{1/3}}\right\},$$

$$\left.\left\{x \to \frac{\left(1-i\sqrt{3}\right)q}{3\,2^{2/3}\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}-\frac{\left(1+i\sqrt{3}\right)\left(-r+\sqrt{4\,q^3+r^2}\right)^{1/3}}{6\,2^{1/3}}\right\}\right\}$$

```
eqns = {x == 1 + 2 a y, y == 9 + 2 x};
sol1 = Solve[eqns, {x, y}]        (*solve for x and y *)
sol2 = Solve[eqns, x, y]          (*solve for x elimenating y *)
```

$$\left\{\left\{x \to -\frac{1+18\,a}{-1+4\,a},\ y \to -\frac{11}{-1+4\,a}\right\}\right\}$$

$$\left\{\left\{x \to -\frac{1+18\,a}{-1+4\,a}\right\}\right\}$$

```
Solve[-Log[3] + 1/2 Log[2 + y/3] - 1/2 Log[y/3] == -i π/2, y]
```

$$\left\{\left\{y \to -\frac{3}{5}\right\}\right\}$$

4.2.2 NSolve

NSolve [*lhs*==*rhs, var*] gives a list of numerical approximations to the roots of a polynomial equation.
NSolve [{*ean*$_1$, *eqn*$_2$, ...}, {*var*$_1$, *var*$_2$, ...}] solves a system of polynomial equations.

```
poly = 3 + 3 x - 7 x^2 - x^3 + 2 x^4 + 3 x^7 - 3 x^8 - x^9 + x^10;
NSolve[poly == 0, x]
```

```
{{x → -1.73205}, {x → -0.868688 - 0.585282 i}, {x → -0.868688 + 0.585282 i},
 {x → -0.496292}, {x → 0.0763556 - 1.14095 i}, {x → 0.0763556 + 1.14095 i},
 {x → 1.}, {x → 1.04048 - 0.56735 i}, {x → 1.04048 + 0.56735 i}, {x → 1.73205}}
```

```
pol1 = x^80 + 4 x^40 + 2 x^2 - 3;
sol = NSolve[pol1 == 0, x];
pol1 /. sol // Chop[#, 10^-2] &
```

```
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
 0, 0, 0, 0, 0, 0, -0.173841 + 0.0985036 i, -0.173841 - 0.0985036 i, 0.312804,
 0.312804, -0.565497 - 1.37761 i, -0.565497 + 1.37761 i, -1.55504 - 0.730422 i,
 -1.55504 + 0.730422 i, 1.30952 + 3.90669 i, 1.30952 - 3.90669 i, -0.731754,
 0, 22.2044 - 21.3828 i, 22.2044 + 21.3828 i, -85.0346 - 1.88577 i,
 -85.0346 + 1.88577 i, 25.8604, 55.4067 + 77.6349 i, 55.4067 - 77.6349 i}
```

```
Clear[eq1, eq2, x, y]
eq1 = x^5 + 4 x^3 + 3 x^2 + 2 x == 10;
NSolve[eq1, x]
```

```
{{x → -1. - 1. i}, {x → -1. + 1. i}, {x → 0.5 - 2.17945 i}, {x → 0.5 + 2.17945 i}, {x → 1.}}
```

```
Clear[eq1, eq2, x, y]
eq1 = x^2 - x y - y^2 == 1;
eq2 = x^3 + 3 x y - y^3 == 9;
NSolve[{eq1, eq2}, {x, y}]
```

```
{{x → 1.76268, y → -2.57952}, {x → -0.43195 - 0.816763 i, y → 0.552813 + 1.71762 i},
 {x → -0.43195 + 0.816763 i, y → 0.552813 - 1.71762 i},
 {x → 1.74511, y → 0.802781}, {x → -2.07194 - 1.87447 i, y → -1.16444 - 1.26905 i},
 {x → -2.07194 + 1.87447 i, y → -1.16444 + 1.26905 i}}
```

4.2.3 DSolve, NDSolve

DSolve[eqns, y, x] solves a differential equation for the function y, with independent variable x.
DSolve[{eqn$_1$, eqn$_2$, eqn$_3$, ..}, {y_1, y_2, y_3, ..}, x] solves a list of differential equations.
DSolve[eqn, y, {x_1, x_2, x_3, ...}] solves a partial differential equation.

```
DSolve[y''[x] == a y'[x] + y[x], y[x], x]
```

$$\left\{\left\{y[x] \to e^{\frac{1}{2}\left(a-\sqrt{4+a^2}\right)x} C[1] + e^{\frac{1}{2}\left(a+\sqrt{4+a^2}\right)x} C[2]\right\}\right\}$$

```
DSolve[{y''[x] == a y'[x] + y[x], y'[0] == 0, y[0] == b}, y[x], x]
```

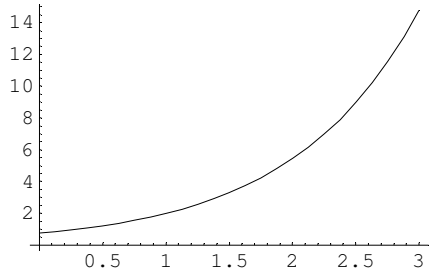
$$\left\{\left\{y[x] \to \frac{1}{2\sqrt{4+a^2}}\left(b\left(a\, e^{\frac{1}{2}\left(a-\sqrt{4+a^2}\right)x} + \sqrt{4+a^2}\, e^{\frac{1}{2}\left(a-\sqrt{4+a^2}\right)x} - a\, e^{\frac{1}{2}\left(a+\sqrt{4+a^2}\right)x} + \sqrt{4+a^2}\, e^{\frac{1}{2}\left(a+\sqrt{4+a^2}\right)x}\right)\right)\right\}\right\}$$

NDSolve [eqns, y, {x, $x_{\min}$, $x_{\max}$}] finds a numerical solution to the ordinary differential equations *eqns* for the function y with the independent variable x in the range x_{min} to x_{max}.
NDSolve [*eqns*, y, {x, x_{min}, x_{max}}, {t, t_{min}, t_{max}}] finds a numerical solution to the partial differential equations *eqns*.
NDSolve [*eqns*, {y_1, y_2, ...}, {x, x_{min}, x_{max}}] finds numerical solutions for the functions y_i.
NDSolve [*eqns*, y[x], {x, x_{min}, x_{max}}] gives solutions for $y[x]$ rather than for the function y itself.

```
sol = NDSolve[{y'[x] == y[x], y[1] == 2}, y, {x, 0, 3}]
{y[1.5], y''[1.5]} /. sol
Plot[y[x] /. sol, {x, 0, 3}, ImageSize → {200, 150}];
```

```
{{y → InterpolatingFunction[{{0., 3.}}, <>]}}
```

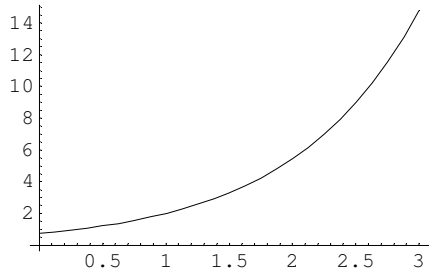
```
{{3.29744, 3.29694}}
```




```
sol = NDSolve[{y'[x] == y[x], y[1] == 2}, y[x], {x, 0, 3}]
{y[x], y''[x]} /. sol /. x → 1.5
Plot[y[x] /. sol, {x, 0, 3}, ImageSize → {200, 150}];
```

```
{{y[x] → InterpolatingFunction[{{0., 3.}}, <>][x]}}
```

```
{{3.29744, y''[1.5]}}
```




```
? Roots
```

```
Roots[lhs==rhs, var] yields a disjunction of
   equations which represent the roots of a polynomial equation. More…
```

4.2.4 Roots & FindRoot

Roots [*lhs == rhs*, *va r*] yields a disjunctions of equations which represent the roots of a polynomial equation.

```
f[x_] := -6 - x + 4 x^2 - x^3
Roots[f[x] == 0, x]
```

```
x == -1 || x == 2 || x == 3
```

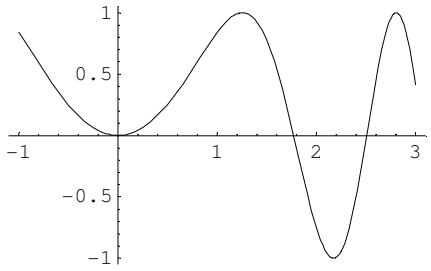
```
Root[f[x], 2]
Table[Root[f[x], n], {n, 1, 3}]
```

```
2
```

```
{-1, 2, 3}
```

FindRoot [*lhs == rhs*, {*x*, x_0}] searches for a numerical solution to the equation *lhs==rhs*, starting with $x=x_0$.
FinRoot [{eqn_1, eqn_2, ...}, {{*x*, x_0}, {*y*, y_0}, ...}] searches for a numerical solution to the simultaneous equations eqn_i.
FindRoot [*lhs == rhs*, {*x*, x_0, x_1}] searches for a solution using x_0 and x_1 as the first two values of *x*, avoiding the use of derivatives.

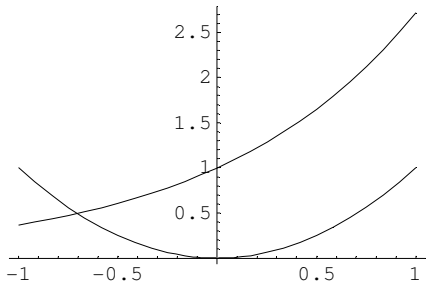
```
Plot[Sin[x^2], {x, -1, 3}, ImageSize → {200, 150}];
FindRoot[Sin[x^2] == 0, {x, 2}]
Sqrt[Pi] // N
```




```
{x → 1.77245}
```

```
1.77245
```

```
Plot[{Exp[x], x^2}, {x, -1, 1}, ImageSize → {200, 150}];
FindRoot[Exp[x] == x^2, {x, -0.5}]
```




```
{x → -0.703467}
```

4.3 Sums And Products

4.3.1 Sum

Sum [f, {i, i_{max}}] evaluates the sum $\sum_{i=1}^{i_{max}} f$.
Sum [f, {i, $i_{\min}$, i_{max}}] starts with $i = i_{min}$. Sum [f, {i, $i_{\min}$, i_{max}, di}] uses steps di.
Sum [f, {i, $i_{\min}$, i_{max}}, {j, $j_{\min}$, j_{max}}, ...] evaluates the multiple sum: $\sum_{i=i_{min}}^{i_{max}} \sum_{j=j_{min}}^{j_{max}} \ldots f$.
Sum [f, {i, $i_{\min}$, i_{max}}] can be entered as $\sum_{i=i_{min}}^{i_{max}} f$.

```
{Sum[2 k - 1, {k, 1, 12}], ∑_{k=1}^{12} (2 k - 1)}
```

```
{144, 144}
```

```
Clear[sinx, cosx, x]
Sum[ (-1) ^ ( n + 2) x^ (2 n) / (2 n) !, {n, 0, ∞}] // FullSimplify
```

```
Cos[x]
```

```
cosx = Sum[ (-1) ^ ( n + 2) x^ (2 n) / (2 n) !, {n, 0, 4}]
Sum[ (-1) ^ ( n / 2) x^n / n !, {n, 0, 8, 2}]
cosx /. x → Pi / 6 // N
With[{x = Pi / 6}, Evaluate[cosx]] // N
```

$$1 - \frac{x^2}{2} + \frac{x^4}{24} - \frac{x^6}{720} + \frac{x^8}{40320}$$

$$1 - \frac{x^2}{2} + \frac{x^4}{24} - \frac{x^6}{720} + \frac{x^8}{40320}$$

```
0.866025
```

```
0.866025
```

```
Clear[sinx]
sinx = Sum[(-1) ^ (n + 2) x^ (2 n + 1) / (2 n + 1) !, {n, 0, 4}]
Sum[(-1) ^ (( n + 1) / 2 + 1) x^n / n !, {n, 1, 9, 2}]
{With[{x = Pi / 6}, Evaluate[sinx]] // N, sinx /. x → Pi / 6 // N}
```

$$x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \frac{x^9}{362880}$$

$$x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \frac{x^9}{362880}$$

```
{0.5, 0.5}
```

```
Sum[Sum[Sin[x^m + y^n], {n, 1, m}], {m, 1, 3}]
Sum[Sin[x^m + y^n], {m, 1, 3}, {n, 1, m}]
```

$$\sum_{m=1}^{3}\sum_{n=1}^{m}\mathrm{Sin}[x^m + y^n]$$

$\mathrm{Sin}[x + y] + \mathrm{Sin}[x^2 + y] + \mathrm{Sin}[x^3 + y] + \mathrm{Sin}[x^2 + y^2] + \mathrm{Sin}[x^3 + y^2] + \mathrm{Sin}[x^3 + y^3]$

$\mathrm{Sin}[x + y] + \mathrm{Sin}[x^2 + y] + \mathrm{Sin}[x^3 + y] + \mathrm{Sin}[x^2 + y^2] + \mathrm{Sin}[x^3 + y^2] + \mathrm{Sin}[x^3 + y^3]$

$\mathrm{Sin}[x + y] + \mathrm{Sin}[x^2 + y] + \mathrm{Sin}[x^3 + y] + \mathrm{Sin}[x^2 + y^2] + \mathrm{Sin}[x^3 + y^2] + \mathrm{Sin}[x^3 + y^3]$

$$\mathrm{With}\left[\{n = 25\},\ \mathrm{Sum}\left[\frac{(2\,n)\,!}{(n + k)\,!\ (n - k)\,!},\ \{k,\ 0,\ n\}\right]\right]$$

$$\mathrm{Sum}\left[\frac{(2\,n)\,!}{(n + k)\,!\ (n - k)\,!},\ \{k,\ 0,\ n\}\right]\ /.\ n \to 25$$

```
626155256640188

626155256640188
```

4.3.2 Product

Product [f, {i, i_{max}}] evaluates the product $\prod_{i=1}^{i_{max}} f$.
Product [f, {i, i_{min}, i_{max}}] starts with $i = i_{min}$. Product [f, {i, i_{min}, i_{max}, di}] uses steps di.
Product [f, {i, i_{min}, i_{max}}, {j, j_{min}, j_{max}}] evaluates the multiple product $\prod_{i=i_{min}}^{i_{max}} \prod_{j=j_{min}}^{j_{max}} \ldots f$.
$\prod$ can be entered as ESC prod ESC or $\prod$.
Product [f, {i, i_{min}, i_{max}}] can be entered as $\prod_{i=i_{min}}^{i_{max}} f$.

$$\left\{\prod_{k=1}^{\infty}\left(1 + \frac{1}{k^2}\right),\ \mathrm{Product}[(1 + 1/k\text{^}2),\ \{k,\ 1,\ \infty\}]\right\}$$

$$\left\{\frac{\mathrm{Sinh}[\pi]}{\pi},\ \frac{\mathrm{Sinh}[\pi]}{\pi}\right\}$$

4.3.3 NSum

NSum [f, {i, i_{min}, i_{max}}] gives a numerical approximation to the sum $\sum_{i=i_{min}}^{i_{max}} f$.
NSum [f, {i, i_{min}, i_{max}, di}] uses a step di in the sum.
NSum can be used for sums with both finite and infinite limits.
NSum [f, {i, ...}, {j, ...}, ...] can be used to evaluate multidimensional sums.

$$\left\{\sum_{i=1}^{\infty}\frac{1}{i^2},\ \mathrm{Sum}[1/i\text{^}2,\ \{i,\ 1,\ \infty\}],\ \mathrm{NSum}[1/i\text{^}2,\ \{i,\ 1,\ \infty\}]\right\}$$

$$\left\{\frac{\pi^2}{6},\ \frac{\pi^2}{6},\ 1.64493\right\}$$

4.3.4 NProduct

NProduct [f, {i, i_{min}, i_{max}}] gives a numerical approximation to the product $\prod_{i=i_{min}}^{i_{max}} f$.
NProduct [f, {i, i_{min}, i_{max}, di}] uses a step di in the product.

```
Product[1 + 1/n^2, {n, 1, 100, 0.5}] // N
```

```
8.35425
```

```
{Product[1 + 1/n^2, {n, 1, ∞}], NProduct[1 + 1/n^2, {n, 1, ∞}]}
```

$$\left\{\frac{\text{Sinh}[\pi]}{\pi},\ 3.67608 + 0.\,i\right\}$$

4.4 Integration

4.4.1 Integrate

Integrate [f, x] gives the indefinite integral $\int f\, dx$.
Integrate [f, {x, x_{min}, x_{max}}] gives the definite integral $\int_{x_{min}}^{x_{max}} f\, dx$.
Integrate [f, {x, x_{min}, x_{max}}, {y, y_{min}, y_{max}}] gives the multiple integral $\int_{x_{min}}^{x_{max}} dx \int_{y_{min}}^{y_{max}} dy\, f$.
Integrate [f, x] can be entered as $\int f\, dx$.

```
{∫x^n dx, Integrate[x^n, x]}
```

$$\left\{\frac{x^{1+n}}{1+n},\ \frac{x^{1+n}}{1+n}\right\}$$

```
{∫Exp[a x^2] dx, Integrate[Exp[a x^2], x]}
```

$$\left\{\frac{\sqrt{\pi}\ \text{Erfi}\left[\sqrt{a}\ x\right]}{2\sqrt{a}},\ \frac{\sqrt{\pi}\ \text{Erfi}\left[\sqrt{a}\ x\right]}{2\sqrt{a}}\right\}$$

```
{Integrate[x^n, {x, 0, 1}, Assumptions → (n > 2)],
 Assuming[n > 2, Integrate[x^n, {x, 0, 1}]]}
```

$$\left\{\frac{1}{1+n},\ \frac{1}{1+n}\right\}$$

```
{Assuming[x ∈ Reals, ∫1/x^(1/3) dx],
 Integrate[1 / x^(1 / 3), x, Assumptions → (x ∈ Reals)]}
```

$$\left\{\frac{3\,x^{2/3}}{2},\ \frac{3\,x^{2/3}}{2}\right\}$$

4.4.2 NIntegrate

NIntegrate [f, {x, x_{min}, x_{max}}] gives a numerical approximation to the integral $\int_{x_{min}}^{x_{max}} f\ dx$.

```
{∫_0^1 Sec[Tan[x]] dx, NIntegrate[Sec[Tan[x]], {x, 0, 1}]}
```

```
{∫_0^1 Sec[Tan[x]] dx, 2.19614}
```

```
Timing[∫_0^∞ Cos[3 x]/Cosh[2 x] dx]
Timing[Integrate[Cos[3 x]/Cosh[2 x], {x, 0, ∞}]] // N
Timing[NIntegrate[Cos[3 x]/Cosh[2 x], {x, 0, ∞}]]
```

```
{1.937 Second, 1/4 π Sech[3 π/4]}
{0.063 Second, 0.147555}
{0.016 Second, 0.147555}
```

4.5 Optimization

4.5.1 NMaximize

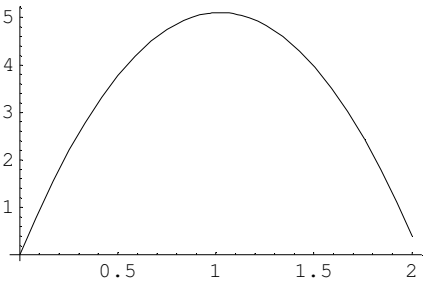
NMaximize [f,{x, y,...}] maximizes f numerically with respect to x, y, … .
NMaximize [{f, *cons*},{x, y,...}] maximizes f numerically subject to the constraints *cons*.
The following gives the maximum value, and where it occurs.

```
NMaximize[x/(1 + Exp[x]), x]
```

```
{0.278465, {x → 1.27846}}
```

```
Clear["Global`*"]
y = v0 t - 0.5 g t^2 /. {v0 → 10., g → 9.8};
NMaximize[y, t]
Plot[y, {t, 0, 2}, ImageSize → {200, 150}];
```

```
{5.10204, {t → 1.02041}}
```



4.5.2 NMinimize

NMinimize [*f*,{*x, y,...*}] minimizes *f* numerically with respect to *x*, *y*, … .
NMinimize [{*f*, *cons*},{*x, y,...*}] minimizes *f* numerically subject to the constraints *cons*.
NMinimize returns a list of the form $\{f_{min}, \{x \to x_{min}, y \to y_{min}, \ldots\}\}$.
The following minimizes the function within the unit circle.

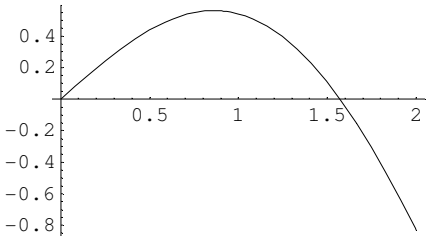
```
Clear["Global`*"]
NMinimize[{Cos[x] - Exp[x y], x^2 + y^2 < 1}, {x, y}]
```

```
{-0.919441, {x → 0.795976, y → 0.605329}}
```

4.5.3 FindMaximum

FindMaximum [*f*, {*x*, x_0}] searches for a local maximum in *f*, starting from the point $x = x_0$.
FindMaximum [*f*, {*x*, x_0}, {*y*, y_0}, ...] searches for a local maximum in a function of several variables.

```
Plot[x Cos[x], {x, 0, 2.}, ImageSize → {200, 150}];
{FindMaximum[x Cos[x], {x, 2}], NMaximize[x Cos[x], x]}
```

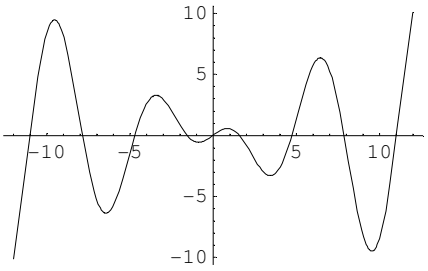



```
{{0.561096, {x → 0.860334}}, {0.561096, {x → 0.860334}}}
```

4.5.4 FindMinimum

FindMinimum [f, {x, x_0}] searches for a local minimum in f, starting from the point $x = x_0$.
FindMinimum [f, {x, x_0}, {y, y_0}, ...] searches for a local minimum in a function of several variables.

```
Plot[x Cos[x], {x, -12, 12.}, ImageSize → {200, 150}];
FindMinimum[x Cos[x], {x, 10}]
NMinimize[x Cos[x], x]
NMaximize[x Cos[x], x]
```




```
{-9.47729, {x → 9.52933}}

{-0.561096, {x → -0.860334}}

{0.561096, {x → 0.860334}}
```

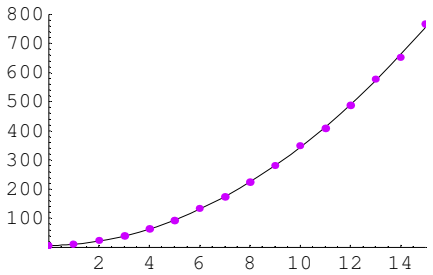
4.5.5 FindFit

FindFit [*data, expr, pars, vars*] finds numerical values of the parameters *pars* that make *expr* give a best fit to *data* as a function of *vars*.
The data can have the form {{x_1, y_1, ..., f_1}, {x_2, y_2, ..., f_2}, ...}, where the number of coordinates x, y, … is equal to the number of variables in the list *vars*.
The data can also be of the form {f_1, f_2, ...}, with a single coordinate assumed to take values 1, 2, ...
FindFit [*data, expr,* {{*par*$_1$, p_1}, {*par*$_2$, p_2}, ...}, *vars*] starts the search for a fit with {par$_1$ → p_1, par$_2$ → p_2, ...}.

```
T1 = Table[{x, 4.5 + 2 x + 3.2 x^2 + Random[Real, {-0.05 x^2, 0.05 x^2}]}, {x, 0, 15}]
f2 = c + d x + e x^2;
f1 = FindFit[T1, f2, {c, d, e}, x]
p1 = Plot[f2 /. f1, {x, -1, 15}, AxesOrigin → {0, 0},
   PlotRange → {{0, 15}, {0, 800}}, DisplayFunction → Identity];
p2 = ListPlot[T1, PlotStyle → {PointSize[0.02], Hue[0.8]},
   DisplayFunction → Identity];
Show[{p1, p2}, DisplayFunction → $DisplayFunction, ImageSize → {200, 150}];
```

```
{{0, 4.5}, {1, 9.72719}, {2, 21.4737}, {3, 39.3622}, {4, 63.9382}, {5, 93.4226},
 {6, 131.029}, {7, 173.059}, {8, 223.948}, {9, 280.355}, {10, 347.388},
 {11, 409.656}, {12, 487.283}, {13, 574.673}, {14, 650.047}, {15, 765.584}}
```

```
{c → 5.79878, d → 1.17288, e → 3.25961}
```



4.6 Data Manipulation

4.6.1 Mean

Mean [*list*] gives the statistical mean of the elements in *list*.
Mean [{{x_1, y_1, ..}, {x_2, y_2, ..}, ...}] gives {Mean[{x_1, x_2, ..}], Mean[{y_1, y_2, ..}, ...}].

```
Mean[{{x1, y1}, {x2, y2}, {x3, y3}}]
```

$$\left\{\frac{1}{3}\,(x1 + x2 + x3),\ \frac{1}{3}\,(y1 + y2 + y3)\right\}$$

```
m = {-1.849637, 4.11, -9.113, -0.4,
   3.40442119, 3.33, 9.193399786, -2.07, 5.32343, 5.9607825};
{Mean[m], Total[m]/Length[m]}
```

```
{1.78894, 1.78894}
```

4.6.2 Variance

Variance[*list*] gives the statistical variance of the elements in *list*.
Variance[*list*] is equivalent to Total [(*list* - Mean[*list*])^2]/(Length[*list*] - 1).

```
m = {-1.849637, 4.11, -9.113, -0.4,
   3.40442119, 3.33, 9.193399786, -2.07, 5.32343, 5.9607825};
{Variance[m], Total[(m - Mean[m])^2] / (Length[m] - 1)}
```

```
{27.4299, 27.4299}
```

4.6.3 StansardDeviation

StandardDeviation [*list*] gives the standard deviation of the elements in *list*.
StandardDeviation [*list*] is equivalent to Sqrt [Variance [*list*]].
StandardDeviation [{{x_1, y_1, ...}, {x_2, y_2, ...}, ...}] gives {StandardDeviation [{x_1, x_2, ...}], StandardDeviation [{y_1, y_2, ...}]}.

```
m = {-1.849637, 4.11, -9.113, -0.4,
   3.40442119, 3.33, 9.193399786, -2.07, 5.32343, 5.9607825};
{StandardDeviation[m], Sqrt[Variance[m]]}
```

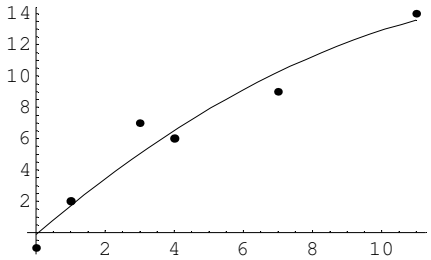
```
{5.23736, 5.23736}
```

4.6.4 Fit

Fit [*data, funs, vars*] finds a least-squares fit to a list of data as a linear combination of the functions *funs* of variables *vars*.
The data can have the form {{x_1, y_1, … , f_1}, {x_2, y_2, … , f_2}, … }, where the number of coordinates x, y, … is equal to the number of variables in the list *vars*.
The data can also be of the form {f_1, f_2, … }, with a single coordinate assumed to take values 1, 2, … .
The argument *funs* can be any list of functions that depend only on the objects *vars*.
Fit [{f_1, f_2, ...}, {1, x, x^2}, x] gives a quadratic fit to a sequence of values f_i. The result is of the form $a_0 + a_1 x + a_2 x^2$, where the a_i are real numbers. The successive values of x_i needed to obtain the f_i are assumed to be 1, 2,....
Fit [{{x_1, f_1}, {x_2, f_2}, ...}, {1, x, x^2}, x] gives does a quadratic fit, assuming a sequence of x values x_i.
Fit [{{x_1, y_1, f_1}, ...}, {1, x, y}, {x, y}] gives finds a fit of the form $a_0 + a_1 x + a_2 y$.

```
Clear["Global`*"]
data = {{0, -1}, {1, 2}, {3, 7}, {4, 6}, {7, 9}, {11, 14}};
p1 = ListPlot[data, PlotStyle → PointSize[0.02], DisplayFunction → Identity];
f1 = Fit[data, {1, x, x^2}, x]
p2 = Plot[f1, {x, 0, 11}, DisplayFunction → Identity];
Show[{p1, p2}, ImageSize → {200, 150}, DisplayFunction -> $DisplayFunction];
```

$$-0.113262 + 1.89613\,x - 0.0592841\,x^2$$



4.6.5 Interpolation

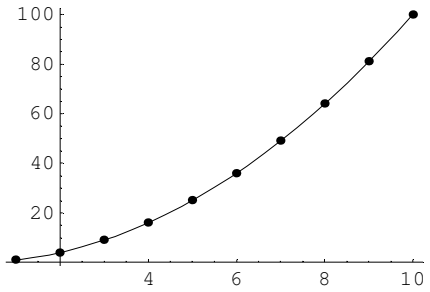
Interpolation [*data*] constructs an InterpolationFunction object which represents an approximate function that interpolates the data.

The data can have the forms $\{\{x_1, f_1\}, \{x_2, f_2\}, \ldots.\}$ or $\{f_1, f_2, \ldots.\}$, where in the second case, the x_i are taken to have values 1, 2, 3, ...

```
data1 = Table[{y, y^2}, {y, 1., 10.}]
f = Interpolation[data1]
p1 = Plot[f[x], {x, 1, 10}, PlotRange → All,
   ImageSize → {200, 150}, DisplayFunction → Identity];
p2 = ListPlot[data1, PlotStyle → PointSize[0.02], DisplayFunction → Identity];
Show[{p1, p2}, ImageSize → {200, 150}, DisplayFunction -> $DisplayFunction];
```

```
{{1., 1.}, {2., 4.}, {3., 9.}, {4., 16.}, {5., 25.},
 {6., 36.}, {7., 49.}, {8., 64.}, {9., 81.}, {10., 100.}}
```

```
InterpolatingFunction[{{1., 10.}}, <>]
```



4.6.6 ListInterpolation

ListInterpolation [*array*] constructs an InterpolationFunction object which represents an approximate function that interpolates the array of values given.
ListInterpolation [array, {{x_{min}, x_{max}}, {y_{min}, y_{max}}, ...}] specifies the domain of the grid from which the values in *array* are assumed to come.
ListInterpolation is similar to Interpolation, but provides a more convenient interface for data that does not include coordinates and for multidimensional data.
Here is a table of values of a function on a regular three dimensional grid.

```
Clear[data, p1, x, y]
data = Table[Cos[x y], {x, -2., 2.}, {y, -2., 2.}]
p1 = ListInterpolation[data, {{-2, 2}, {-2, 2}}]
{Cos[x y], p1[x, y]} /. {x → 2., y → 2.}
```

```
{{-0.653644, -0.416147, 1., -0.416147, -0.653644},
 {-0.416147, 0.540302, 1., 0.540302, -0.416147},
 {1., 1., 1., 1., 1.}, {-0.416147, 0.540302, 1., 0.540302, -0.416147},
 {-0.653644, -0.416147, 1., -0.416147, -0.653644}}

InterpolatingFunction[{{-2., 2.}, {-2., 2.}}, <>]

{-0.653644, -0.653644}
```

4.6.7 FunctionInterpolation

FunctionInterpolation [*expr*, {x, $x_{\min}$, $x_{\max}$}] evaluates *expr* with x running from x_{min} to x_{max} and constructs an InterpolationFunction object which represents an approximate function corresponding to the result.
FunctionInterpolation [*expr*, {x, $x_{\min}$, $x_{\max}$}, {y, $y_{\min}$, $y_{\max}$}, ...] constructs an InterpolatingFunction object with several arguments.
The following user defined function f is an InterpolatingFunction object that interpolates over a two-dimensional domain, t and x.

```
f = FunctionInterpolation[t^2 + Sqrt[x],
  {x, 0, 1}, {t, 0, 2}]
{f[x, t], t^2 + Sqrt[x]} /. {x → .51, t → 1.1}
```

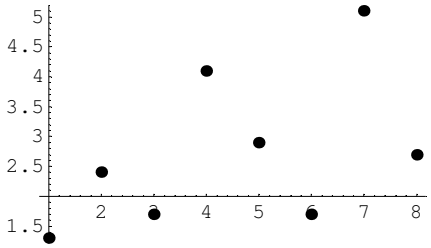
```
InterpolatingFunction[{{0, 1}, {0, 2}}, <>]

{1.92415, 1.92414}
```

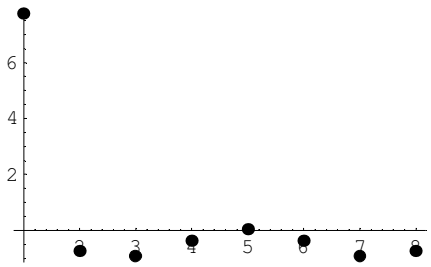
4.6.8 Fourier

Fourier [*list*] finds the discrete Fourier transform of a list of complex numbers.
The discrete Fourier transform v_s of a list u_r of length n is by default defined to be $\frac{1}{\sqrt{n}} \sum_{r=1}^{n} u_r \, e^{2\pi i (r-1)(s-1)/n}$.
With the setting FourierParameters → {a, b} the discrete Fourier transform computed by Fourier is $\frac{1}{n^{(1-a)/2}} \sum_{r=1}^{n} u_r \, e^{2\pi i b (r-1)(s-1)/n}$.

```
Clear[data, p1]
data = {1.3, 2.4, 1.7, 4.1, 2.9, 1.7, 5.1, 2.7};
p1 = ListPlot[data, PlotStyle → PointSize[0.03], ImageSize → {200, 150}];
f1 = Fourier[data]
ListPlot[Re[f1], PlotStyle → PointSize[0.03], ImageSize → {200, 150}];
{InverseFourier[f1], data}
```




```
{7.74282 + 0. i, -0.740685 - 0.677082 i, -0.919239 - 0.954594 i, -0.390685 + 1.72708 i,
 0.0353553 + 0. i, -0.390685 - 1.72708 i, -0.919239 + 0.954594 i, -0.740685 + 0.677082 i}
```




```
{{1.3, 2.4, 1.7, 4.1, 2.9, 1.7, 5.1, 2.7}, {1.3, 2.4, 1.7, 4.1, 2.9, 1.7, 5.1, 2.7}}
```

4.6.9 InverseFourier

InverseFourier [*list*] finds the discrete inverse Fourier transform of a list of complex numbers.
The discrete Fourier transform v_s of a list u_r of length n is by default defined to be $\frac{1}{\sqrt{n}} \sum_{r=1}^{n} u_r \, e^{2\pi i (r-1)(s-1)/n}$.
With the setting FourierParameters → {a, b} the discrete Fourier transform computed by Fourier is $\frac{1}{n^{(1+a)/2}} \sum_{r=1}^{n} u_r \, e^{2\pi i b (r-1)(s-1)/n}$.

```
{InverseFourier[f1], data}
```

```
{{1.3, 2.4, 1.7, 4.1, 2.9, 1.7, 5.1, 2.7}, {1.3, 2.4, 1.7, 4.1, 2.9, 1.7, 5.1, 2.7}}
```

4.7 Number Representation

Four underlying types of numbers are built into *Mathematica*.

Integer : arbitrary-length exact integer,
Rational : integer / integer in lowest terms,
Real : approximate real number, with any specified precision,
Complex : complex number of the form number + number I
NumberQ[*x*] : test whether *x* is any kind of number
IntegerQ[*x*] : test whether *x* is an integer
EvenQ[*x*] : test whether *x* is even
OddQ[*x*] : test whether *x* is odd
PrimeQ[*x*] : test whether *x* is a prime integer
Head[*x*] === type : test the type of a number

4.8 Problems

Q1) Plot the following function in the range x = 0 to x = 3, and find all roots of this equation in the given range:

$$2\,x^3 - 5\,x^2 + \frac{\text{Sin}(x)}{x^2} = 0\,;$$

Q2) Generate a list with elements $\{x, \frac{\text{Cos}(x)}{x}\}$, for x = 1 to x = 12. Interpolate this list and show both plots of the list and of the interpolatiig function on one graph.

Q3) Solve the simultaneous equations and substitute the answer in one of the equations as a test : (a)

$$4\,x + 5\,y = 5;\ \text{and}\ 6\,x + 7\,y = 7;\quad \text{(b)}\ t^2 + 4\,t - 8 = 0\,;\ \text{(c)}\ \sqrt{x+2} + 4 = x\ .$$

Q4) Expand the following summation function *f*, and plot it for $x = -4$ to $x = 4$. Find the maximum of this function around $x = 3$.

$$\mathbf{f} = \sum_{\mathbf{n=1}}^{\mathbf{3}} \sum_{\mathbf{m=1}}^{\mathbf{4}} \frac{\mathbf{Exp[n\,x]\ Sin[m\,x]}}{\mathbf{x^m}}$$

Q5) Define the function $f = \sum_{n=0}^{4} (\frac{a}{R})^n P_n(x)$ and integrate $\int f(x)\, d\, x$. Plot the result for $a = 2$, and $R = 5$, in the range $0 \le x \le 10$.

Q6) Evaluate : $\int_0^1 \frac{4}{1+x^2}\, dx$; What is special about this integral ?

Q7) Consider the integral $\int \frac{x}{a^3+x^3}\, dx$; (a) Evaluate the integral ; (b) Differentiate to recover the integrand.

Q8) Determine the sum of the infinite series : $1 + \frac{1}{3^4} + \frac{1}{5^4} + \frac{1}{7^4} + \ldots\ldots$

Q9) Solve Numerically: $\frac{d^2 y}{\mathrm{dx}^2} + \sin^2 x \frac{\mathrm{dy}}{\mathrm{dx}} + 3\, y^2 = e^{-x^2}$, with initial conditions: $y(0) = 1$, $y'(0) = 0$. Determine $y(1)$, $y(3)$, and $y(5)$. Plot $y(x)$ for $0 \le x \le 5$.

Q10) Generate data using Gaussian Function $\frac{1}{\sqrt{2\,\pi\sigma^2}}\, e^{\frac{-(x-\mathrm{xm})}{2\sigma^2}}$ for the range $3.5 \le x \le 6.5$. Fit the data and plot the function, the data, and the fitting function on one graph. Interpolate this data and plot the interpolation function and the data on one graph.