New developments in statistical methods

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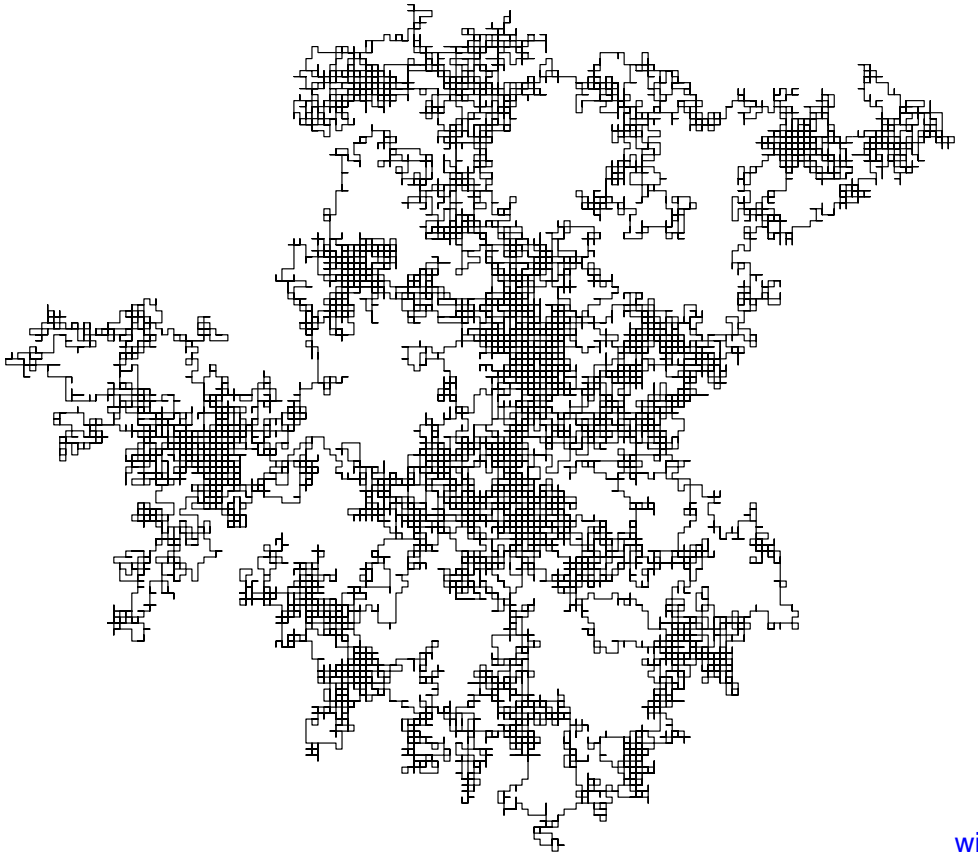
IWHSS 2016

Getting home

restnova.com

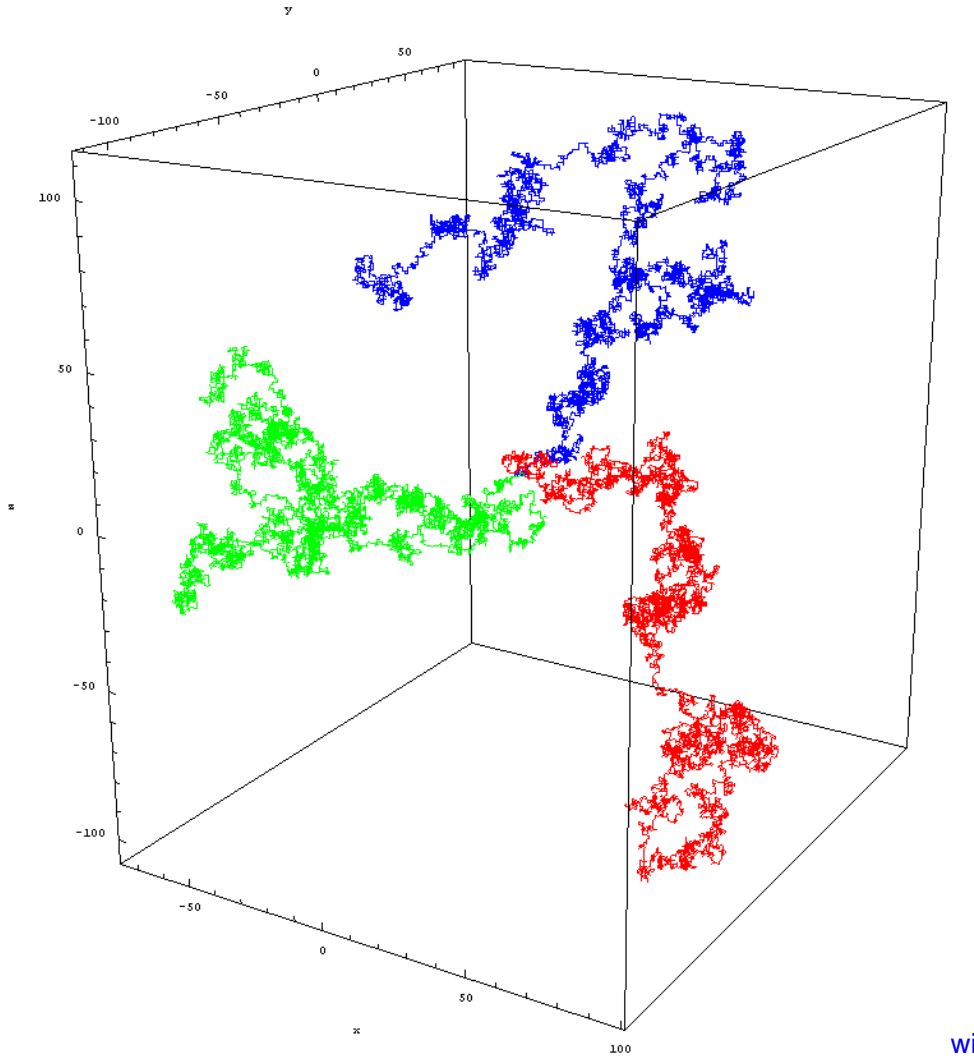
Getting home



wikipedia

symmetric random walk $P(\text{return}|1D) = P(\text{return}|2D) = 1$

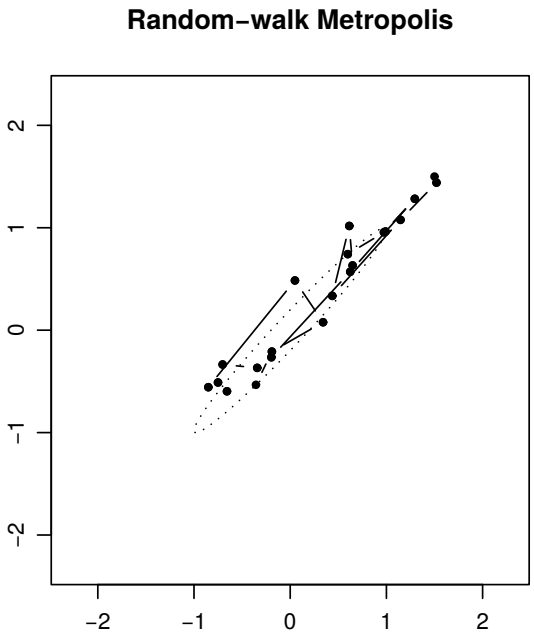
Getting home



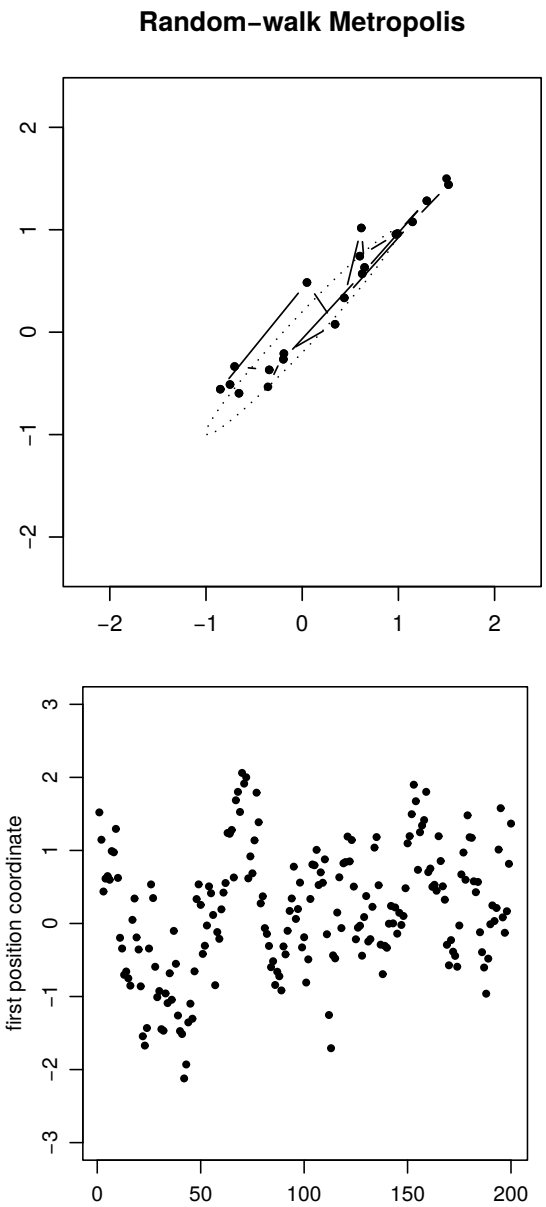
wikipedia

symmetric random walk $P(\text{return}|1D) = P(\text{return}|2D) = 1$
but $P(\text{return}|n > 3) < 1$

Random walk in 2D



Random walk in 2D



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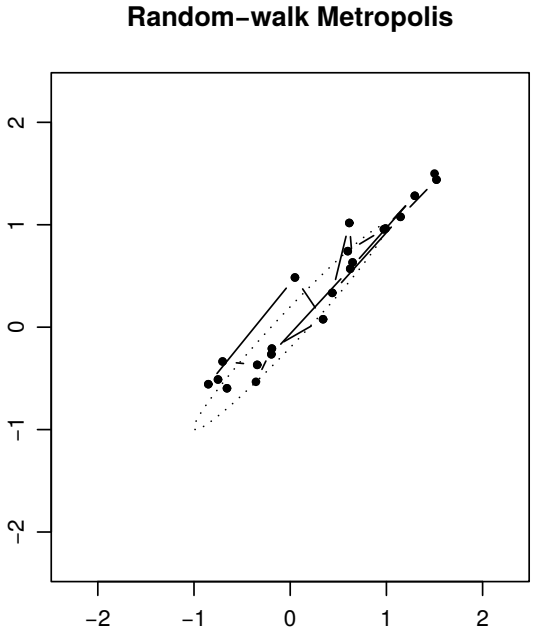

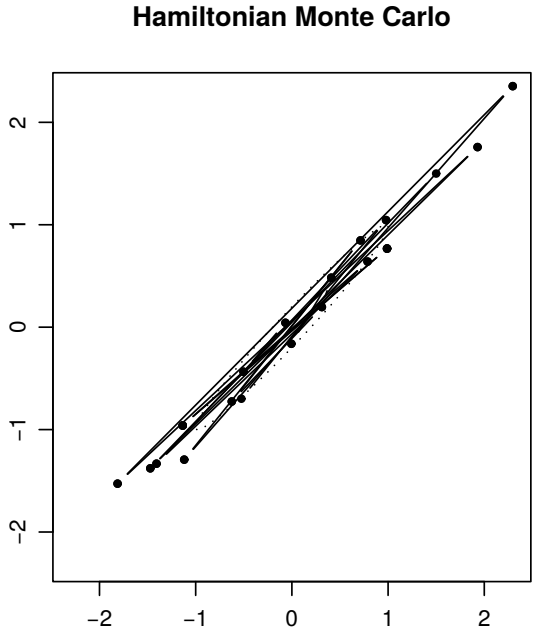

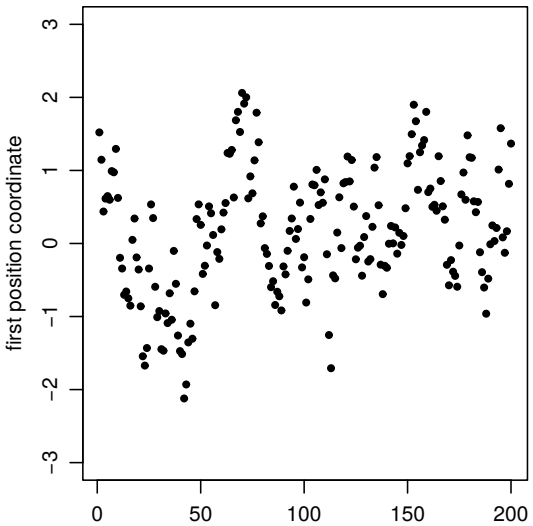

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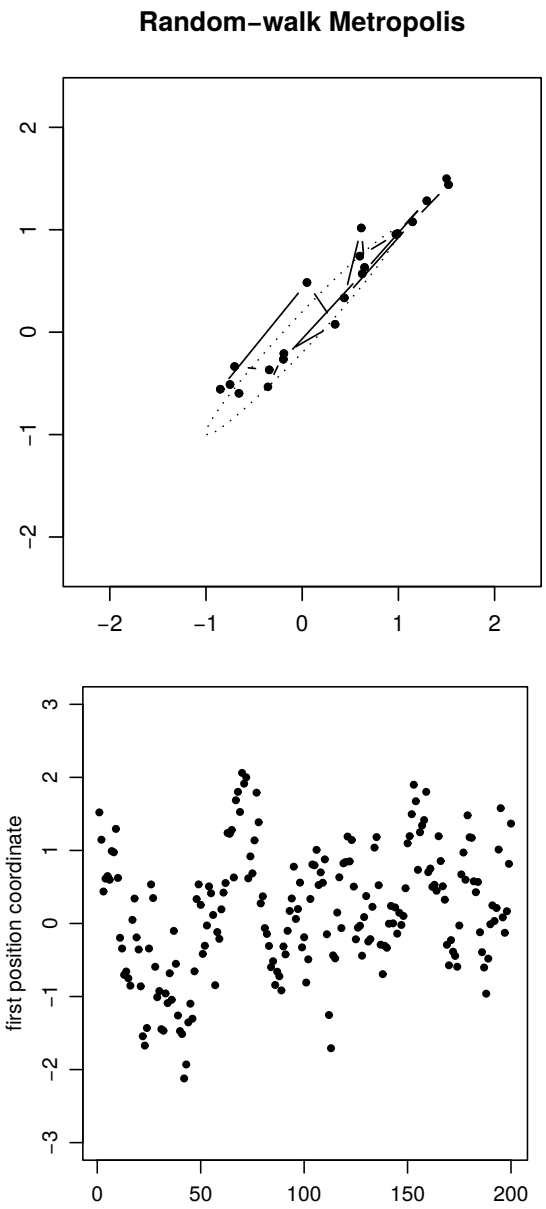
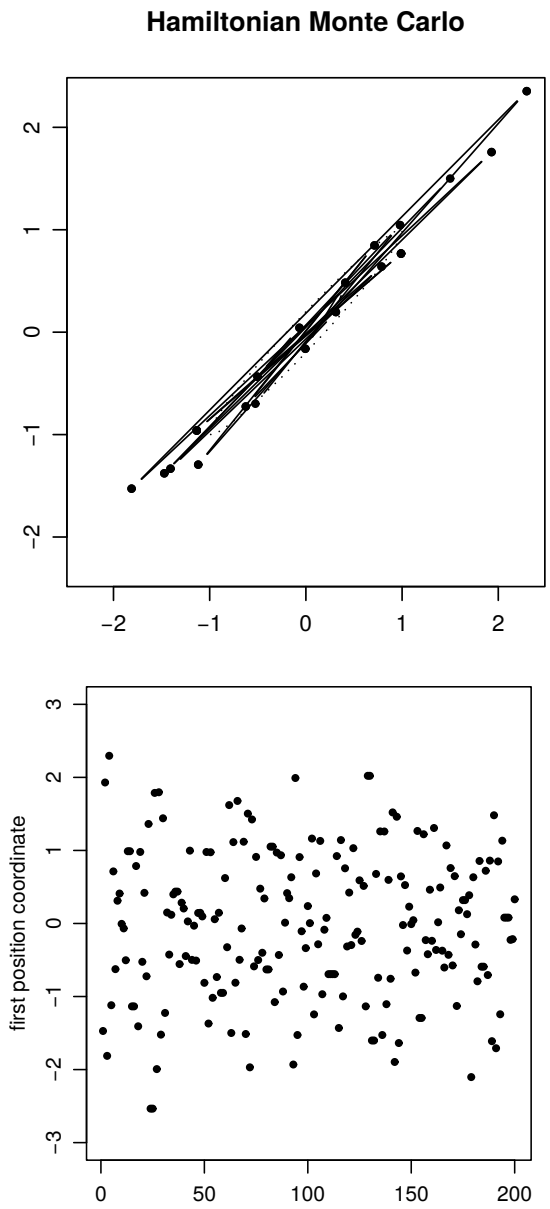
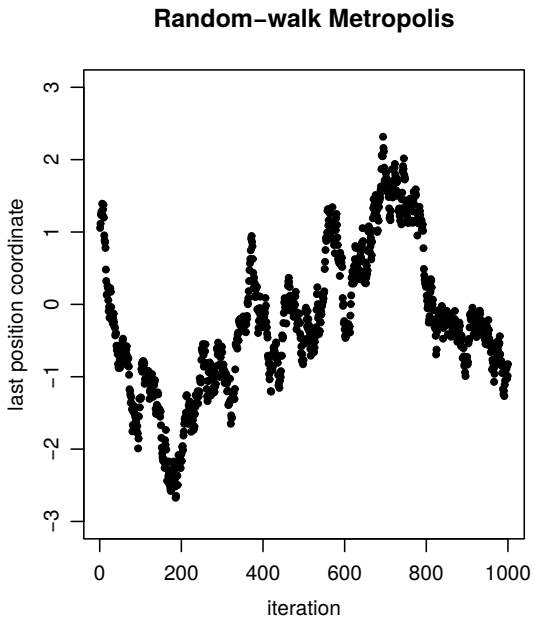




R. Neal, Handbook of MCMC methods

Random walk in 100D



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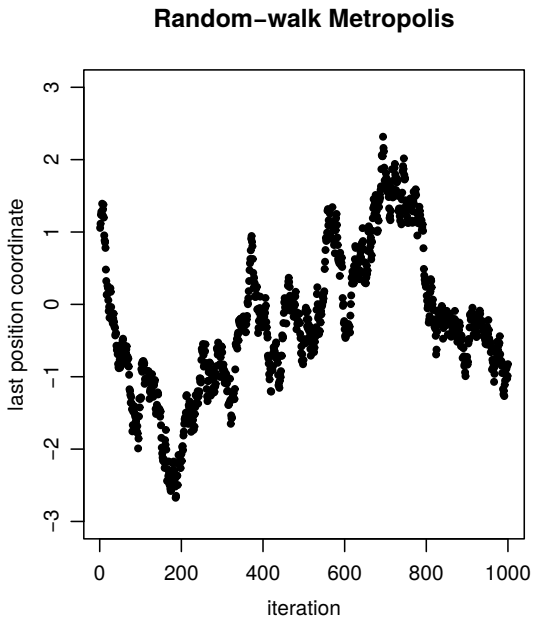

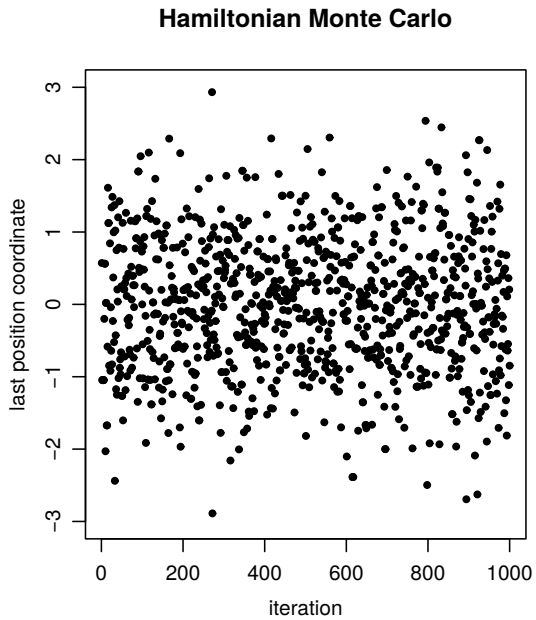

R. Neal, Handbook of MCMC methods

Hamiltonian Monte Carlo

Classical mechanics

- potential $U(\boldsymbol{x}) = -\log P(\boldsymbol{x})$
- add auxiliary momenta $\boldsymbol{p}$ in kin. energy
- Hamiltonian $H = \frac{1}{2}\boldsymbol{p}^T \boldsymbol{M}^{-1}\boldsymbol{p} + U(x)$

Update equations

From $(\boldsymbol{x}, \boldsymbol{p}) \to (\boldsymbol{x}', \boldsymbol{p}')$ by discretizing

$$\dot{\boldsymbol{x}} = \frac{\partial H}{\partial \boldsymbol{p}} = \boldsymbol{M}^{-1}\boldsymbol{p}$$

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{x}} = -\nabla U(\boldsymbol{x})$$

Draw $\boldsymbol{p}'$, accept $\boldsymbol{x}'$ with prob. $\min(1, e^{-(H'-H)})$

How HMC beats "curse of dimensionality"

- gradient ∇U provides direction in space
- conserved quantities
- work even in $512^3 \approx 10^7$ dimensions J. Jasche (2015)

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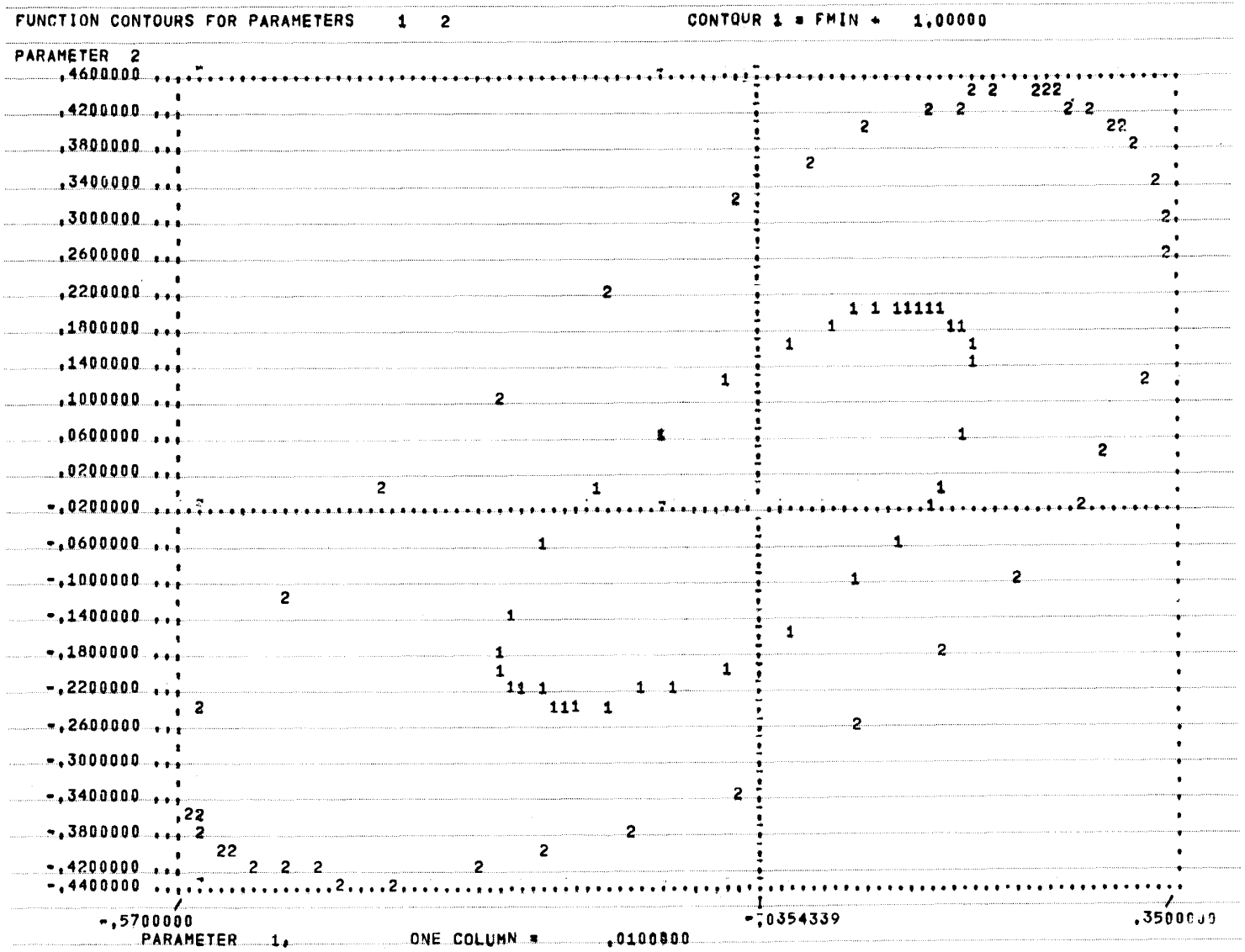
Optimization

Minuit

- called from `hist.Fit()` in ROOT
- quasi-Newton method
  $f(\boldsymbol{x}_k + \boldsymbol{s}_k) = f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{s}_k + \frac{1}{2} \boldsymbol{s}_k^T B_k \boldsymbol{s}_k$
- update of inverse Hessian B_k needs ∇f, too
- default: estimate ∇f by central finite differencing
- problems in 1000D: 2001 calls of f + small error in each dimension but f falls off very rapidly
- minuit accepts user-supplied gradient, too
- pretty robust but dates back to late 1960s
- most popular in high dim.: L-BFGS (1980), e.g. in nlopt



F. James and M. Roos (1975)

automatic differentiation

- derivative via chain chain rule for basic operations
- get ∇f for $\lesssim 5$ calls of f
- more than 20 packages for C/C++ on wikipedia
- source-code transformation vs. operator overloading
- tuned for statistics: STAN math library, released 2015

Normal example

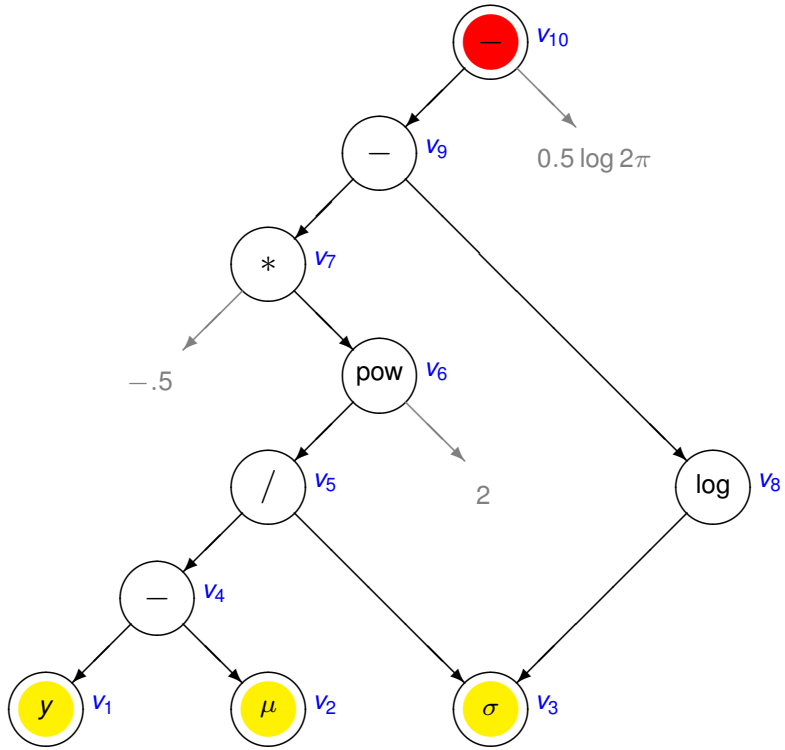
$$f(y, \mu, \sigma) = \log\left(\text{Normal}(y|\mu, \sigma)\right) = -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

forward mode

- trace calculation from input y, μ, σ to output f
- need n passes for gradient of n inputs

reverse mode

- single forward pass to compute derivatives between nodes
- single reverse pass to compute gradient
- larger memory footprint: store derivatives and adjoints



STAN math documentation

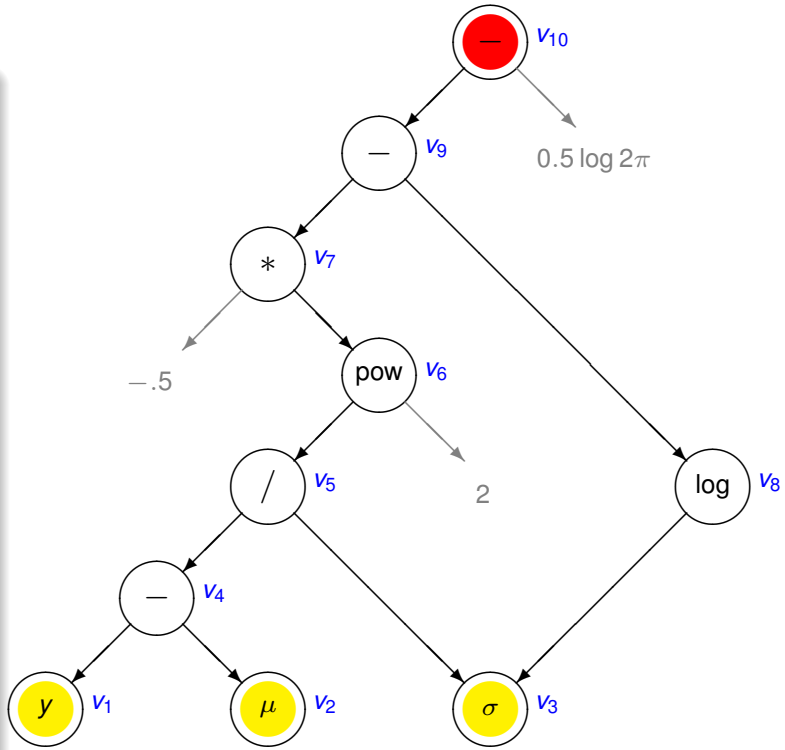
Applying the chain rule

$$f(y,\mu,\sigma) = \log\left(\text{Normal}(y|\mu,\sigma)\right) = -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

forward pass

forward pass

var	*value*	*partials*
v_1	y	
v_2	μ	
v_3	σ	
v_4	$v_1 - v_2$	$\partial v_4/\partial v_1 = 1$ $\quad$ $\partial v_4/\partial v_2 = -1$
v_5	v_4/v_3	$\partial v_5/\partial v_4 = 1/v_3$ $\quad$ $\partial v_5/\partial v_3 = -v_4 v_3^{-2}$
v_6	$(v_5)^2$	$\partial v_6/\partial v_5 = 2v_5$
v_7	$(-0.5)v_6$	$\partial v_7/\partial v_6 = -0.5$
v_8	$\log v_3$	$\partial v_8/\partial v_3 = 1/v_3$
v_9	$v_7 - v_8$	$\partial v_9/\partial v_7 = 1$ $\quad$ $\partial v_9/\partial v_8 = -1$
v_{10}	$v_9 - (0.5\log 2\pi)$	$\partial v_{10}/\partial v_9 = 1$



STAN math documentation

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial v_{10}}\frac{\partial v_{10}}{\partial \sigma} = \frac{\partial f}{\partial v_{10}}\frac{\partial v_{10}}{\partial v_9}\frac{\partial v_9}{\partial \sigma} = \frac{\partial f}{\partial v_{10}}\frac{\partial v_{10}}{\partial v_9}\left(\frac{\partial v_9}{\partial v_7}\frac{\partial v_7}{\partial \sigma} + \frac{\partial v_9}{\partial v_8}\frac{\partial v_8}{\partial \sigma}\right) = \dots$$

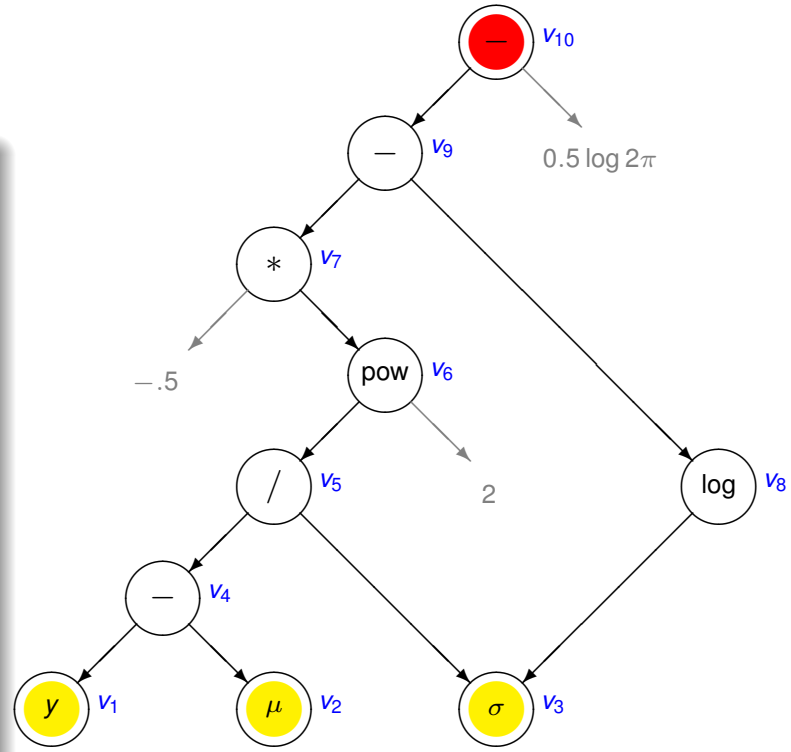
Applying the chain rule

$$f(y,\mu,\sigma) = \log\left(\text{Normal}(y|\mu,\sigma)\right) = -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

reverse pass

duplicate graph with adjoints a_i

var	*operation*	*adjoint*	*result*
$a_{1:9}$	$=$	0	$a_{1:9} = 0$
a_{10}	$=$	1	$a_{10} = 1$
a_9	$+=$	$a_{10} \times \partial v_{10}/\partial v_9$	$a_9 = 1 \times 1 = 1$
$\dots$			
a_3	$+=$	$a_8 \times \partial v_8/\partial v_3$	$a_3 = -1 \times 1/v_3$
$\dots$			
a_3	$+=$	$a_5 \times \partial v_5/\partial v_3$	$a_3 = -1/v_3 + v_5 v_4 v_3^{-2}$
a_1	$+=$	$a_4 \times (1)$	$a_1 = -v_5/v_3$
a_2	$+=$	$a_4 \times (-1)$	$a_2 = v_5/v_3$



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operator overloading in C++

$$f(y, \mu, \sigma) = \log\left(\text{Normal}(y|\mu, \sigma)\right) = -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

```
template <typename T1, typename T2, typename T3>
typename boost::math::tools::promote_args<T1, T2, T3>::type
normal_log(const T1& y, const T2& mu, const T3& sigma) {
using std::pow; using std::log;
return -0.5 * pow((y - mu) / sigma, 2.0) - log(sigma)
       -0.5 * log(2 * stan::math::pi());
}
```

regular evaluation: `T = double`, autodiff: `T = stan::math::var`

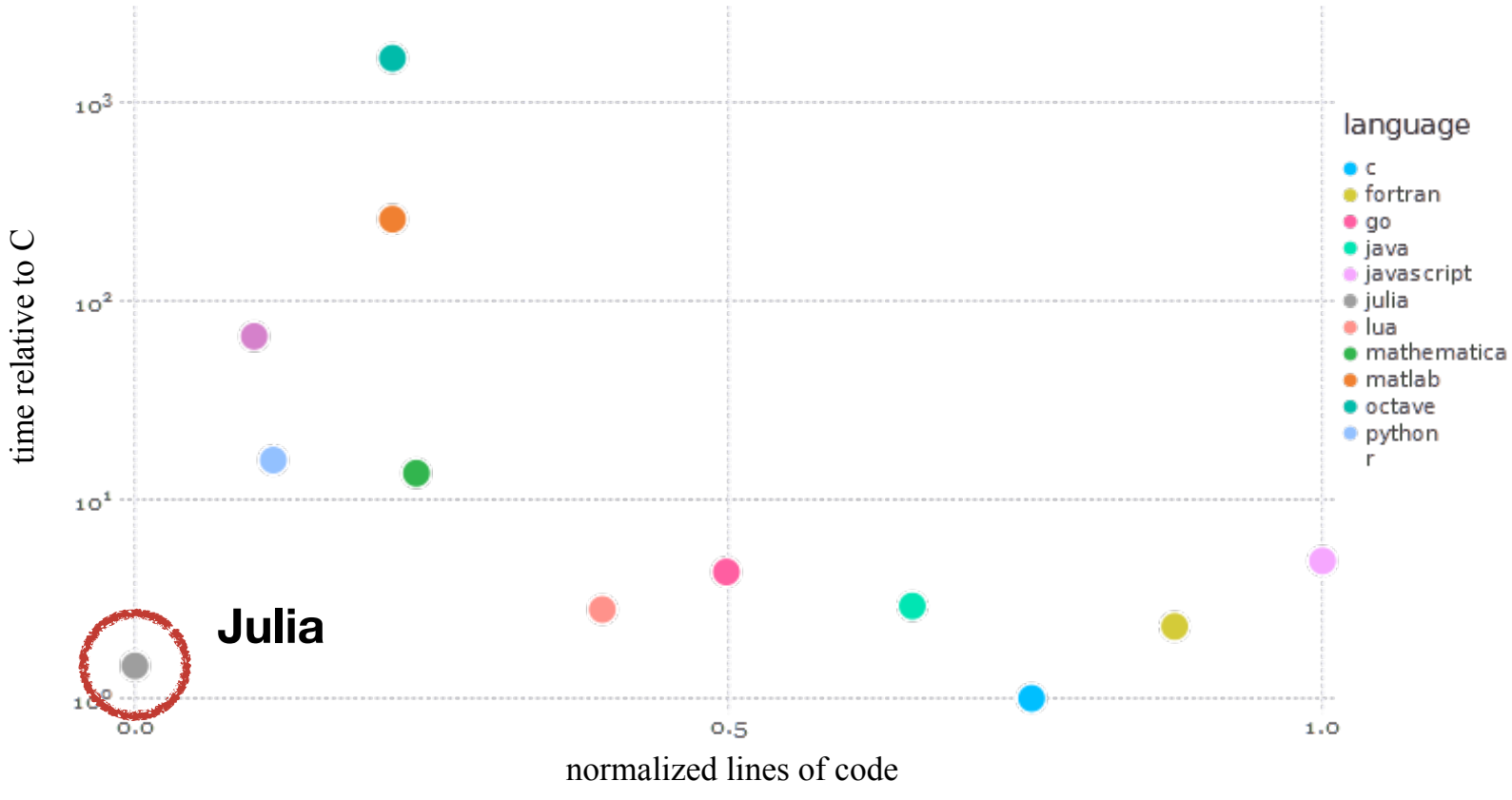
invasive, hard to use in existing projects

Julia

Main features

- new open-source language (2012), julialang.org
- designed for technical computing
- as expressive and interactive as python
- just-in-time compiled via LLVM, near C speed
- call C, Fortran, python, R w/o glue code
- advanced code inspection: codes can inspect itself
- multiple dispatch instead of classes with methods

Speed vs. Productivity



Stefan Karpinski, DIANA meeting at CERN, Jul 2016

julia functions and automatic differentiation

```
# define function w/o types
julia> f(x) = x^3
f (generic function with 1 method)

# 1st call: compile
julia> @time f(5.0)
  0.000600 seconds (149 allocations: 10.167 KB)
125.0

# 2nd call: use compiled version
julia> @time f(5.0)
  0.000004 seconds (5 allocations: 176 bytes)

# specific code for Float64 argument
julia> code_llvm(f, (Float64,))
define double @julia_f_22990(double) {
top:
  %1 = fmul double %0, %0
  %2 = fmul double %1, %0
  ret double %2
}
```

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```

```
# install package from internet
# including dependencies
julia> Pkg.add("ReverseDiffSource")
INFO: Installing ReverseDiffSource v0.2.3
INFO: Package database updated

# import symbols of the package
julia> using ReverseDiffSource

# generate source of gradient
# from source code
julia> rdiff( :(x^3), x=5.)
quote
    (x ^ 3,3 * x ^ 2)
end

# function and gradient from a function
julia> f_gradf = rdiff(f, (5.0,))
(anonymous function)

# evaluate function and gradient together
julia> f_gradf(5)
(125,75)
```

reverse mode: source transformation

julia functions and automatic differentiation

```
using Optim, ForwardDiff

# .^ = square elementwise
h(x::Vector) = sum(x.^2)

# Newton's method needs gradient and Hessian
julia> res = optimize(h, [111, -2222.2], Newton(), OptimizationOptions(autodiff=true))
 ...
 * Minimizer: [-1.4210854715202004e-14,0.0]
 * Minimum: 2.019484e-28
 * Iterations: 1
 ...
 * Objective Function Calls: 5
 * Gradient Calls: 5

julia> ForwardDiff.gradient(h, [0.0, 0.0])
2-element Array{Float64,1}:
 0.0
 0.0

julia> ForwardDiff.hessian(h, Optim.minimizer(res))
2x2 Array{Float64,2}:
 2.0  0.0
 0.0  2.0
```

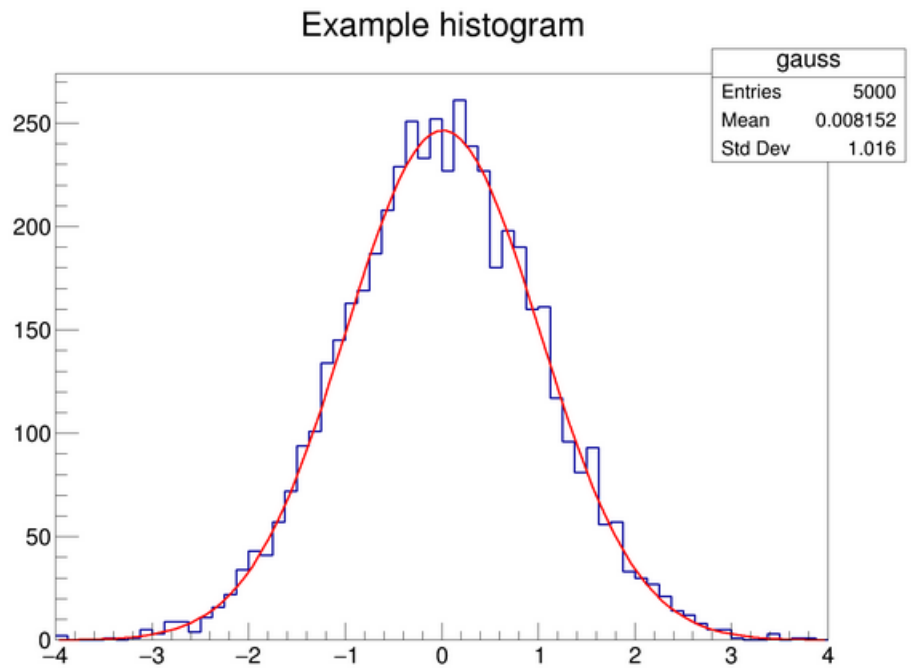
forward mode: operator overloading

notebooks

- ipython notebook $\Rightarrow$ jupyter
- supports over 40 languages
- explore data from the browser
- try C++ online via cling at CERN
- try julia online on juliabox

Let's now fit the histogram.

In [6]:
```
h.Fit("gaus", "S");
c.Draw();
```




```
 FCN=47.4997 FROM MIGRAD    STATUS=CONVERGED      53 CALLS          54 TOTA
L
                     EDM=8.44224e-09    STRATEGY= 1      ERROR MATRIX ACCUR
ATE
  EXT PARAMETER                                   STEP         FIRST
  NO.   NAME      VALUE            ERROR          SIZE      DERIVATIVE
   1  Constant     2.46469e+02   4.31494e+00   1.19094e-02  -2.44811e-05
   2  Mean         1.04782e-02   1.43576e-02   4.87656e-05  -6.34020e-03
   3  Sigma        1.00315e+00   1.03818e-02   9.45504e-06  -2.70309e-02
```

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In [7]:
```
const ⊗ = kron
eye(2,2) ⊗ rand(2,2)
```

Out[7]:
```
4x4 Array{Float64,2}:
 0.68628   0.553253  0.0       0.0
 0.141211  0.25523   0.0       0.0
 0.0       0.0       0.68628   0.553253
 0.0       0.0       0.141211  0.25523
```

Functions and JIT-compilation

Functions can be defined in several ways, and *don't*

In [8]:
```
# verbose form:
function foo(x)
    return x + 1
end

# one-line form:
foo(x) = x + 1

# anonymous function
x -> x + 1
```

Out[8]:
```
(anonymous function)
```

Conclusion

- optimizing/sampling w/o gradient = driving w/o a map
- automatic differentiation $\Rightarrow$ gradient, Hessian
- will julia replace python in 5–10 years?
- notebooks can change the way we work and teach