New Developments in Minuit2

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Introduction

- **Minuit**
  - Popular minimisation program developed in the 1970s by *F. James*.
  - It is a **variable-metric method** (quasi-Newton method) based on the DFP / BFGS update of the inverse Hessian matrix.
  - Works extremely well for fitting (e.g. parameter estimation) and it is has been used extensively in HEP.
  - Available in ROOT since the beginning in the `TMinuit` class.
- **Minuit2**
  - Improved version re-written in C++ classes of same algorithm (MIGRAD)
  - Available both in ROOT and as a standalone version
  - Being used in the statistical analysis of LHC experiments
  - **iMinuit** : python package built on top of Minuit2
    - used in large astroparticle physics experiments

Characteristics of Minuit

- **Works very well,** superior to gradient descent methods
  - Much less number of iterations to converge
  - No need to perform matrix inversion at each iteration
  - Approximate Hessian converges to true Hessian at the minimum
  - Regularisation when Hessian is not positive defined
    - add offset to the diagonal of H to make it positively defined
  - Self-correcting if the Hessian approximation is not good enough
- Disadvantages:
  - Sensitive to initial parameters, it is a local minimiser and can get stuck in local minima
  - Sensitive to bad numerical precision in function and gradient calculation
  - Does not scale to problems with a huge number of parameters
    - proven to work to > ~ 1000 parameters (e.g Higgs combination fits)
    - will not work for training deep-learning models with millions of parameters
      - need to use gradient descent in these cases

External Gradient and Hessian

- Minuit requires the function gradient at each iteration
  - computed by default numerically using a 3 points rule and adaptive step sizes
    - well-tested and robust method
    - essential to having good precision when the gradient is close to zero (near the minimum) to converge rapidly
- Support for external gradients provided by user
  - needed for users exploiting Automatic Differentiation (AD)
- **New**: Option in Minuit2 to provide external Hessian or only the diagonal of the Hessian (G2) for seeding
  - without providing Hessian, Minuit2 computes G2 numerically
  - using initial user steps is often not good (need good estimates)

New improvements in Minuit2

- Improved debugging
  - can log and return to user all minimisation iteration states
  - can provide a detailed output of each iteration (in debug mode)
- Possibility to add users callback functions at each iteration
- Thread-safety: Minuit2 can work in multi-threads if user provided function can
  - support for likelihood or gradient parallelisation
- Addition of new minimization methods:
  - **BFGS**: use only standard BFGS formula instead of the default mode of using both BFGS or DFP formula depending on some conditions

Specialized Algorithms for Fitting

- When minimising Least-square functions:

$$F(x) = \sum_{k=1}^{n} f_k^2 = \sum_{k=1}^{n} \left(\frac{y_k - T_k(x)}{\sigma_k} \right)^2$$

Hessian $$H_{ij} = \frac{\partial^2 F(x)}{\partial x_i \partial x_j} = \sum_{k=1}^{n} 2 \frac{\partial f_k \partial f_k}{\partial x_i \partial x_j} + 2 f_k \frac{\partial^2 f_k}{\partial x_i \partial x_j} \approx \sum_{k=1}^{n} 2 \frac{\partial f_k \partial f_k}{\partial x_i \partial x_j}$$

$$\Rightarrow \quad \mathbf{H} \approx \mathbf{J}^T \mathbf{J}$$

this can be neglected when residuals f are small

Neglect second derivatives of model function: linearisation

- Many algorithms have been developed on this approximation:
  - e.g. Levenberg-Marquardt (GSL), Fumili, …

Likelihood Fits

- **For likelihood functions:**

$$\mathcal{L}(x) = -\sum_{k=1}^{n} \log f(y_k|x) \quad \text{and} \qquad H_{ij} = \frac{\partial^2 \mathcal{L}(\theta)}{\partial\theta_i \partial\theta_j} = -\sum_{k=1}^{n} \frac{\partial}{\partial x_i}\left(\frac{1}{f_k}\frac{\partial f_k}{\partial x_j}\right) = \sum_{k=1}^{n} \frac{1}{f_k^2}\frac{\partial f_k \partial f_k}{\partial x_i \partial x_j} - \sum_{k=1}^{n} \frac{1}{f_k}\frac{\partial^2 f_k}{\partial x_i \partial x_j}$$

  - the linear approximation is not always valid!

- **For binned likelihood fits**, can write the likelihood as

$$\mathcal{L}(x) = -\sum_{k=1}^{n} \log P(n_k|\mu_k(x)) = -\sum_{k=1}^{n} \log \frac{e^{-\mu_k(x)}\mu_k(x)^{n_k}}{n_k!}$$

and after removing constant terms

$$\mathcal{L}(x) = \sum_{k=1}^{n} \left(\mu_k(x) - n_k \log \mu_k(x)\right)$$

$$H_{ij} = \frac{\partial^2 \mathcal{L}(\theta)}{\partial\theta_i \partial\theta_j} = \sum_{k=1}^{n} \frac{\partial}{\partial x_i}\left(\frac{\partial \mu_k}{\partial x_j} - \frac{n_k}{\mu_k}\frac{\partial \mu_k}{\partial x_j}\right) = \sum_{k=1}^{n} \frac{n_k}{\mu_k^2}\frac{\partial \mu_k \partial \mu_k}{\partial x_i \partial x_j} - \sum_{k=1}^{n} \frac{(n_k - \mu_k)}{\mu_k}\frac{\partial^2 \mu_k}{\partial x_i \partial x_j} \approx \sum_{k=1}^{n} \frac{n_k}{\mu_k^2}\frac{\partial \mu_k \partial \mu_k}{\partial x_i \partial x_j}$$

$$\mathbf{H} \approx \mathbf{J}^T \mathbf{J}$$

this can be neglected
it is like a residual f_k

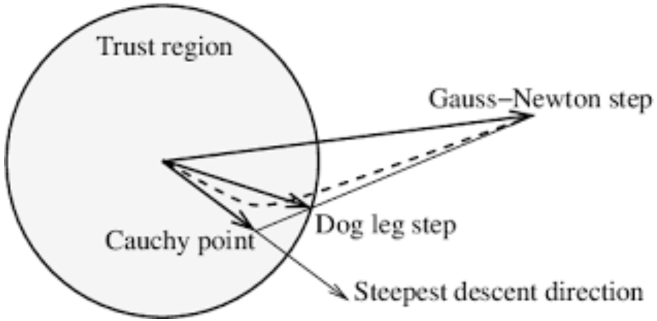
- **The same algorithms used for least-square fitting can be used !**

Specialized Fitting Methods

- Hessian can be computed directly from the first derivatives of the model function
  - It is like a linear fit approximation
- This approximation is also good in the case of binned likelihood fits but not always for standard unbinned maximum likelihood fits
- **Advantage of linearisation:**
  - positive defined Hessian and easy to calculate gradients (one can use a 2-point rule)
  - faster to converge than standard methods (Minuit/BFGS)
- Disadvantage:
  - Initial point need to be close enough to the minimum to consider the approximation $\mathbf{H}_k \approx \mathbf{J}_k^T \mathbf{J}_k$ valid
  - require a more complex interface, needed the Jacobian matrix (number of fit points $\times$ number of parameters) at each iteration

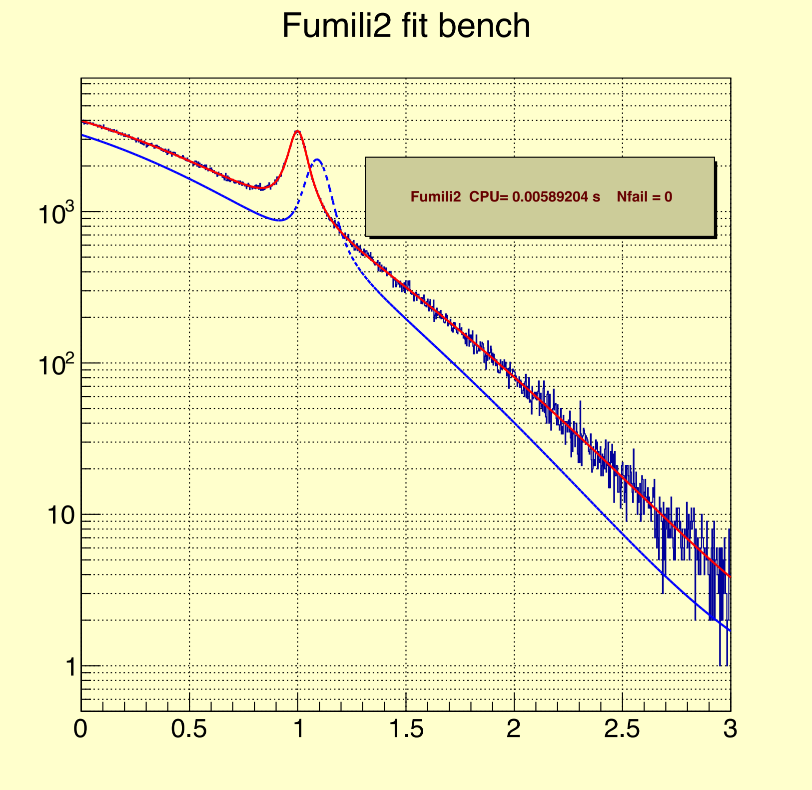
New Fumili Algorithm

- New implementation of Fumili algorithm: **Fumili2**
  - original algorithm from I. Silin implemented in the Cernlib and `TFumili` class
- It is integrated into Minuit2 library
  - re-using Minuit2 interfaces classes
  - working for both least-square and binned likelihood fits
- Based on trust-region using dogleg step
  - trust region can be scaled using a metric defined by the diagonal of the approximated Hessian



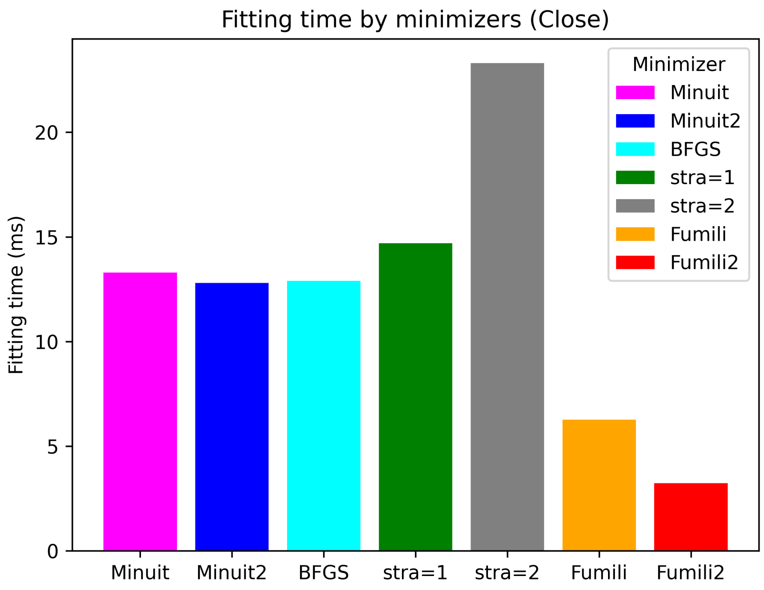
Benchmark Results

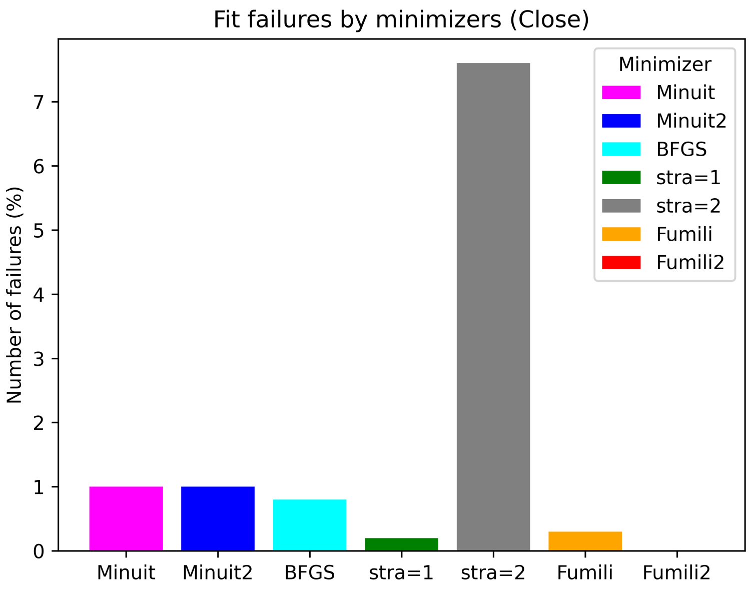
- Use a binned likelihood to fit signal peak over some background in a histogram
  - 1000 bins
  - 7 parameter fits performing numerical convolution
  - repeat fit 1000 times with different data and different initial random parameter values
    - not too far from the minimum



Benchmark Results

- Binned likelihood fit to signal peak over some background

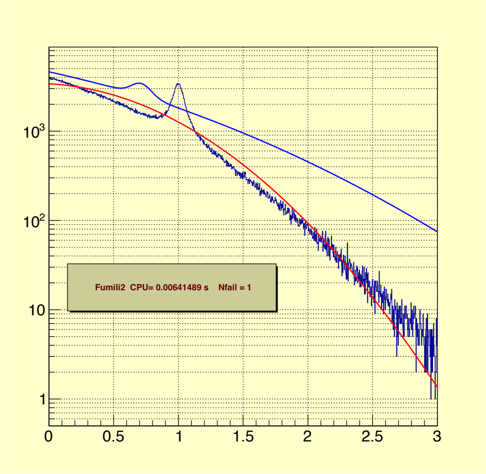


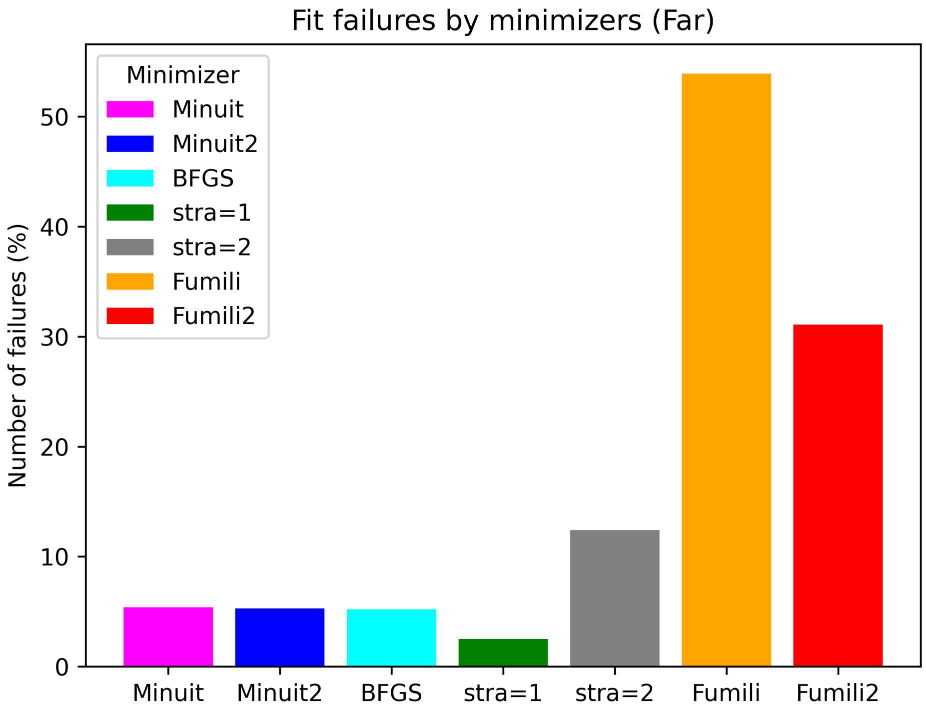


- New Fumili algorithm (**Fumili2**) works very well !

Benchmark Results (2)

- **With initial parameters values further away from minimum**





Using a starting point further away we start to see more fit failures !

ROOT Minimization Interface

- ROOT provides class **`ROOT::Math::Minimizer`** as general interface for minimization
- Current default is TMinuit (old Minuit implementation)
  - plan to switch to use Minuit2 as default in the next release
- Implemented by several algorithms:
  - `TMinuit`
  - Minuit2
  - `TFumili`
  - GSL minimisers and fitters algorithms (Levenberg-Marquardt)
  - Simulated annealing and Genetic algorithm
  - R-Minimizer : minimiser based on algorithms from R
  - and now from Python: `scipy.optimize`

Scipy optimizers

- New implementation of ROOT::Math::Minimizer using `scipy.optimize` (from *O. Zapata)*
- `scipy.optimize.minimize` provides several minimization algorithms

scipy.optimize.minimize

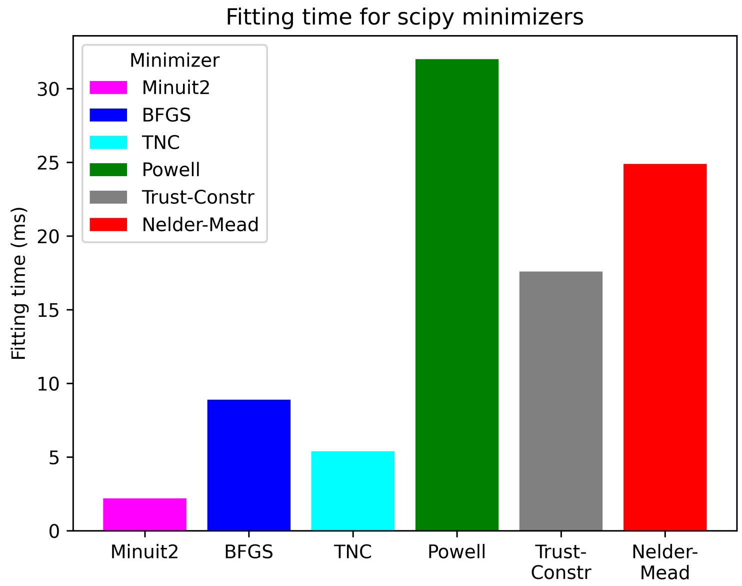
```
scipy.optimize.minimize(fun, x0, args=(), method=None, jac=None, hess=None,
hessp=None, bounds=None, constraints=(), tol=None, callback=None, options=None)
```

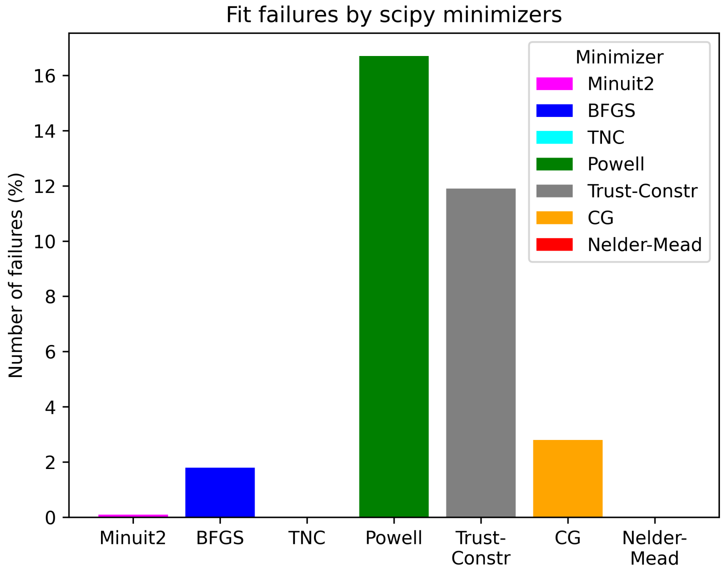
method : ***str or callable, optional***

Type of solver. Should be one of

- 'Nelder-Mead' (see here)
- 'Powell' (see here)
- 'CG' (see here)
- 'BFGS' (see here)
- 'Newton-CG' (see here)
- 'L-BFGS-B' (see here)
- 'TNC' (see here)
- 'COBYLA' (see here)
- 'SLSQP' (see here)
- 'trust-constr'(see here)
- 'dogleg' (see here)
- 'trust-ncg' (see here)
- 'trust-exact' (see here)
- 'trust-krylov' (see here)

Benchmark with Scipy





Time for CG is > 600 ms

- Varying performance of `scipy` minimisers
  - Minuit2 performs better!
- Fitting using AD *(with a different fit than before)*
  - without providing gradients `scipy` optimisers perform worse
    - *e.g. number of failures for TNC is more than 80%*

iminuit

(from Hans Dembinsky)

- Jupyter-friendly Python frontend to Minuit2 C++ library in ROOT
- Part of Scikit-HEP project, developed in sync with ROOT
- Backend in particle and astroparticle physics libraries zfit, pyhf, gammapy, flavio, ctapipe, ...
- Easy to install: *pip install iminuit* installs precompiled binary package on all major platforms
- Comprehensive documentation with many tutorials
- 100 % test coverage

- Batteries included: shipped with common cost functions for statistical fits
  - Binned and unbinned maximum-likelihood
  - **Template fits (new):** including mix of templates and parametric models HD, A. Abdelmotteleb EPJ C 82, 1043 (2022)
  - Non-linear regression with (optionally robust) weighted least-squares
  - Gaussian penalty terms
  - Cost functions can be combined by adding: *total_cost = cost_1 + cost_2*
- Support for SciPy minimisers as alternatives to Minuit's Migrad algorithm
- Smart visualization of fit results in Jupyter notebooks + **interactive fits**

iMinuit benchmarks available at https://iminuit.readthedocs.io/en/stable/benchmark.html

Example fit with interactive fitting widget

```python
import numpy as np
from iminuit import Minuit
from scipy.stats import norm

x = norm.rvs(size=1000, random_state=1)

# Negative unbinned log-likelihood with a normal PDF;
# ready-made cost functions like this are in iminuit.cost
def nll(mu, sigma):
    return -np.sum(norm.logpdf(x, mu, sigma))

m = Minuit(nll, mu=0, sigma=1)
m.limits["mu"] = (-1, 1)
m.limits["sigma"] = (0, np.inf)
m.migrad()  # find minimum
m.hesse()   # compute uncertainties
```

[17] ✓ 0.0s Python

Migrad	
FCN = 1400	Nfcn = 34
EDM = 1.5e-07 (Goal: 0.0002)	
Valid Minimum	No Parameters at limit
Below EDM threshold (goal x 10)	Below call limit

Covariance	Hesse ok	Accurate	Pos. def.	Not forced

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	mu	0.04	0.04			-1	1	
1	sigma	0.981	0.031			0		

	mu	sigma
mu	0.00192	0
sigma	0	0.000962

Conclusions

- Minuit is more than 50 years old but it seems to be still the best minimization algorithm for HEP fitting problems
- New algorithm (Fumili2) for least-square and binned likelihood fit
- Recent improvements in Minuit2:
  - support for external gradient and Hessian (for AD users)
  - improve logging and usability
- Minuit2 will be made the default minimiser in the next ROOT version
- Python version (***iminuit***) available also for the Python user community
- Future work:
  - implement support for non-trivial parameter constraints

References

- Minuit2:
  - Users guide
  - Minuit Tutorial on Function Minimization (*F. James*)
- ROOT Minimisers
  - ROOT::Math::Minimizer
- scipy:
  - scipy.optimize.minimize documentation
  - scipy ROOT interface
- iMinuit
  - https://iminuit.readthedocs.io/en/stable/

Backup Slides

Minuit Algorithm

- Start with an initial approximation of inverse Hessian, $H = (\nabla^2 f(x))^{-1}$
  - e.g. use diagonal second derivatives
- Iterate :
  - compute new step direction as $p_k = -Hg$ where $g = \nabla f(x_k)$
  - perform line search for optimal point $x_{k+1} = x_k + \alpha p_k$
    - $s_k = x_{k+1} - x_k$
  - compute the new gradient g at x_{k+1} and $y_k = g_{k+1} - g_k$
  - Update inverse Hessian matrix H_k according to BFGS or DFP update formula

BFGS : $H_{k+1} = (I - \frac{s_k y_k^T}{y_k^T s_k}) H_k (I - \frac{y_k s_k^T}{y_k^T s_k}) + \frac{s_k s_k^T}{y_k^T s_k}$ DFP: $H_{k+1} = H_k + \frac{s_k s_k^T}{s_k^T y_k} - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k}$

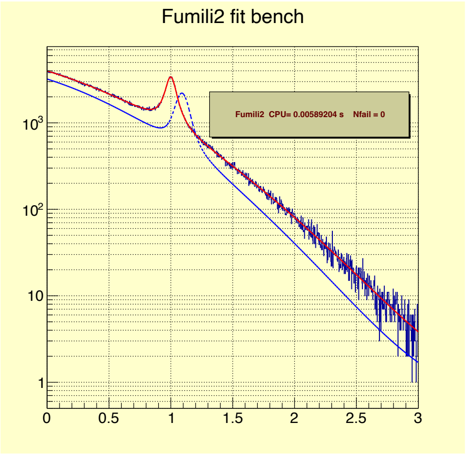
  - stop iteration when the Expected Distance from the Minimum (EDM) $\rho = g^T H g$ is small
- EDM provides a scale-invariant quantity to tell the convergence of method.
  - This is unique in Minuit!

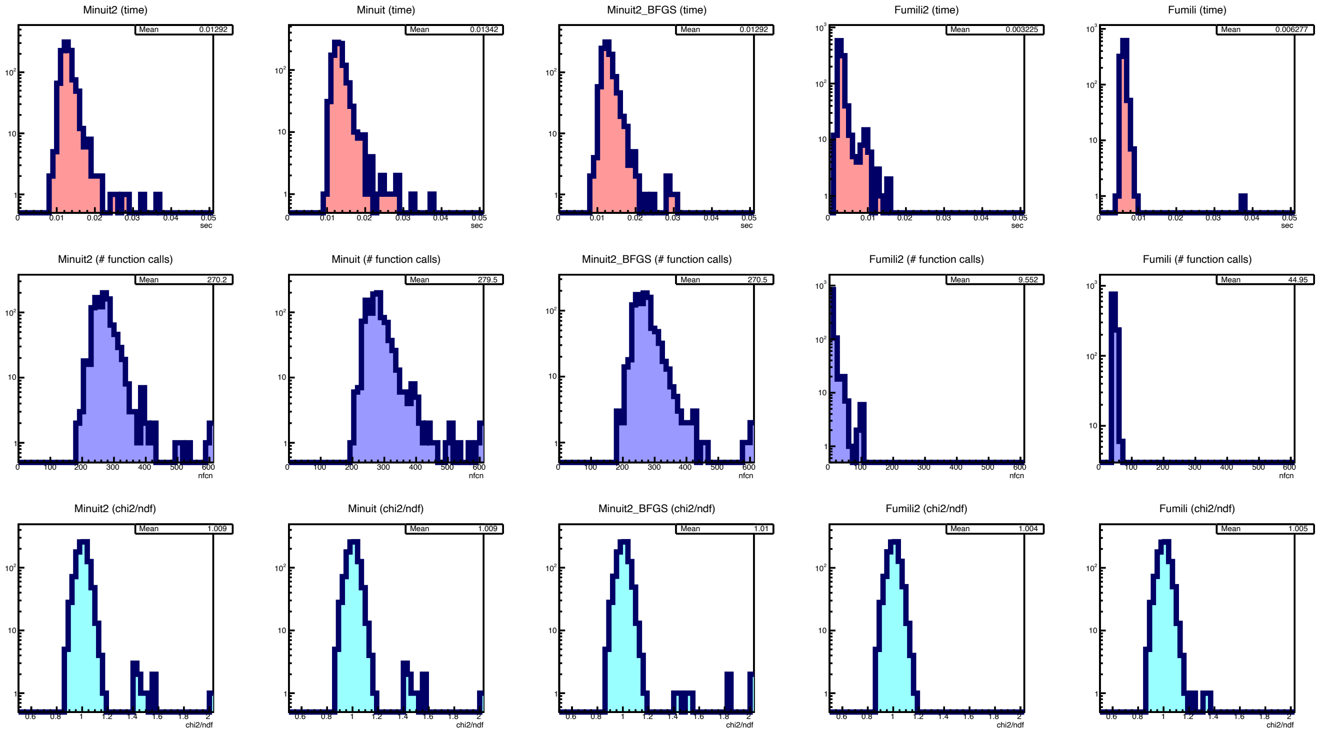
Fumili Algorithm

- Old algorithm proposed already in 1961 by I. Silin
- Implemented later in the CERN library and made also available to ROOT with TFumili class.
  - It uses the Hessian approximation combined with a trust region method.
    - a multidimensional parallelepiped ("box") is defined around the point and used its intersection with the Newton direction for the next step
    - size of the parallelepiped changes dynamically
      - depending on the function improvements and the expectation from a quadratic approximation.
- Faster than Minuit for least-square fits when the starting point is close enough to the solution

Benchmark Results

- Use a binned likelihood to fit signal peak over some background

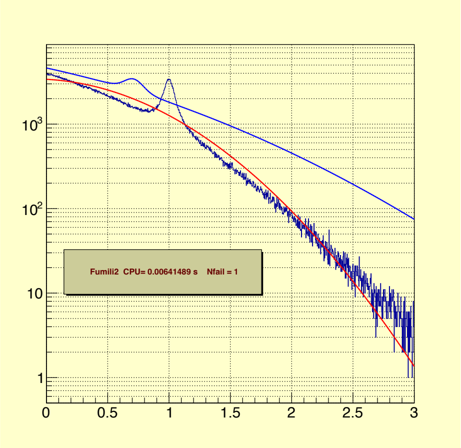


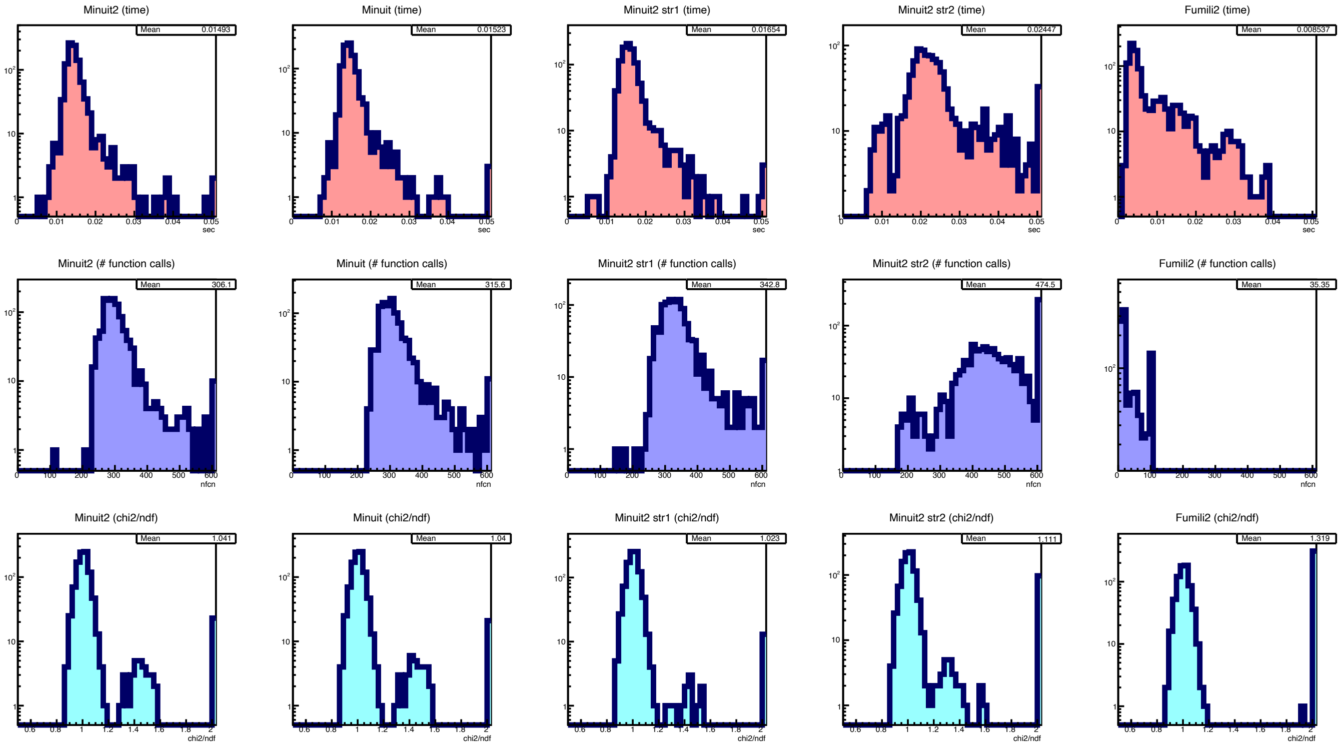


1000 bins - 7 parameters
repeat fit 1000 times with different data and different initial parameter values

Benchmark Results (2)

- Using initial parameters values further away from minimum solution

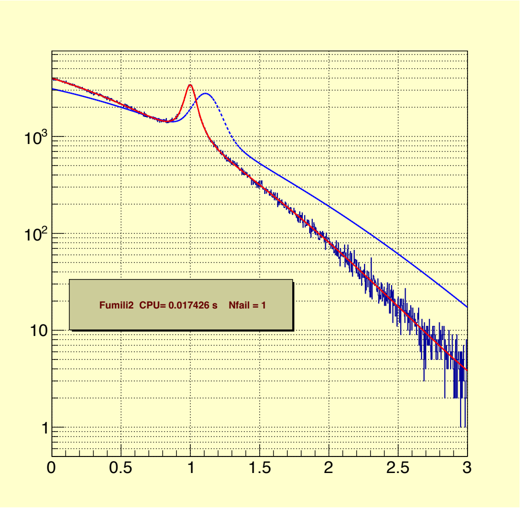




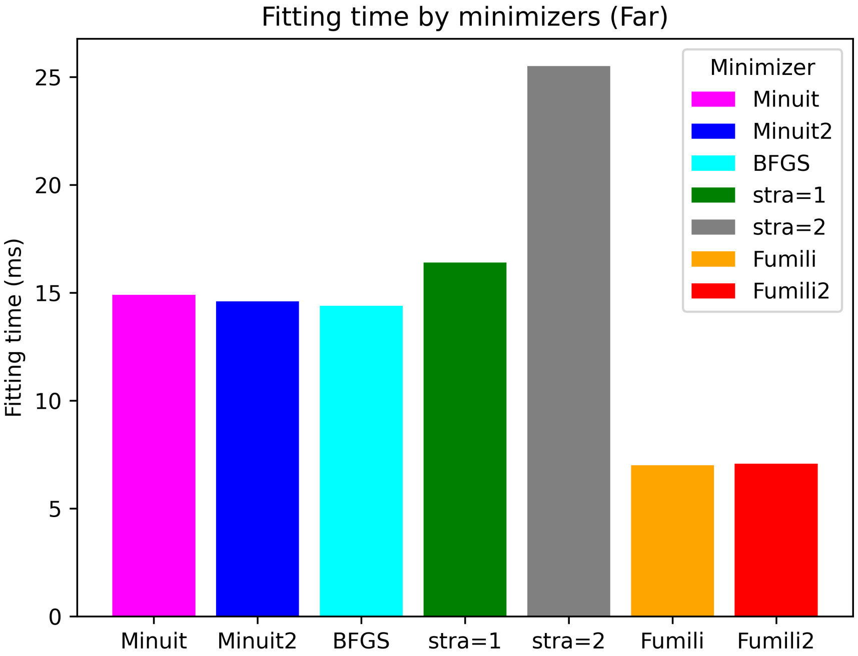
Using a starting point further away we start to see more fit failures !

Benchmark Results (2)

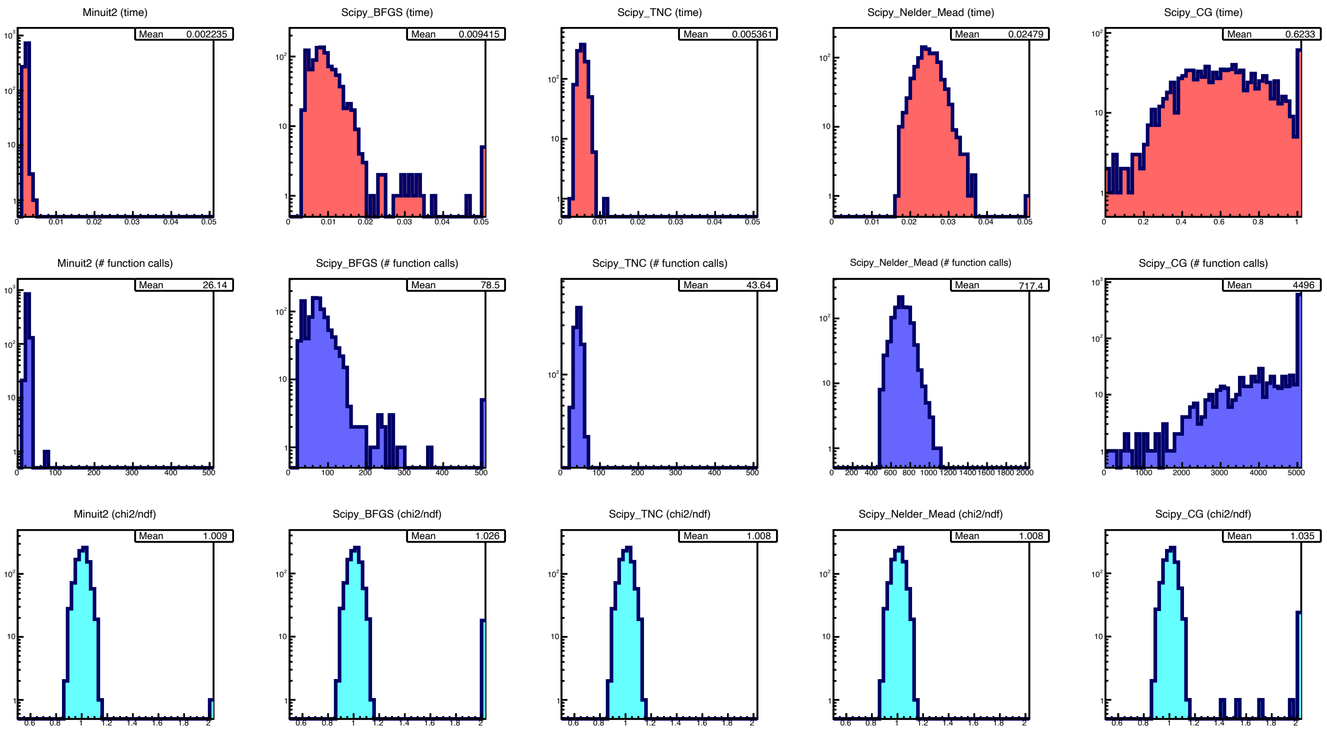
- Using initial parameters values further away from minimum solution



Using a starting point further away we see also longer fitting time



Benchmark using Scipy Minimisers

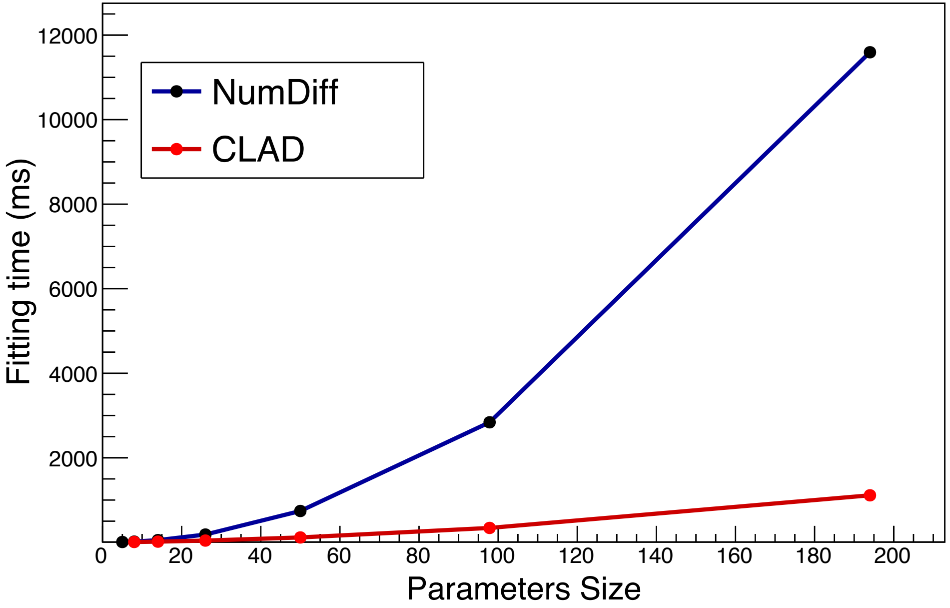


Poor performance of `scipy` with respect to Minuit!

Using Scipy Minimizer interface from *O. Zapata*

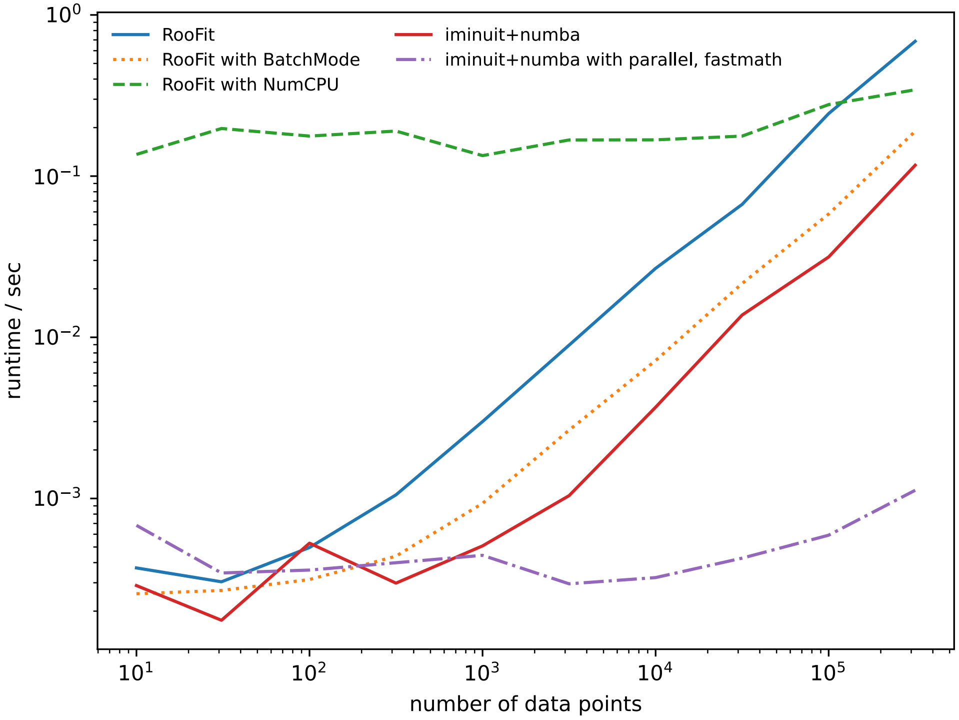
Fitting time using AD

- Fitting time in Minuit2 for different sizes: AD vs Numerical differentiation



High performance fitting in Python with iminuit

- Using Python not performance bottleneck, if numerical code is accelerated with Numba JIT
- Crucial for high performance: accelerated parallelized SIMD-friendly PDF and accelerated unbinned likelihood function
- Benchmarks for unbinned likelihood fit of normal distribution with parameters μ, σ



- iminuit
- iminuit.cost.UnbinnedNLL
- numba-accelerated normal distribution from numba-stats package
- automatic parallelization and fastmath

Up to 100x faster than RooFit (C++)
with NumCPU (parallel computation)
and BatchMode (≈ fastmath) options

Scipy using Numerical Derivatives

- Fitting time and failures in Scipy with numerical gradients