Phys 512: PS4

1) a) First we consider Newton's method to find optimal parameters for a given fit

↳ Whereas gradient descent simply follows the gradient ∇f along the χ^2 manifold, Newton's method takes into account the curvature & follows $H^{-1}\nabla f$, where H^{-1} is the Hessian (inverse). Thus our step looks like:

$$x \longrightarrow x + \delta x \; : \; \delta x = -\eta H^{-1} \nabla f \; , \quad \eta \in \mathbb{R}$$

The following are the derivatives of the Lorentzian:

- $f(t) = \dfrac{a}{1 + (t-t_0)^2/w^2} = a\left[1 + w^{-2}(t-t_0)^2\right]^{-1}$. $\partial_a f(t) = \left[1 + w^{-2}(t-t_0)^2\right]^{-1}$
- $\partial_{t_0} f(t) = (2a(t-t_0)w^2)/((t-t_0)^2 + w^2)^2$
- $\partial_w f(t) = (2a(t-t_0)^2 w/((t-t_0)^2 + w^2)^2$

This will be useful for the calculations:

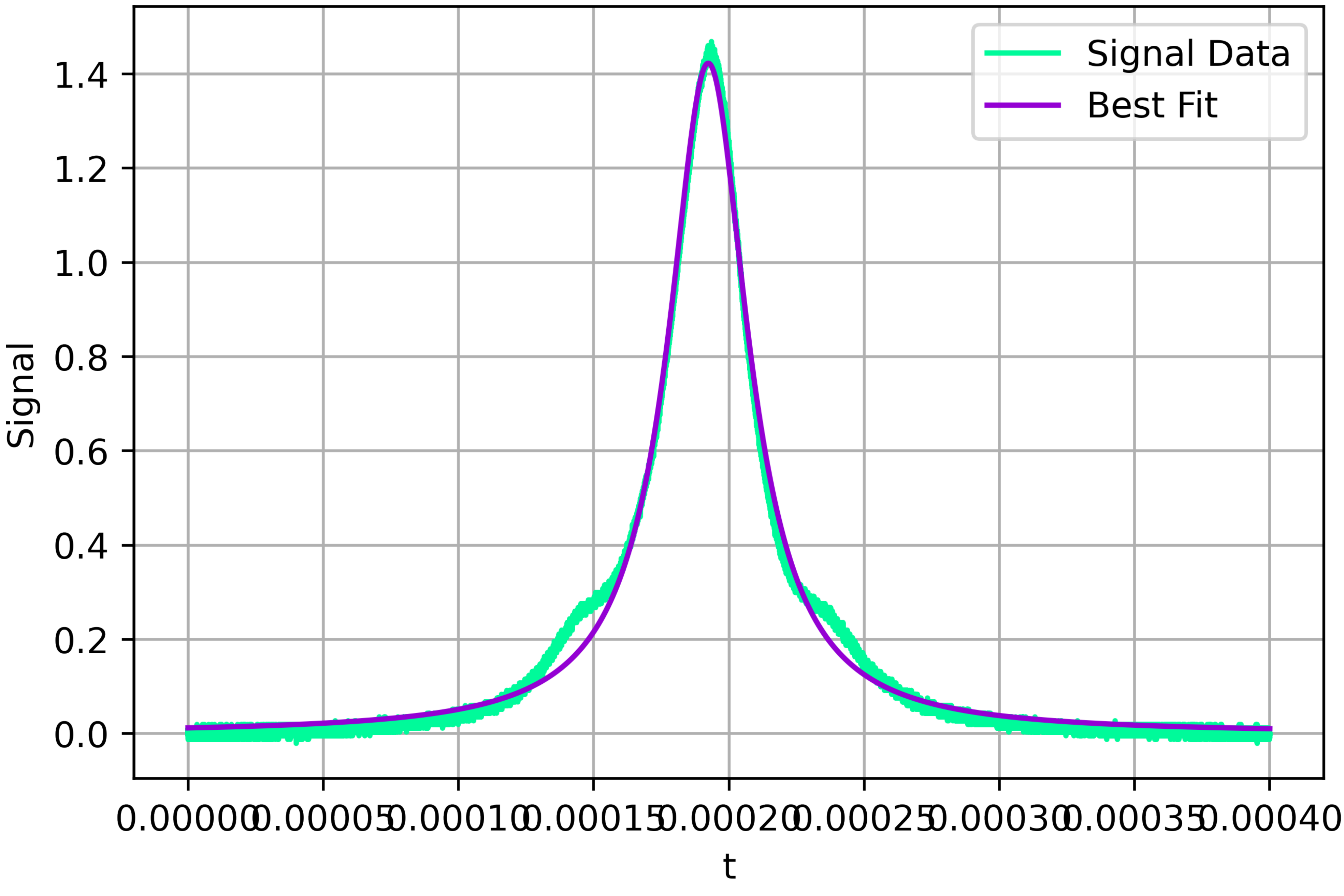
- $f(t;m) \equiv A(m)$, $r \equiv d - A(m)$ · $\chi^2 = r^T N^{-1} r$ · $\nabla \chi^2 = -2A'^T N^{-1} r$
- $\nabla^2 \chi^2 \simeq 2A'^T N^{-1} A'$ · $\delta m = (A'^T N^{-1} A')^{-1} (A'^T N^{-1} r)$

<u>Note:</u> We initially (for 1a)) assume $N = \mathbb{1}$ & thus get:

- $\delta m = [\nabla f^T \nabla f]^{-1} [\nabla f^T r] = [\nabla f^T \nabla f]^{-1} [\nabla f^T (d - f)]$

For an initial guess of $a, t_0, w = [1.5, 2\times10^{-4}, 1\times10^{-4}]$ we get the following best fit parameters, & the plot looks like:

25 steps $a = 1.4228$, $t_0 = 1.9236 \times 10^{-4}$, $w = 1.7924 \times 10^{-5}$



Signal Data
Best Fit
Signal
t
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035
0.00040

b) Our estimate for computing the error was derived from discussions w/ Guillaume

↳ The procedure for estimating N will be done via taking the standard deviation (at a point x_0) of a small, compact neighborhood of data point surrounding x_0

↳ Moreover we assume the standar error on each data point is $\simeq 5 \times 10^{-3} \equiv \sigma$ ($\simeq$ the std of 25 points)

With this we can estimate the covariance matrix:

$$N^{-1} = \mathbb{1}/\sigma^2 \quad \Rightarrow \quad N = A'^T N^{-1} A' = \frac{1}{\sigma^2} \nabla f^T \nabla f$$

Using this, we get the parameter uncertainties:

$$\sigma_a = 8.4304 \times 10^{-5}, \quad \sigma_{t_0} = 1.0618 \times 10^{-9}, \quad \sigma_w = 1.5036 \times 10^{-4}$$

c) We redo part a) w/ numerical derivaties & get the following best-fit parameters:

$$a = 1.4228, \quad t_0 = 1.9236 \times 10^{-4}, \quad w = 1.7923 \times 10^{-5}$$

It is somewhat suspicious that they are the exact same values (on python they agree to a lot more digits), but it suffices to say they are not statistically different from the answers in a)

↳ The diffrence is less then σ we computed in b)

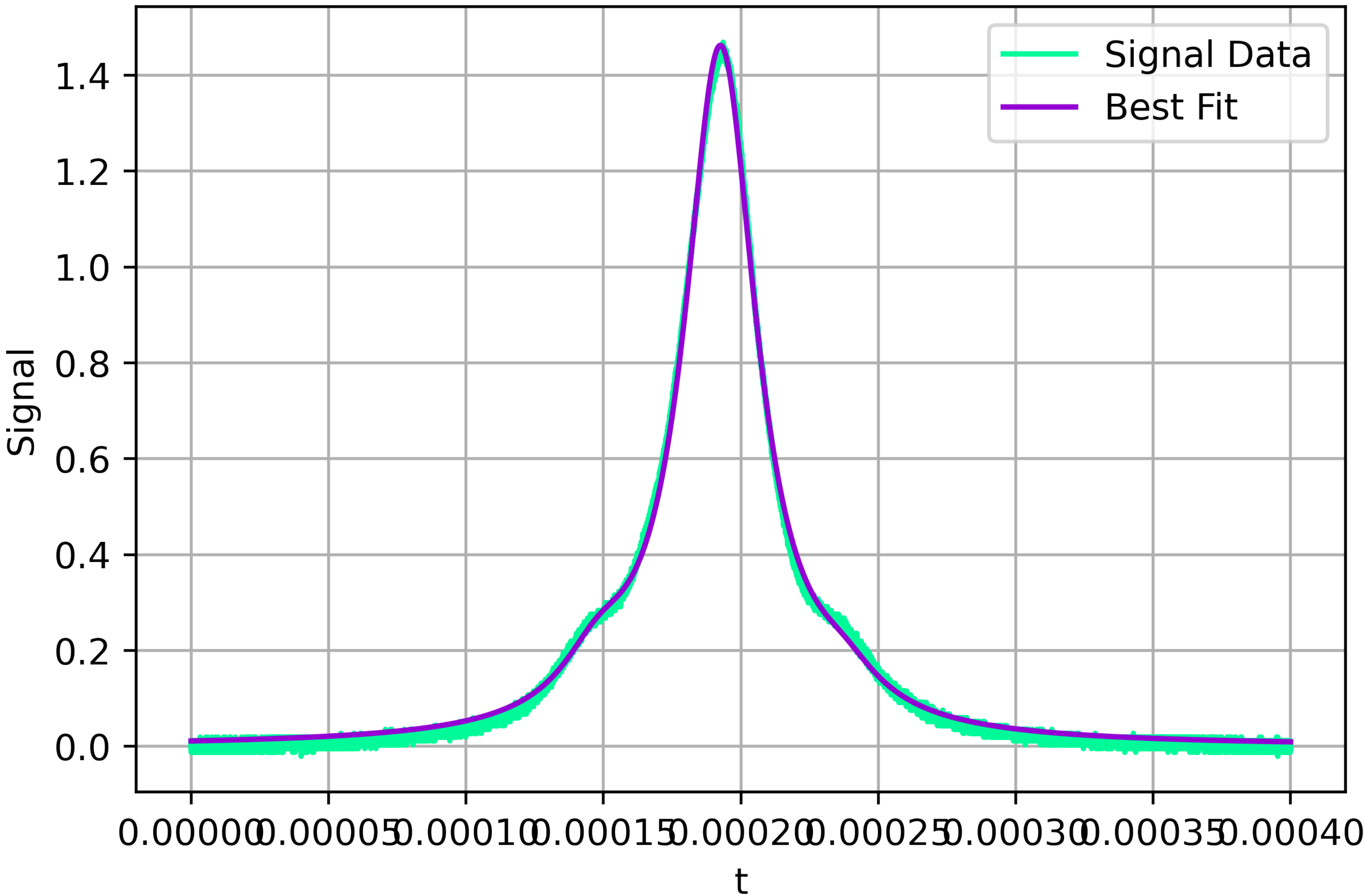
d) We repeat what is done in c) (numerical derivatives), except now with:

$$f(t) = a\left[1 + (t-t_0)^2/w^2\right]^{-1} + b\left[1 + (t-t_0+dt)^2/w^2\right]^{-1} + c\left[1 + (t-t_0-dt)^2/w^2\right]^{-1}$$

Following the procedure we've done in a-c), we have the following best fit parameters & their uncertainties:

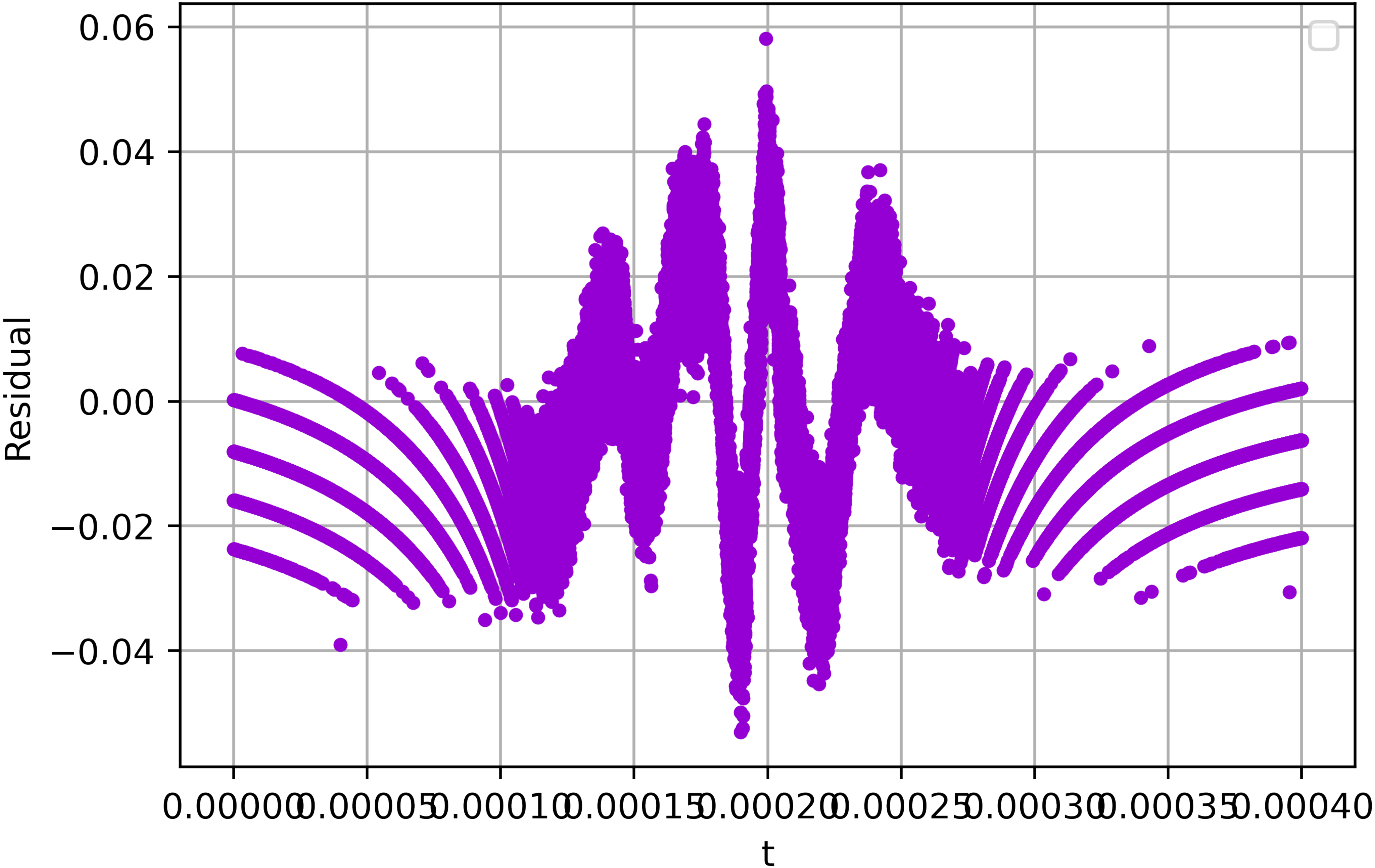
$a = 1.4430 \pm 9.1390 \times 10^{-5}$, $b = 1.0391 \times 10^{-1} \pm 8.7167 \times 10^{-5}$
$c = 6.4733 \times 10^{-2} \pm 8.5381 \times 10^{-5}$, $t_0 = 1.9258 \times 10^{-4} \pm 1.0820 \times 10^{-9}$
$w = 1.6065 \times 10^{-5} \pm 1.9378 \times 10^{-9}$, $dt = 4.457 \times 10^{-5} \pm 1.3044 \times 10^{-8}$

Moreover, the prediction fits the data better, as seen in:



Signal Data
Best Fit
Signal
t
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035
0.00040

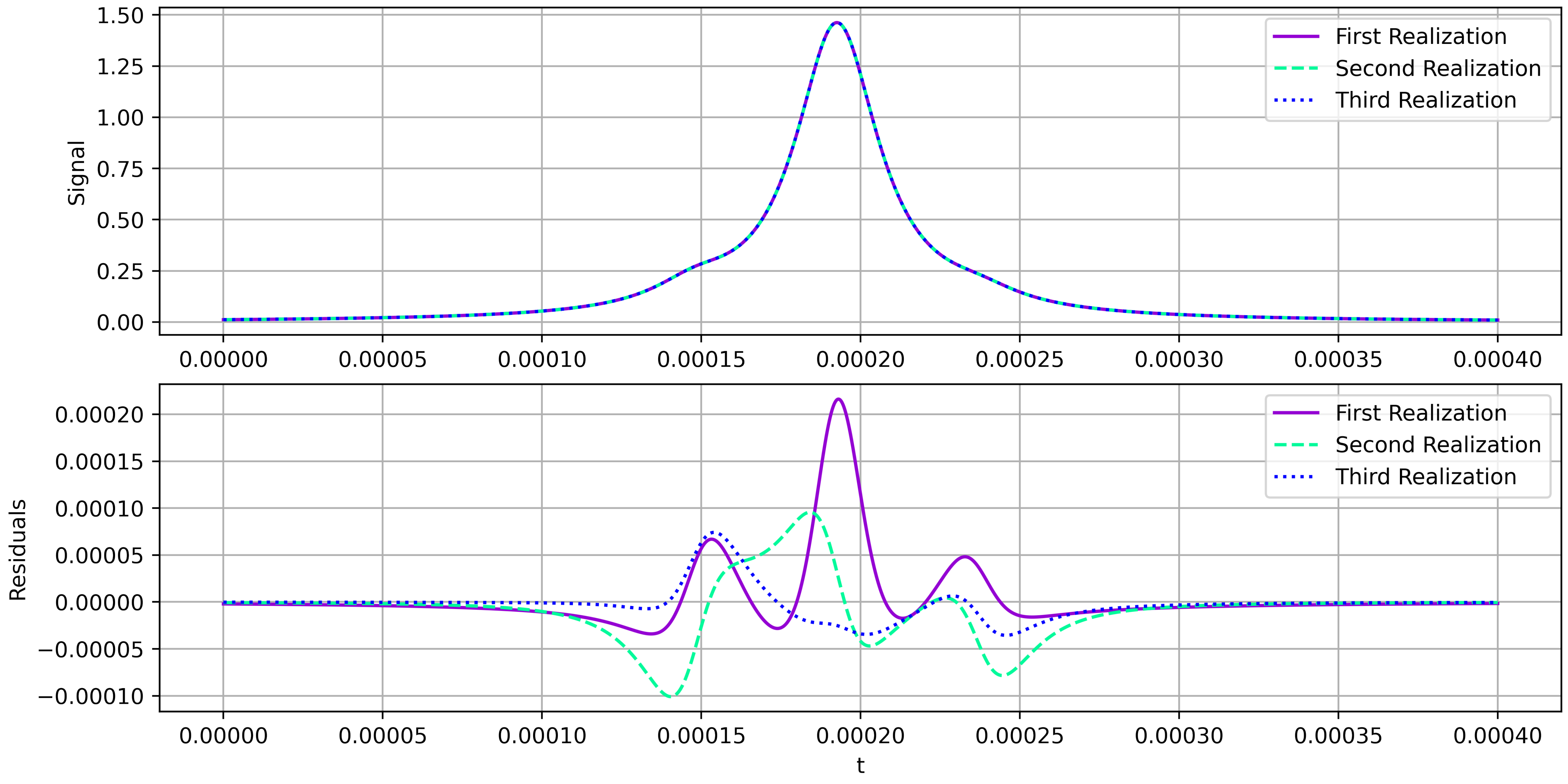
e) The residuals (data - fit) have the following plot: (2



0.06
0.04
0.02
0.00
−0.02
−0.04
Residual
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035
0.00040
t

The residuals clearly contain a structure & are thus correlated. This tells us the error bars we got by assuming independence is not a full description of the data.

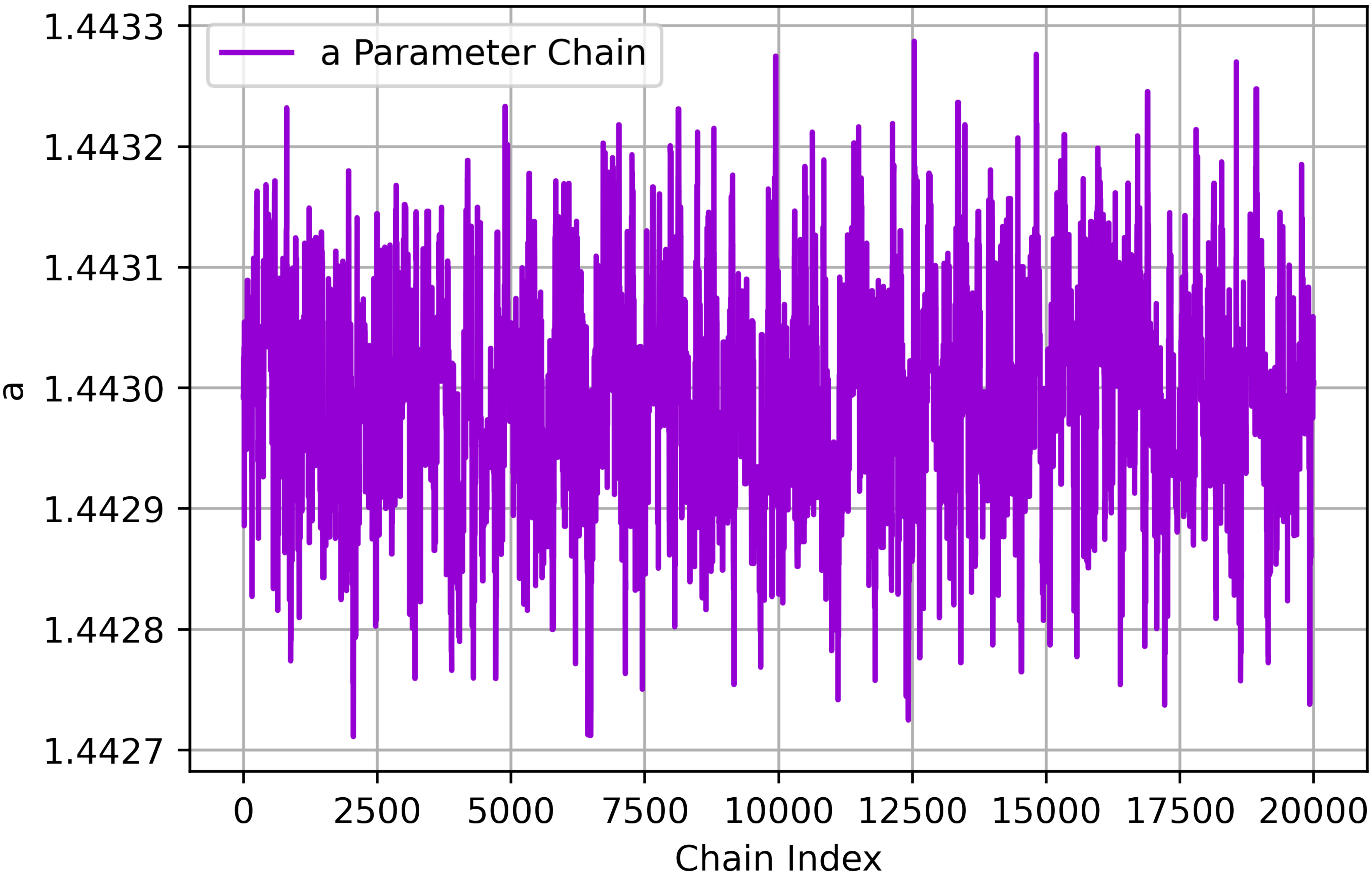
f) We consider three different realizations for randomly i.i.d perturbed parameters & it has the following plot (& their corresponding residuals):



1.50
1.25
1.00
0.75
0.50
0.25
0.00
Signal
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035
0.00040
First Realization
Second Realization
Third Realization
0.00020
0.00015
0.00010
0.00005
0.00000
−0.00005
−0.00010
Residuals
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035
0.00040
t
First Realization
Second Realization
Third Realization

Computing the typical difference in χ^2 gives us 8.5200×10^{-5} which is reasonable at is much less than 1 & we only perturbed the parameters by a small, random amount.

g) After computing the MCMC algorithm for 20,000 steps, we have the chain plot for the 'a' parameter:



a Parameter Chain
a
1.4433
1.4432
1.4431
1.4430
1.4429
1.4428
1.4427
0
2500
5000
7500
10000
12500
15000
17500
20000
Chain Index

As we can see from above, the chain doesn't have an inherent structure & have stabilized around the mean a ~ 1.4430.

↳ Moreover, the best-fit parameters & their uncertainties are:

- $a = 1.4430 \pm 9.0059 \times 10^{-5}$
- $b = 0.1039 \pm 8.7292 \times 10^{-5}$
- $c = 0.0647 \pm 8.6482 \times 10^{-5}$
- $t_0 = 0.0002 \pm 1.0569 \times 10^{-4}$
- $\omega = 1.16065 \times 10^{-5} \pm 1.8700 \times 10^{-9}$
- $\delta t = 4.4567 \times 10^{-5} \pm 1.1778 \times 10^{-8}$

My error bars have not changed by a significant amount (less than 1σ).

h) Using our best fit parameters, we can compute the width μ of the resonance cavity:

$$\mu = dt/w \cdot 9\,GHz = (24.9674 \pm 0.0280)\ GHz$$