Title: Numerical Methods Lecture - 230117

Speakers: Erik Schnetter

Collection: Numerical Methods (2022/2023)

Date: January 17, 2023 - 9:15 AM

URL: https://pirsa.org/23010004

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README.md

FittingAModel2023

Repository for PSI Numerical Method 2023 lesson on "Fitting a model to data"

This lesson uses some ideas from the paper https://arxiv.org/abs/1008.4686 and Table 1 from that paper has been copied into `data.csv`.

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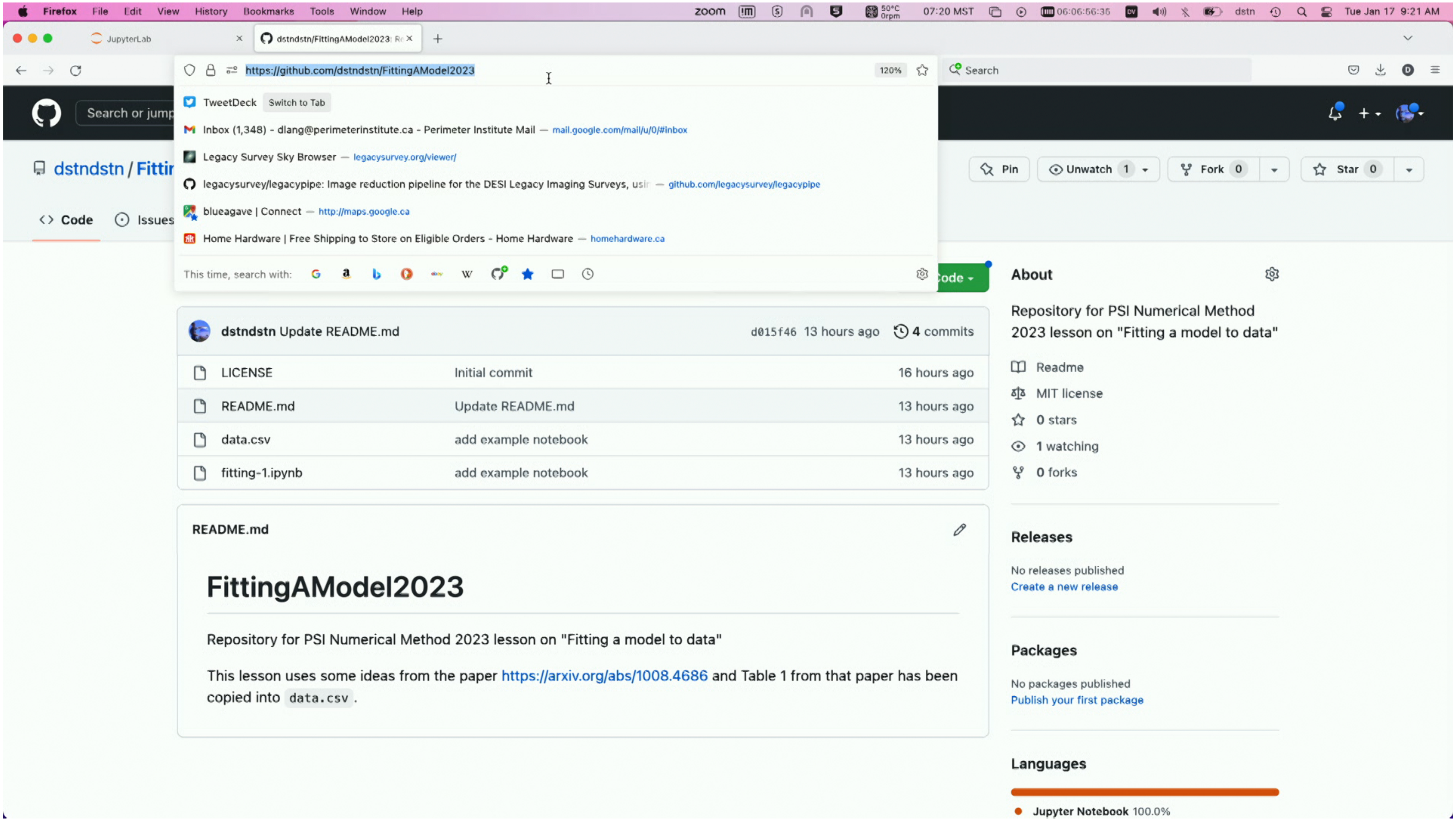
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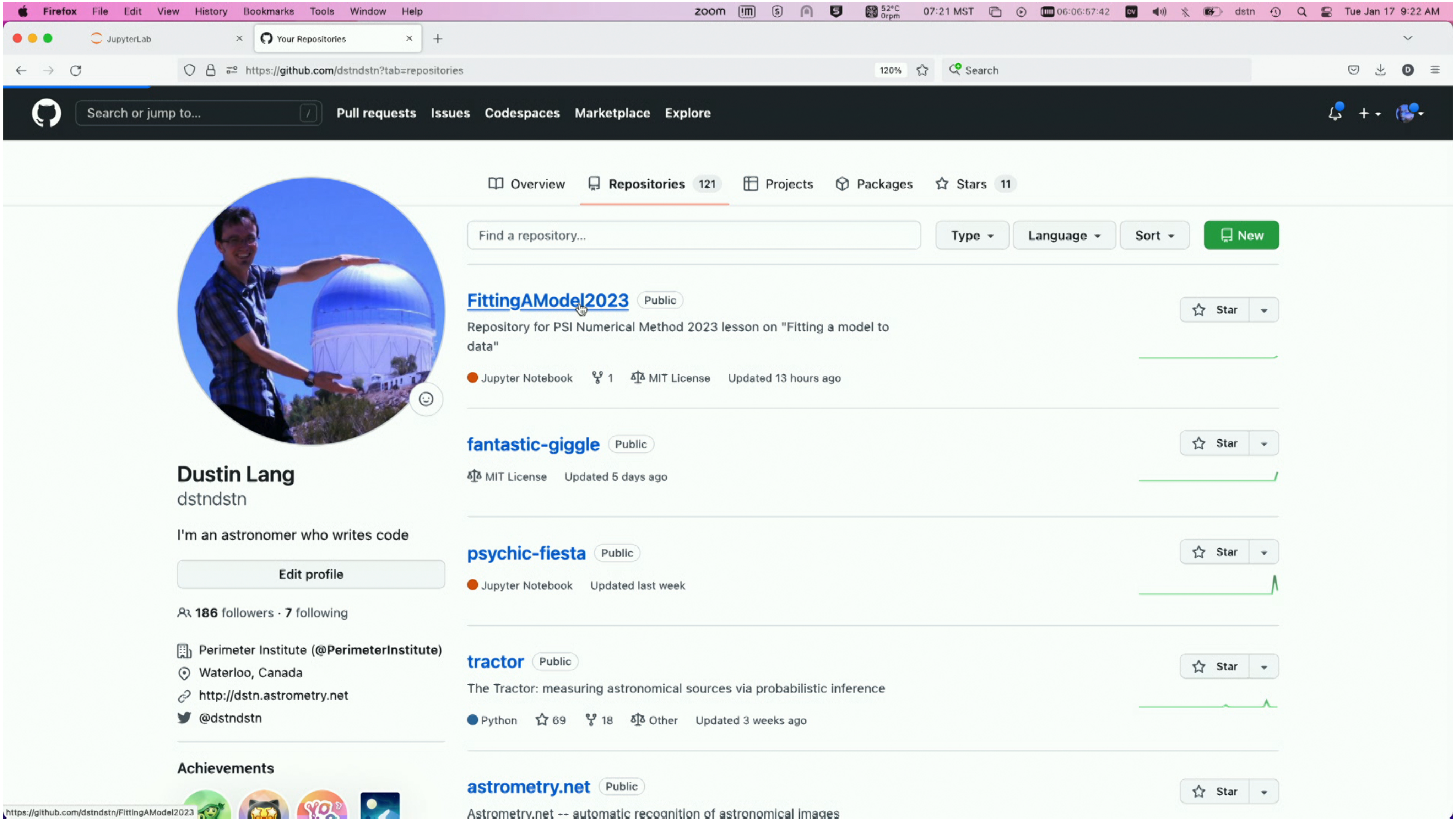
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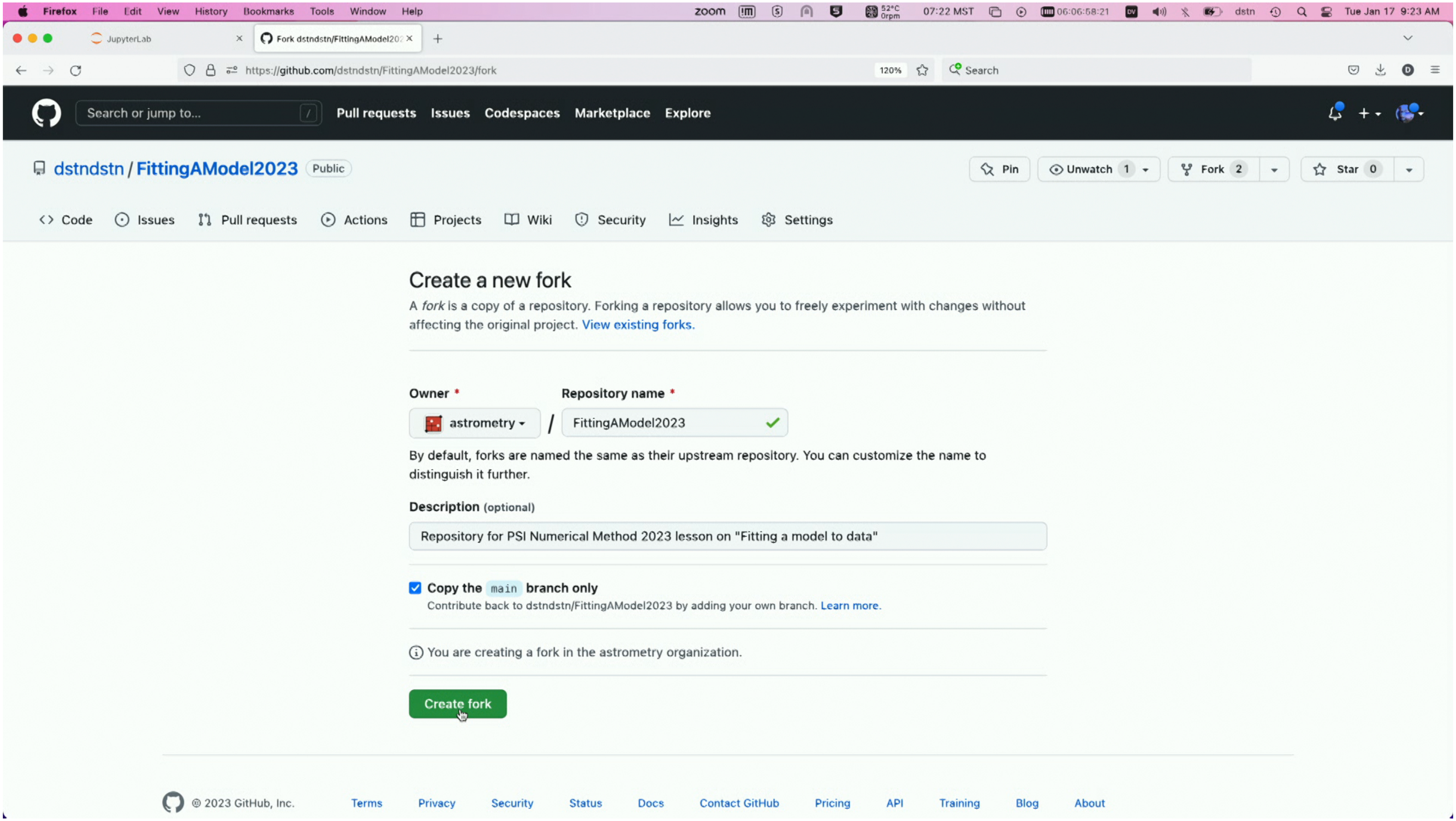
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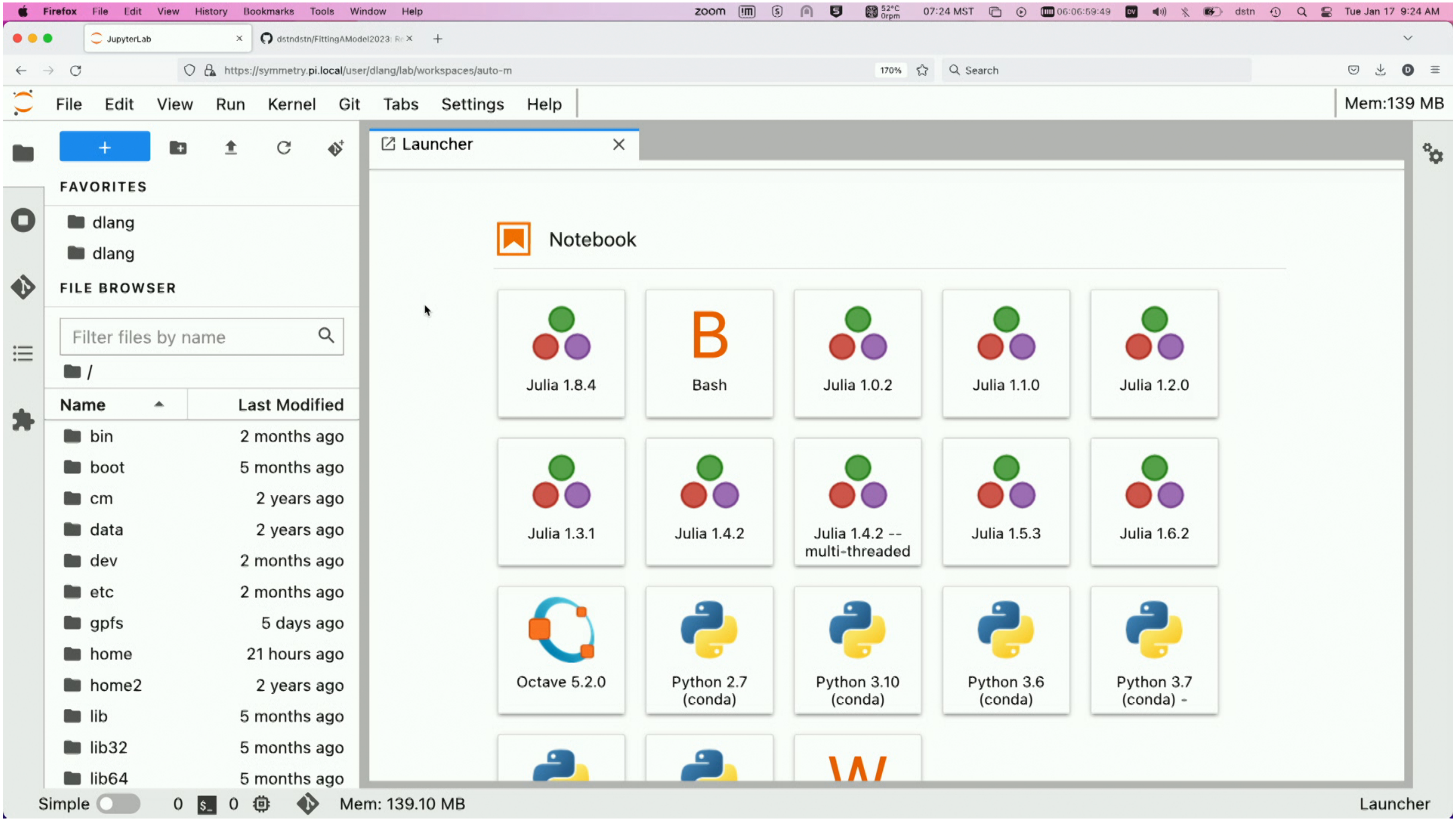

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bin 2 months ago
boot 5 months ago
cm 2 years ago
data 2 years ago
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gpfs 5 days ago
home 21 hours ago
home2 2 years ago
lib 5 months ago
lib32 5 months ago
lib64 5 months ago
Notebook
Julia 1.8.4
Bash
Julia 1.0.2
Julia 1.1.0
Julia 1.2.0
Julia 1.3.1
Julia 1.4.2
Julia 1.4.2 -- multi-threaded
Julia 1.5.3
Julia 1.6.2
Octave 5.2.0
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Python 3.10 (conda)
Python 3.6 (conda)
Python 3.7 (conda) -
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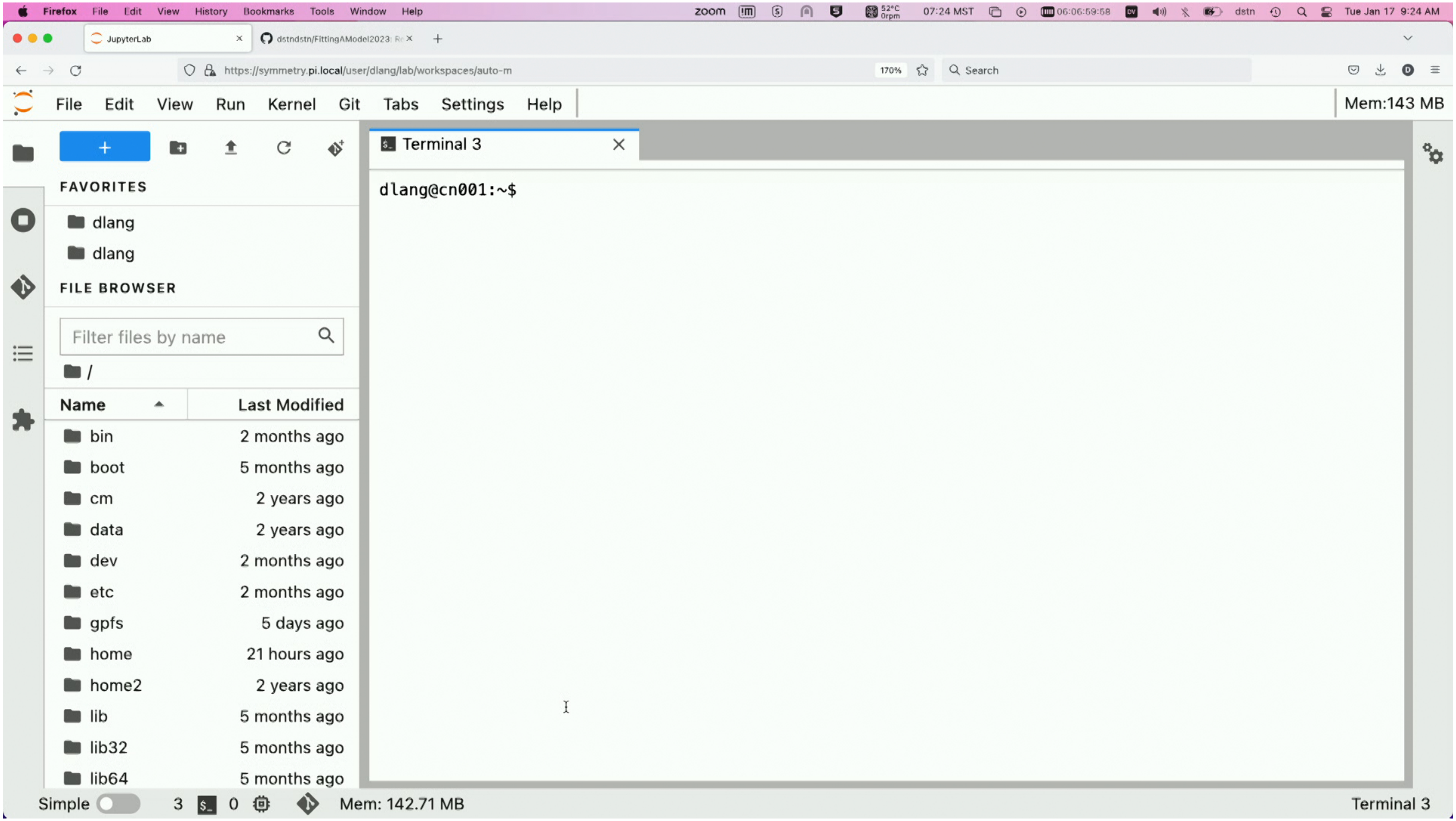
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Mem:143 MB
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Terminal 3
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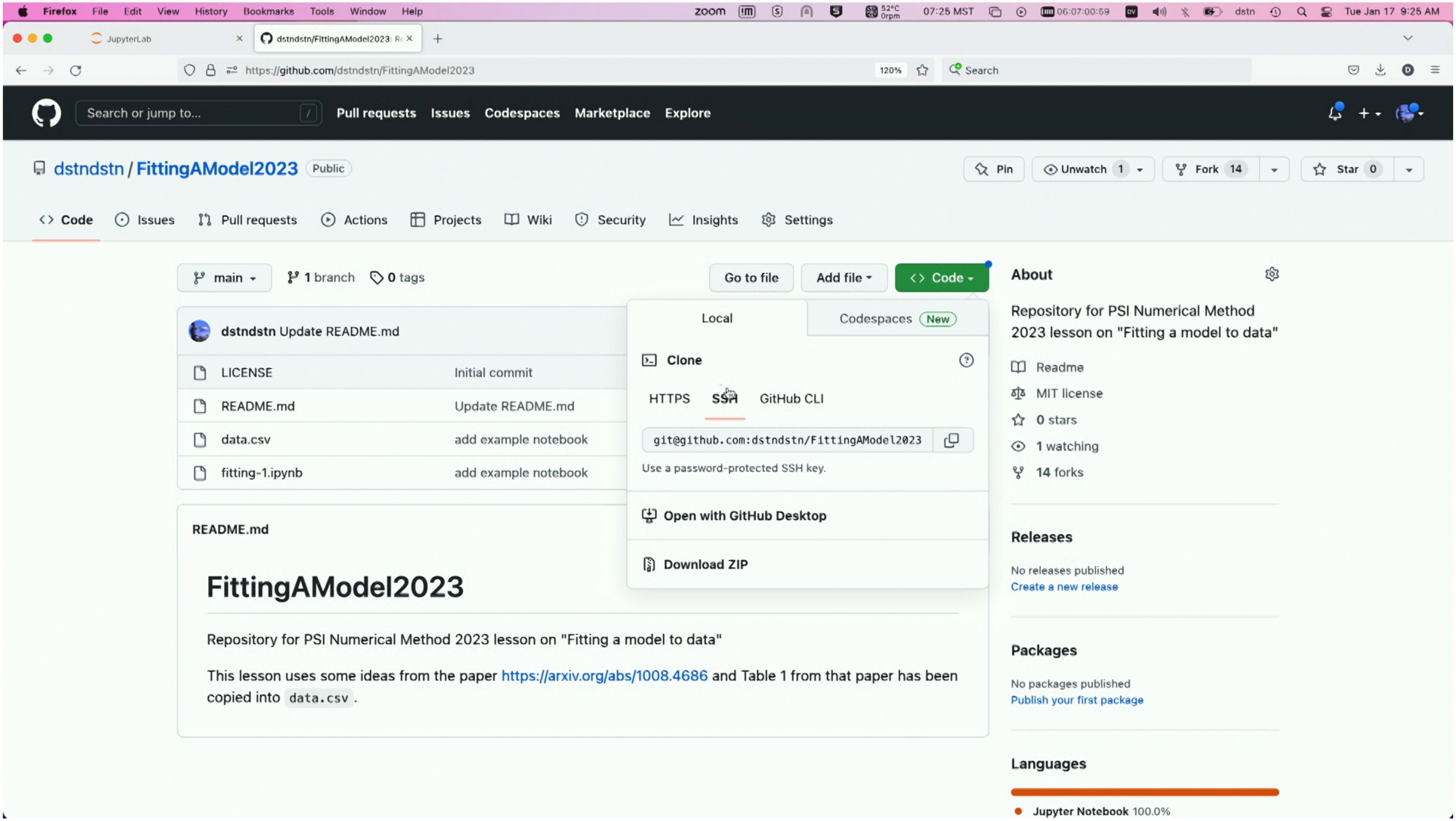
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Go to file Add file Code
dstndstn Update README.md
LICENSE Initial commit
README.md Update README.md
data.csv add example notebook
fitting-1.ipynb add example notebook
Local Codespaces New
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git@github.com:dstndstn/FittingAModel2023
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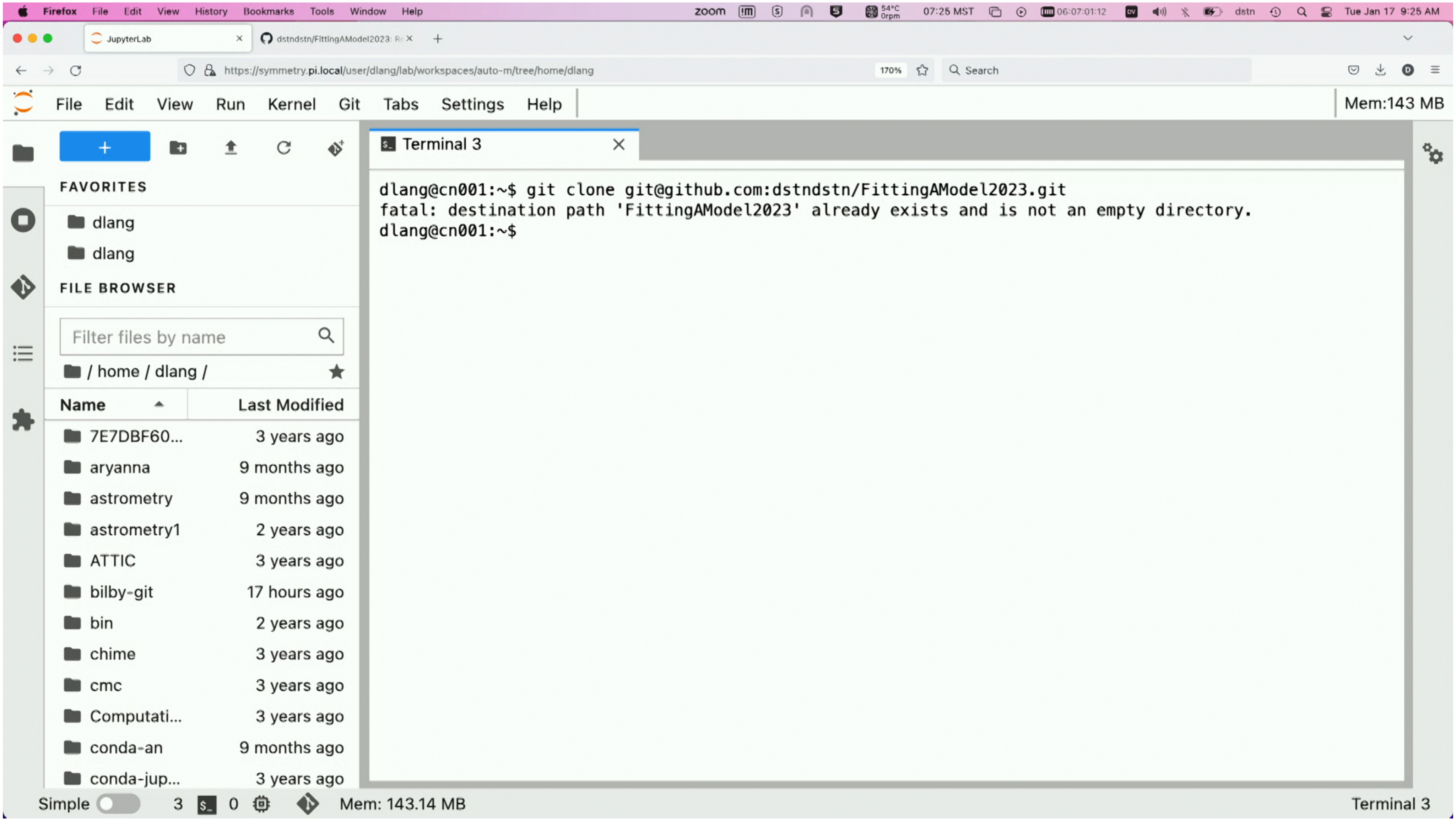
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https://symmetry.pi.local/user/dlang/lab/workspaces/auto-m/tree/home/dlang
File Edit View Run Kernel Git Tabs Settings Help
Mem:143 MB
Terminal 3
dlang@cn001:~$ git clone git@github.com:dstndstn/FittingAModel2023.git
fatal: destination path 'FittingAModel2023' already exists and is not an empty directory.
dlang@cn001:~$
FAVORITES
dlang
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FILE BROWSER
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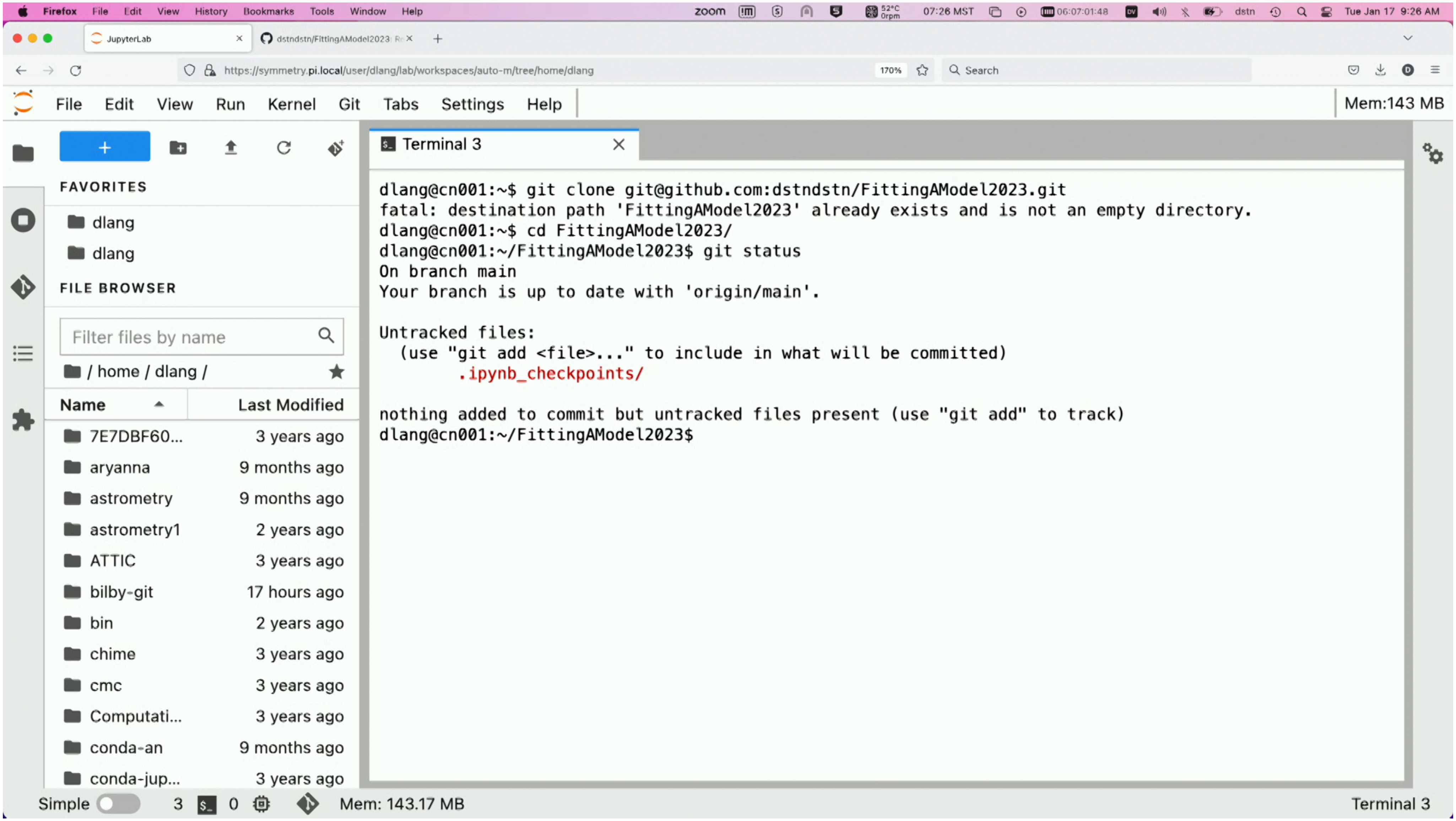
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FAVORITES
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chime 3 years ago
cmc 3 years ago
Computati... 3 years ago
conda-an 9 months ago
conda-jup... 3 years ago
Terminal 3
dlang@cn001:~$ git clone git@github.com:dstndstn/FittingAModel2023.git
fatal: destination path 'FittingAModel2023' already exists and is not an empty directory.
dlang@cn001:~$ cd FittingAModel2023/
dlang@cn001:~/FittingAModel2023$ git status
On branch main
Your branch is up to date with 'origin/main'.
Untracked files:
(use "git add <file>..." to include in what will be committed)
.ipynb_checkpoints/
nothing added to commit but untracked files present (use "git add" to track)
dlang@cn001:~/FittingAModel2023$
Simple
Mem: 143.17 MB
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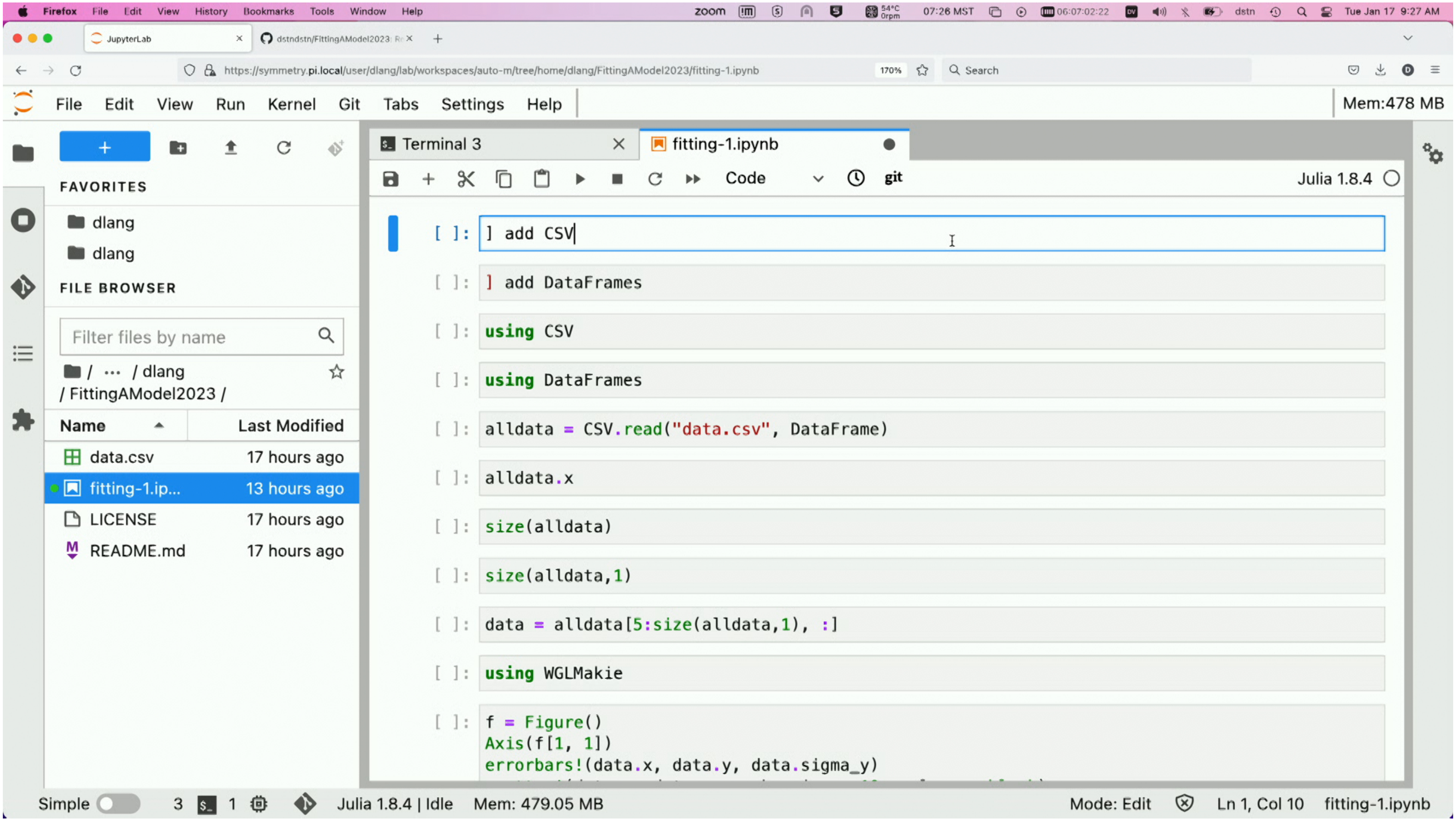
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Name
Last Modified
data.csv 17 hours ago
fitting-1.ip... 13 hours ago
LICENSE 17 hours ago
README.md 17 hours ago
Terminal 3
fitting-1.ipynb
Code
git
Julia 1.8.4
[ ]:] add CSV
[ ]:] add DataFrames
[ ]: using CSV
[ ]: using DataFrames
[ ]: alldata = CSV.read("data.csv", DataFrame)
[ ]: alldata.x
[ ]: size(alldata)
[ ]: size(alldata,1)
[ ]: data = alldata[5:size(alldata,1), :]
[ ]: using WGLMakie
[ ]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
Simple
Julia 1.8.4 | Idle
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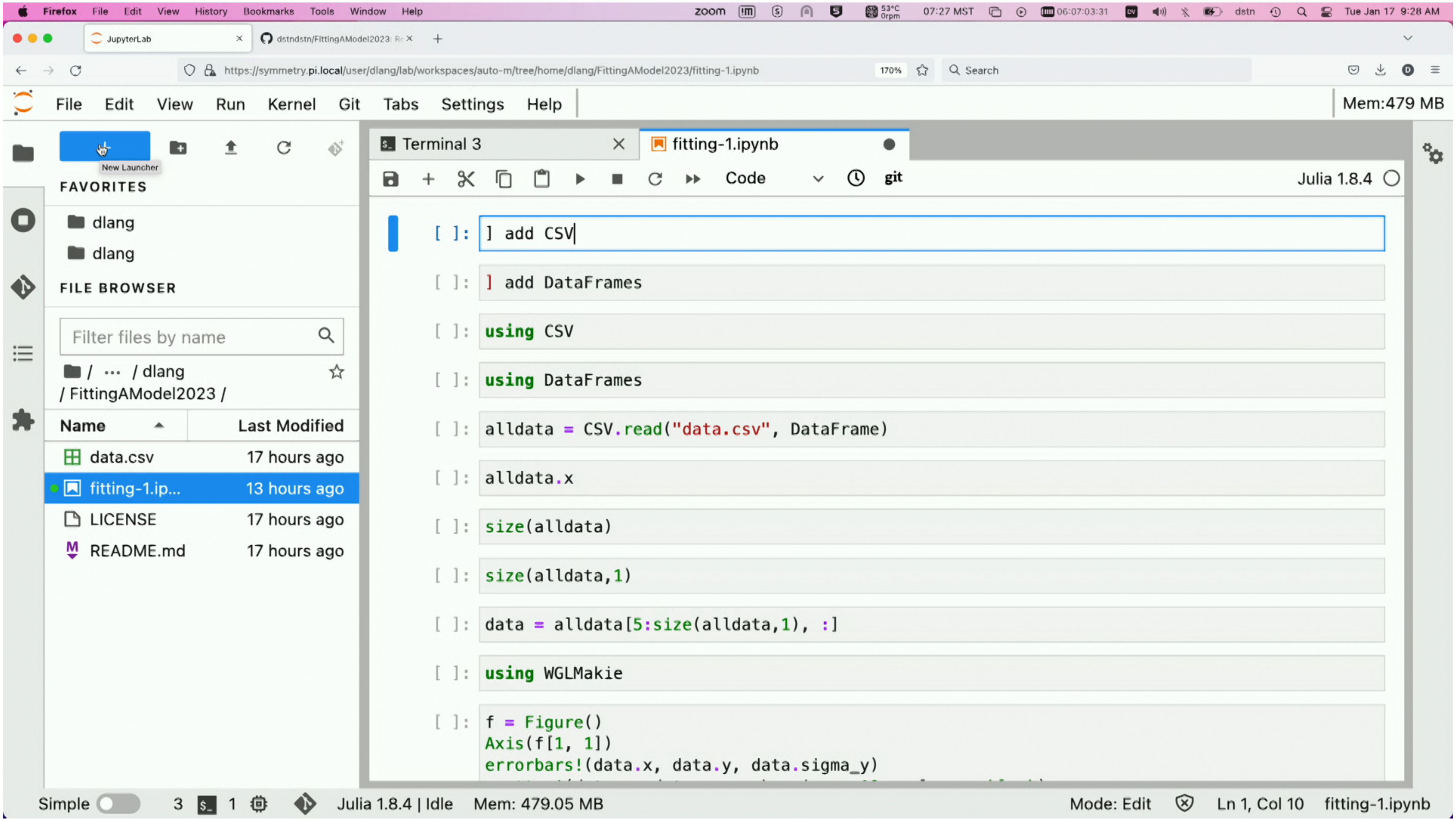
Ln 1, Col 10
fitting-1.ipynb



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data.csv 17 hours ago
fitting-1.ip... 13 hours ago
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README.md 17 hours ago
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fitting-1.ipynb
Code
git
Julia 1.8.4
[ ]:] add CSV
[ ]:] add DataFrames
[ ]: using CSV
[ ]: using DataFrames
[ ]: alldata = CSV.read("data.csv", DataFrame)
[ ]: alldata.x
[ ]: size(alldata)
[ ]: size(alldata,1)
[ ]: data = alldata[5:size(alldata,1), :]
[ ]: using WGLMakie
[ ]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
Simple
Julia 1.8.4 | Idle
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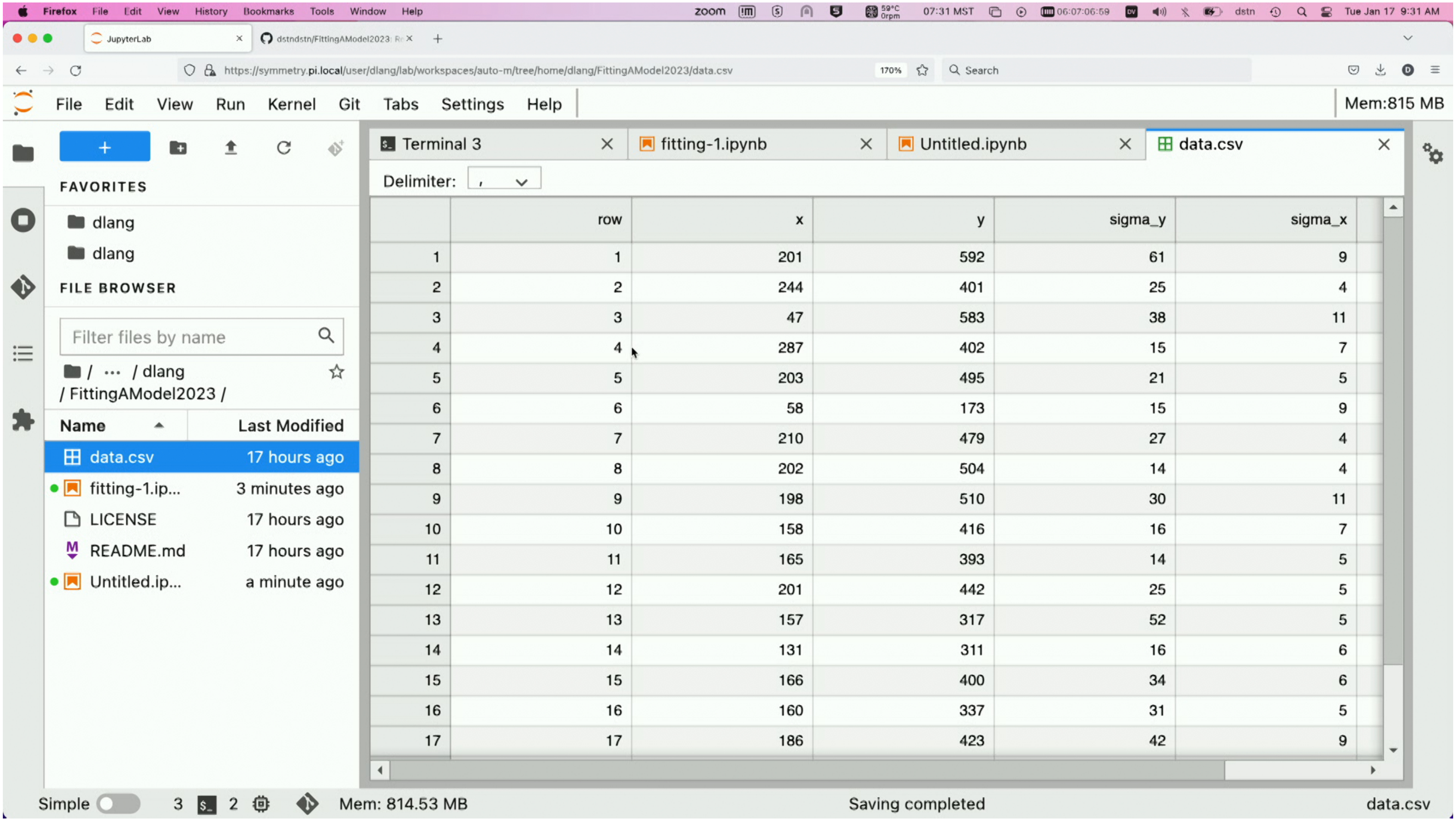
fitting-1.ipynb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7 7 210 479 27 4
8 8 202 504 14 4
9 9 198 510 30 11
10 10 158 416 16 7
11 11 165 393 14 5
12 12 201 442 25 5
13 13 157 317 52 5
14 14 131 311 16 6
15 15 166 400 34 6
16 16 160 337 31 5
17 17 186 423 42 9
Simple 3 2 Mem: 814.53 MB
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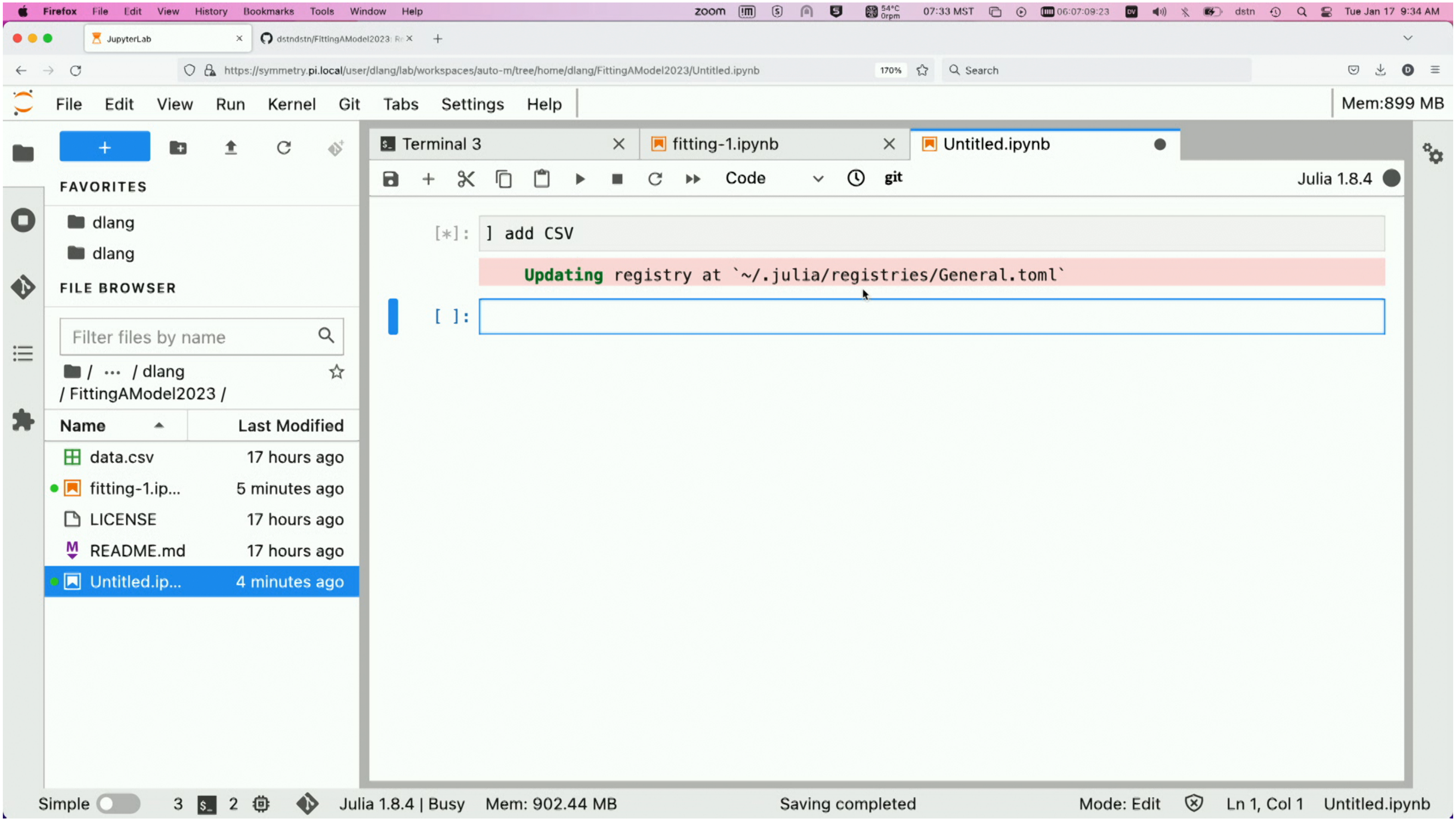
data.csv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Untitled.ip... 4 minutes ago
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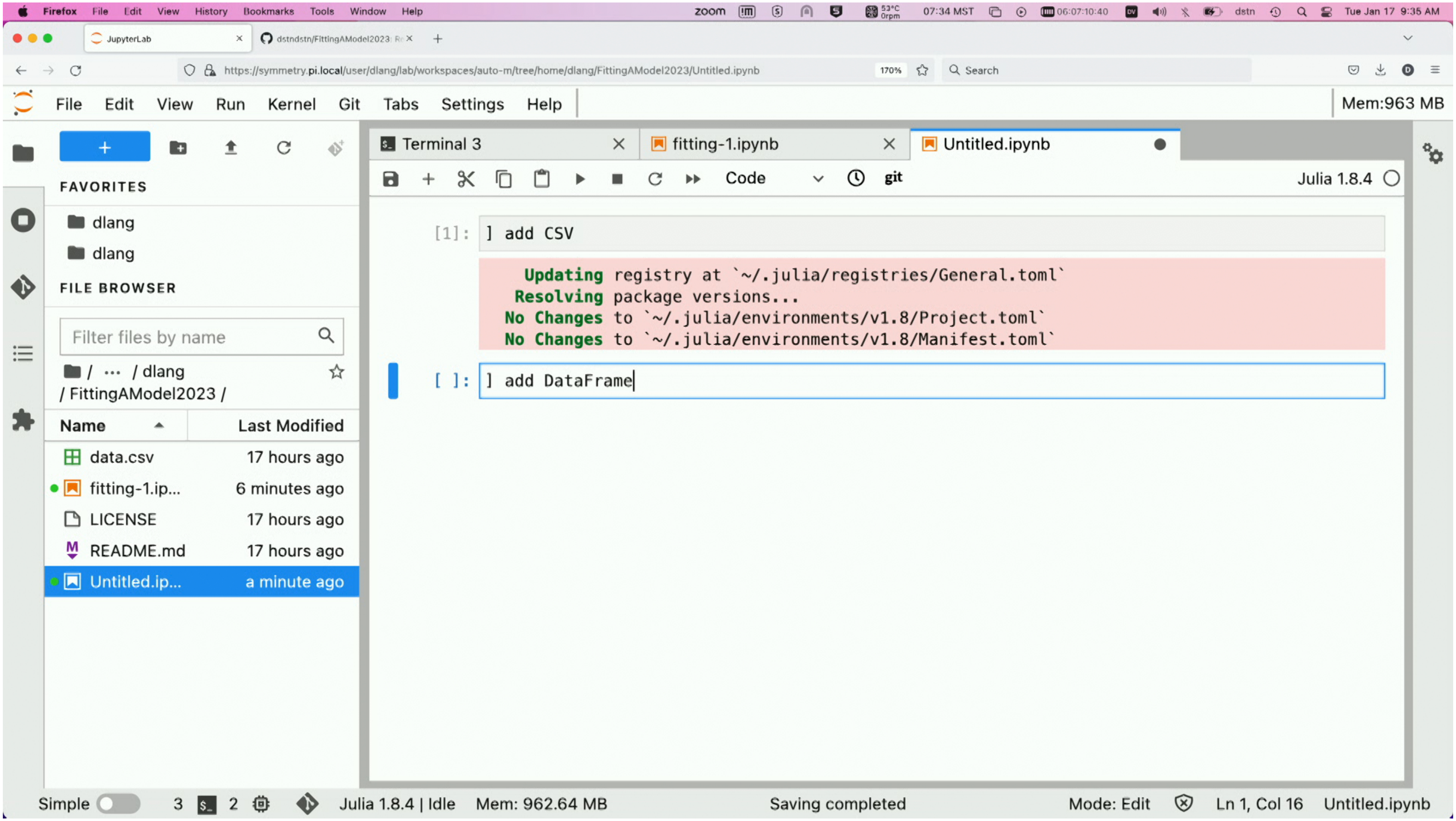
fitting-1.ipynb
Untitled.ipynb
Code
git
Julia 1.8.4
[*]:] add CSV
Updating registry at `~/.julia/registries/General.toml`
[ ]:
Simple 3 2 Julia 1.8.4 | Busy Mem: 902.44 MB Saving completed Mode: Edit Ln 1, Col 1 Untitled.ipynb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fitting-1.ipynb
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Last Modified
data.csv 17 hours ago
fitting-1.ip... 6 minutes ago
LICENSE 17 hours ago
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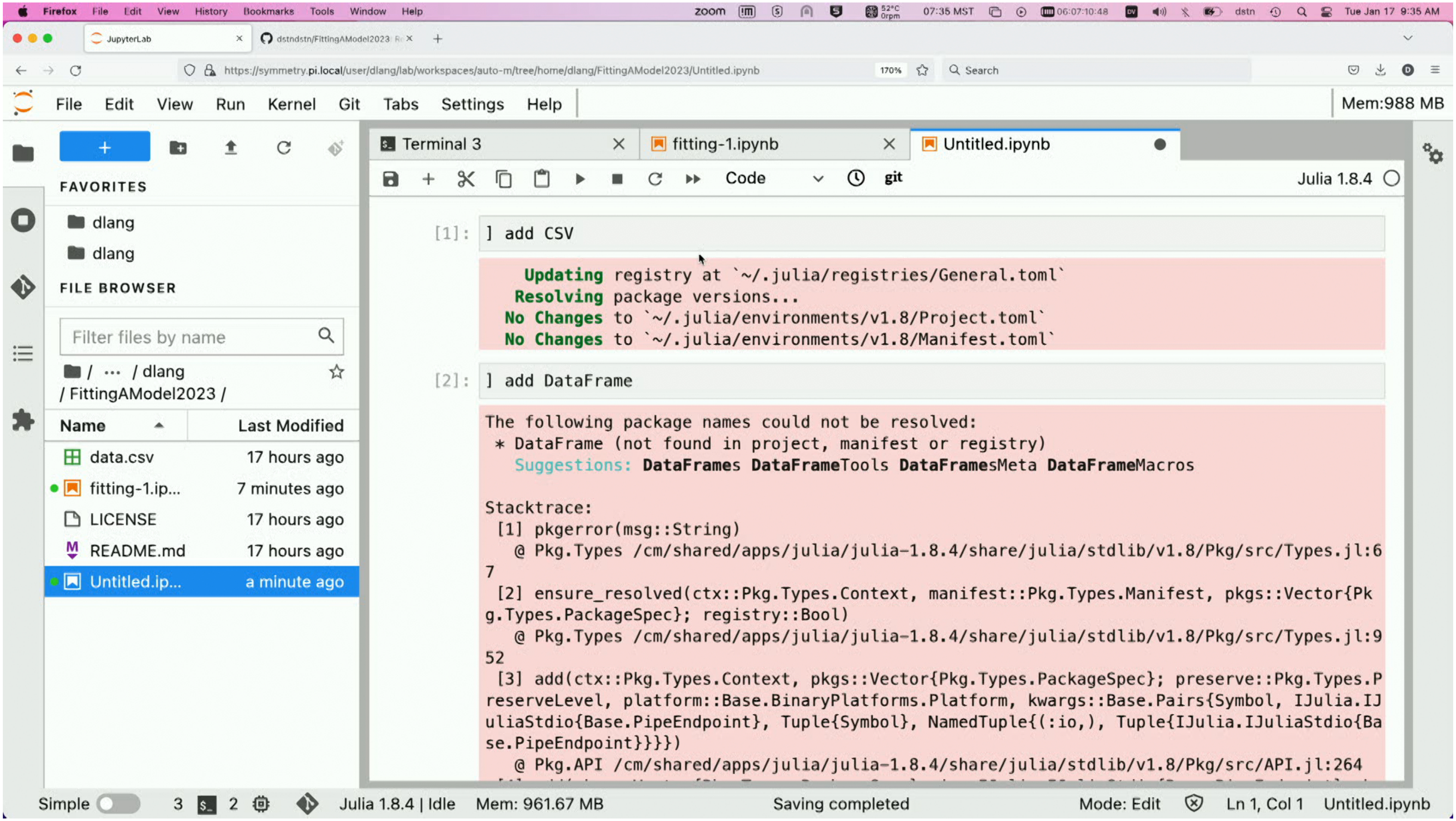
[1]:] add CSV
Updating registry at `~/.julia/registries/General.toml`
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[ ]:] add DataFrame
Simple 3 2 Julia 1.8.4 | Idle Mem: 962.64 MB Saving completed Mode: Edit Ln 1, Col 16 Untitled.ipynb



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LICENSE 17 hours ago
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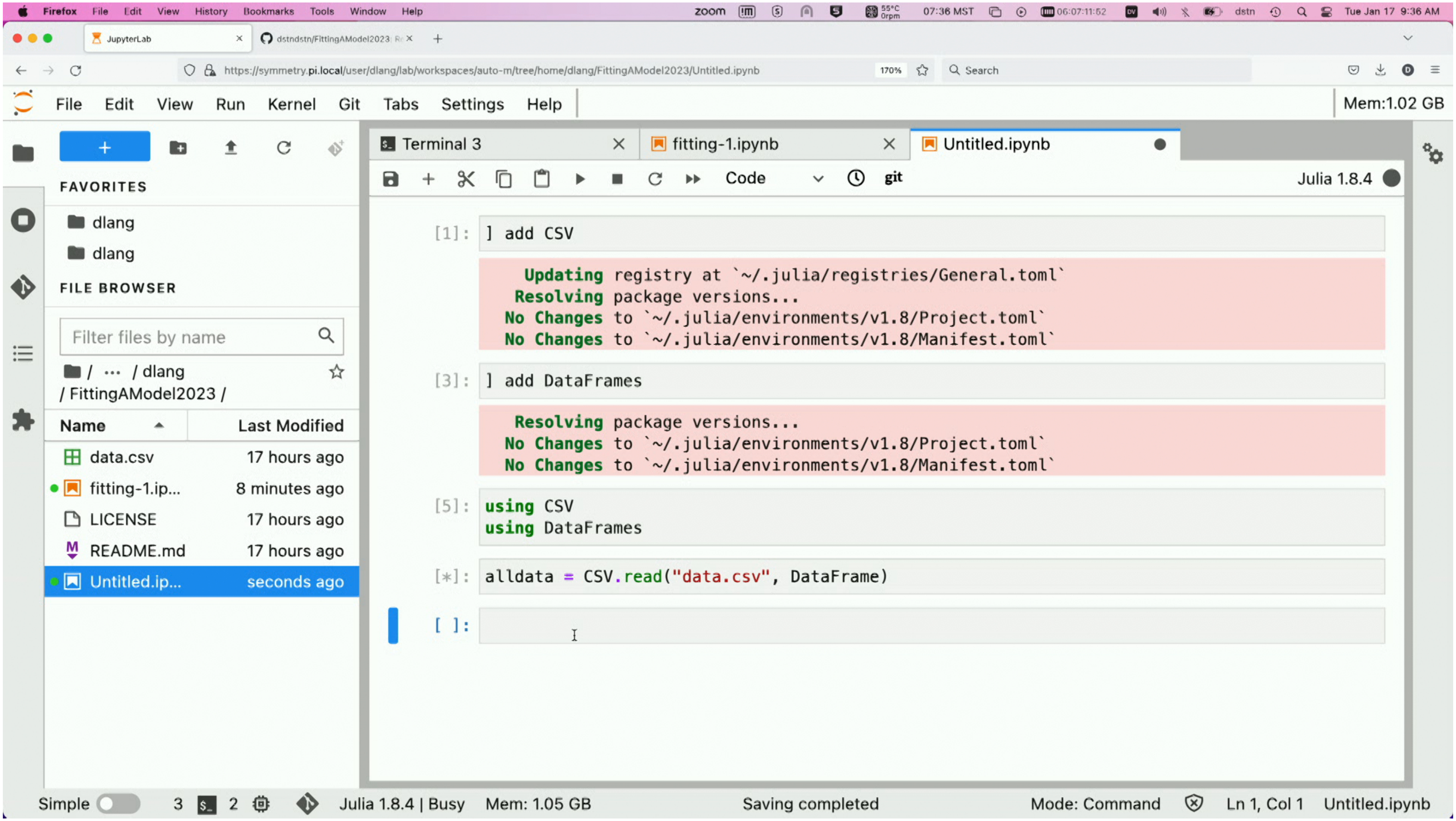
Untitled.ip... a minute ago
Terminal 3
fitting-1.ipynb
Untitled.ipynb
Code
git
Julia 1.8.4
[1]:] add CSV
Updating registry at `~/.julia/registries/General.toml`
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[2]:] add DataFrame
The following package names could not be resolved:
* DataFrame (not found in project, manifest or registry)
Suggestions: DataFrames DataFrameTools DataFramesMeta DataFrameMacros
Stacktrace:
[1] pkgerror(msg::String)
@ Pkg.Types /cm/shared/apps/julia/julia-1.8.4/share/julia/stdlib/v1.8/Pkg/src/Types.jl:67
[2] ensure_resolved(ctx::Pkg.Types.Context, manifest::Pkg.Types.Manifest, pkgs::Vector{Pkg.Types.PackageSpec}; registry::Bool)
@ Pkg.Types /cm/shared/apps/julia/julia-1.8.4/share/julia/stdlib/v1.8/Pkg/src/Types.jl:952
[3] add(ctx::Pkg.Types.Context, pkgs::Vector{Pkg.Types.PackageSpec}; preserve::Pkg.Types.PreserveLevel, platform::Base.BinaryPlatforms.Platform, kwargs::Base.Pairs{Symbol, IJulia.IJuliaStdio{Base.PipeEndpoint}, Tuple{Symbol}, NamedTuple{(:io,), Tuple{IJulia.IJuliaStdio{Base.PipeEndpoint}}}})
@ Pkg.API /cm/shared/apps/julia/julia-1.8.4/share/julia/stdlib/v1.8/Pkg/src/API.jl:264
Simple 3 2 Julia 1.8.4 | Idle Mem: 961.67 MB Saving completed Mode: Edit Ln 1, Col 1 Untitled.ipynb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Terminal 3
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[1]:] add CSV
Updating registry at `~/.julia/registries/General.toml`
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[3]:] add DataFrames
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[5]: using CSV
using DataFrames
[*]: alldata = CSV.read("data.csv", DataFrame)
[ ]:
Simple
Julia 1.8.4 | Busy
Mem: 1.05 GB
Saving completed
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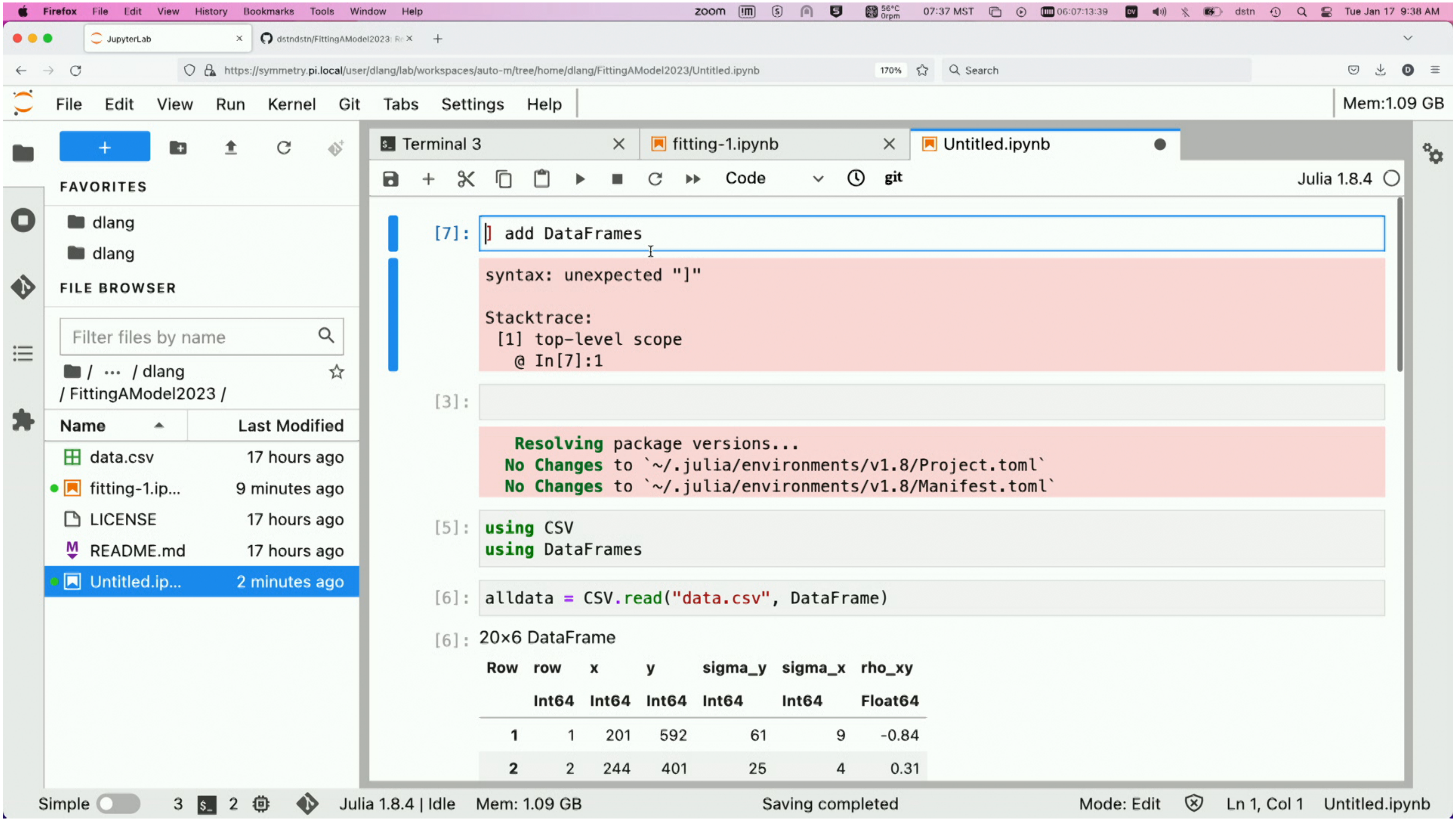
Untitled.ipynb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Name
Last Modified
data.csv 17 hours ago
fitting-1.ip... 9 minutes ago
LICENSE 17 hours ago
README.md 17 hours ago
Untitled.ip... 2 minutes ago
[7]:] add DataFrames
syntax: unexpected "]"
Stacktrace:
[1] top-level scope
@ In[7]:1
[3]:
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
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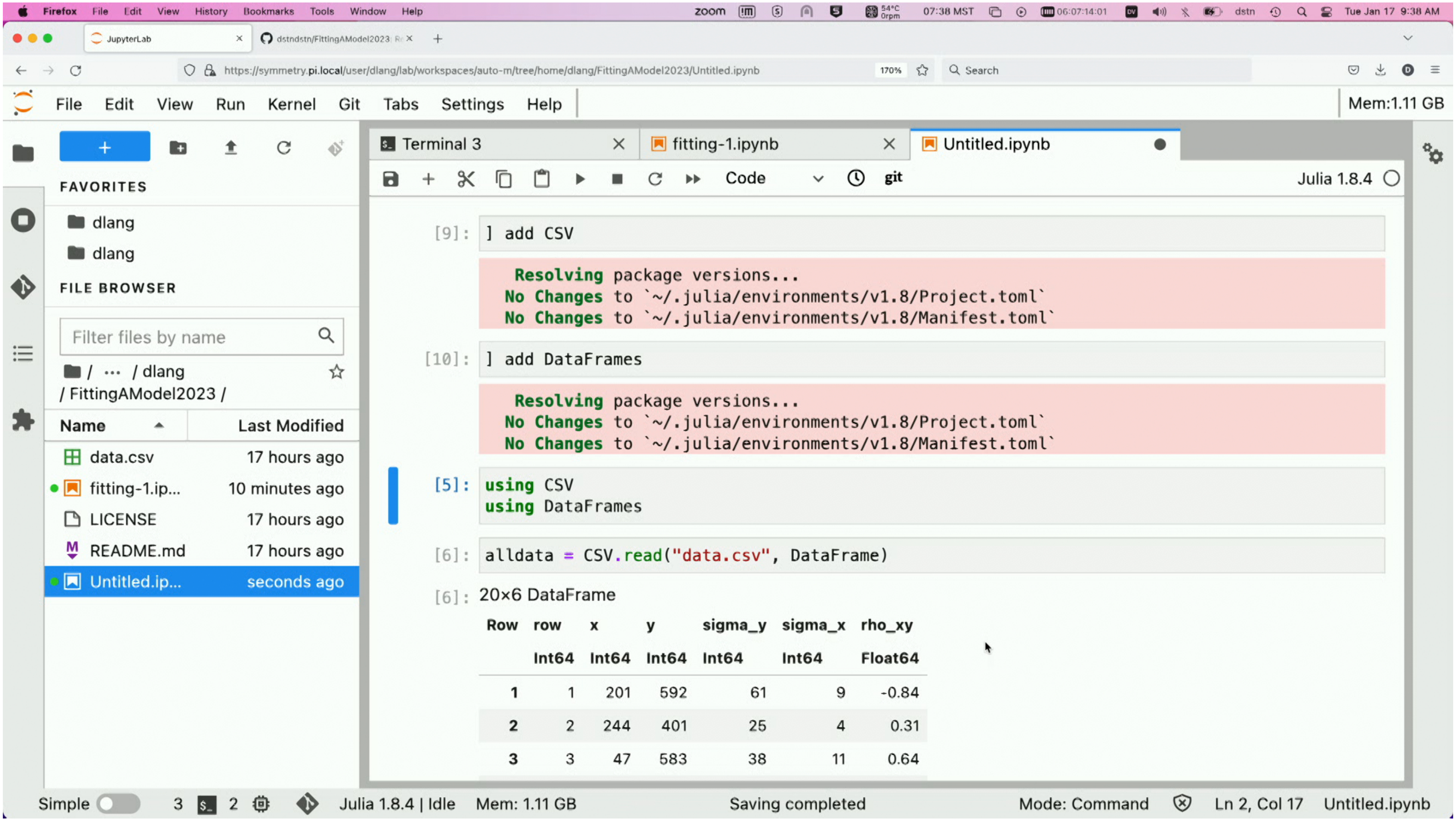
[5]: using CSV
using DataFrames
[6]: alldata = CSV.read("data.csv", DataFrame)
[6]: 20×6 DataFrame
Row row x y sigma_y sigma_x rho_xy
Int64 Int64 Int64 Int64 Int64 Float64
1 1 201 592 61 9 -0.84
2 2 244 401 25 4 0.31
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.09 GB Saving completed Mode: Edit Ln 1, Col 1 Untitled.ipynb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README.md 17 hours ago
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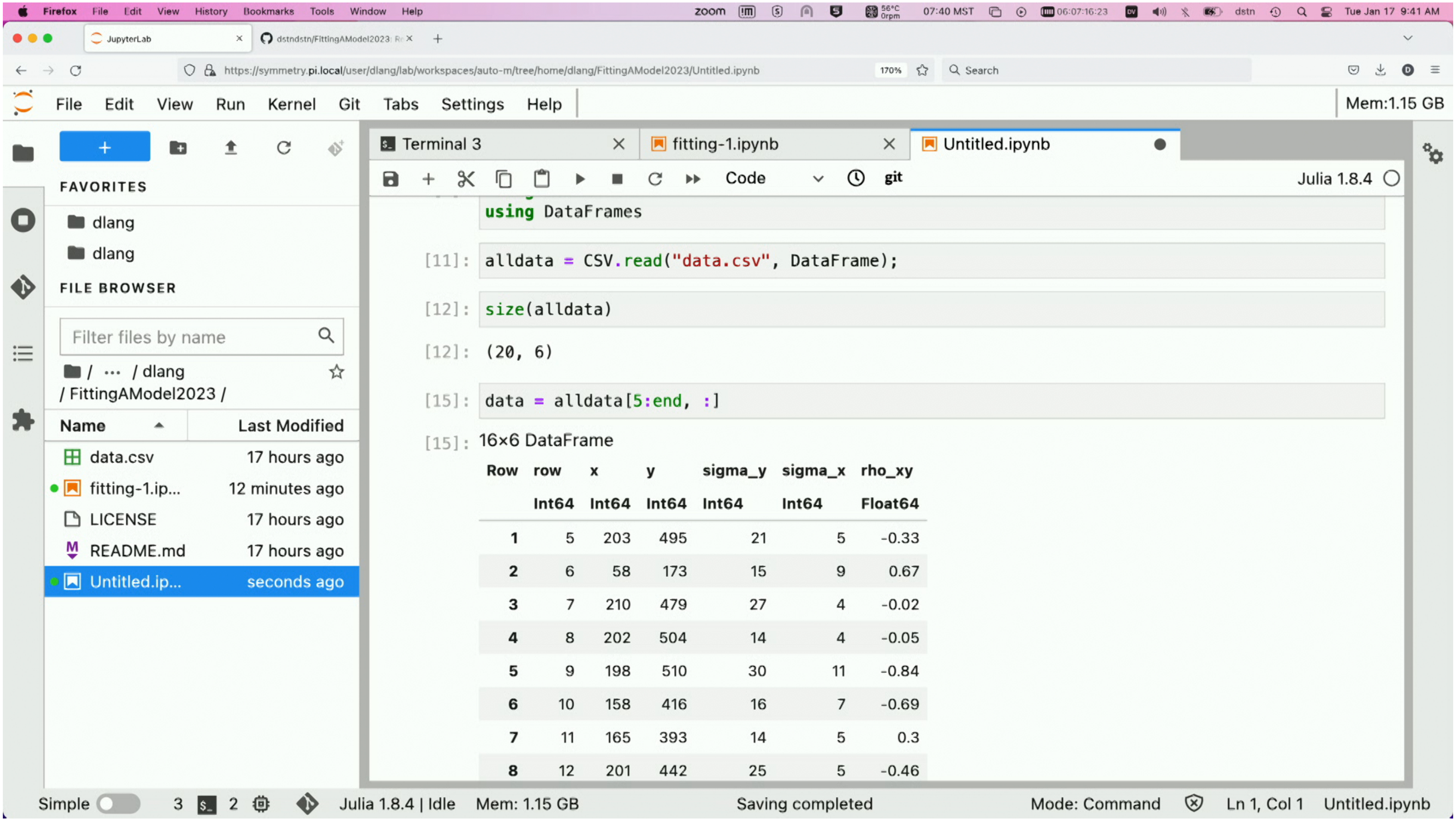
[9]:] add CSV
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[10]:] add DataFrames
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[5]: using CSV
using DataFrames
[6]: alldata = CSV.read("data.csv", DataFrame)
[6]: 20×6 DataFrame
Row row x y sigma_y sigma_x rho_xy
Int64 Int64 Int64 Int64 Int64 Float64
1 1 201 592 61 9 -0.84
2 2 244 401 25 4 0.31
3 3 47 583 38 11 0.64
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.11 GB Saving completed Mode: Command Ln 2, Col 17 Untitled.ipynb

[6]: 20×6 DataFrame

Row	row	x	y	sigma_y	sigma_x	rho_xy
	Int64	Int64	Int64	Int64	Int64	Float64
1	1	201	592	61	9	-0.84
2	2	244	401	25	4	0.31
3	3	47	583	38	11	0.64
4	4	287	402	15	7	-0.27
5	5	203	495	21	5	-0.33
6	6	58	173	15	9	0.67
7	7	210	479	27	4	-0.02
8	8	202	504	14	4	-0.05
9	9	198	510	30	11	-0.84
10	10	158	416	16	7	-0.69
11	11	165	393	14	5	0.3
12	12	201	442	25	5	-0.46
13	13	157	317	52	5	-0.03
14	14	131	311	16	6	0.5
15	15	166	400	34	6	0.73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data.csv 17 hours ago
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using DataFrames
[11]: alldata = CSV.read("data.csv", DataFrame);
[12]: size(alldata)
[12]: (20, 6)
[15]: data = alldata[5:end, :]
[15]: 16×6 DataFrame
Row row x y sigma_y sigma_x rho_xy
Int64 Int64 Int64 Int64 Int64 Float64
1 5 203 495 21 5 -0.33
2 6 58 173 15 9 0.67
3 7 210 479 27 4 -0.02
4 8 202 504 14 4 -0.05
5 9 198 510 30 11 -0.84
6 10 158 416 16 7 -0.69
7 11 165 393 14 5 0.3
8 12 201 442 25 5 -0.46
Simple
Julia 1.8.4 | Idle
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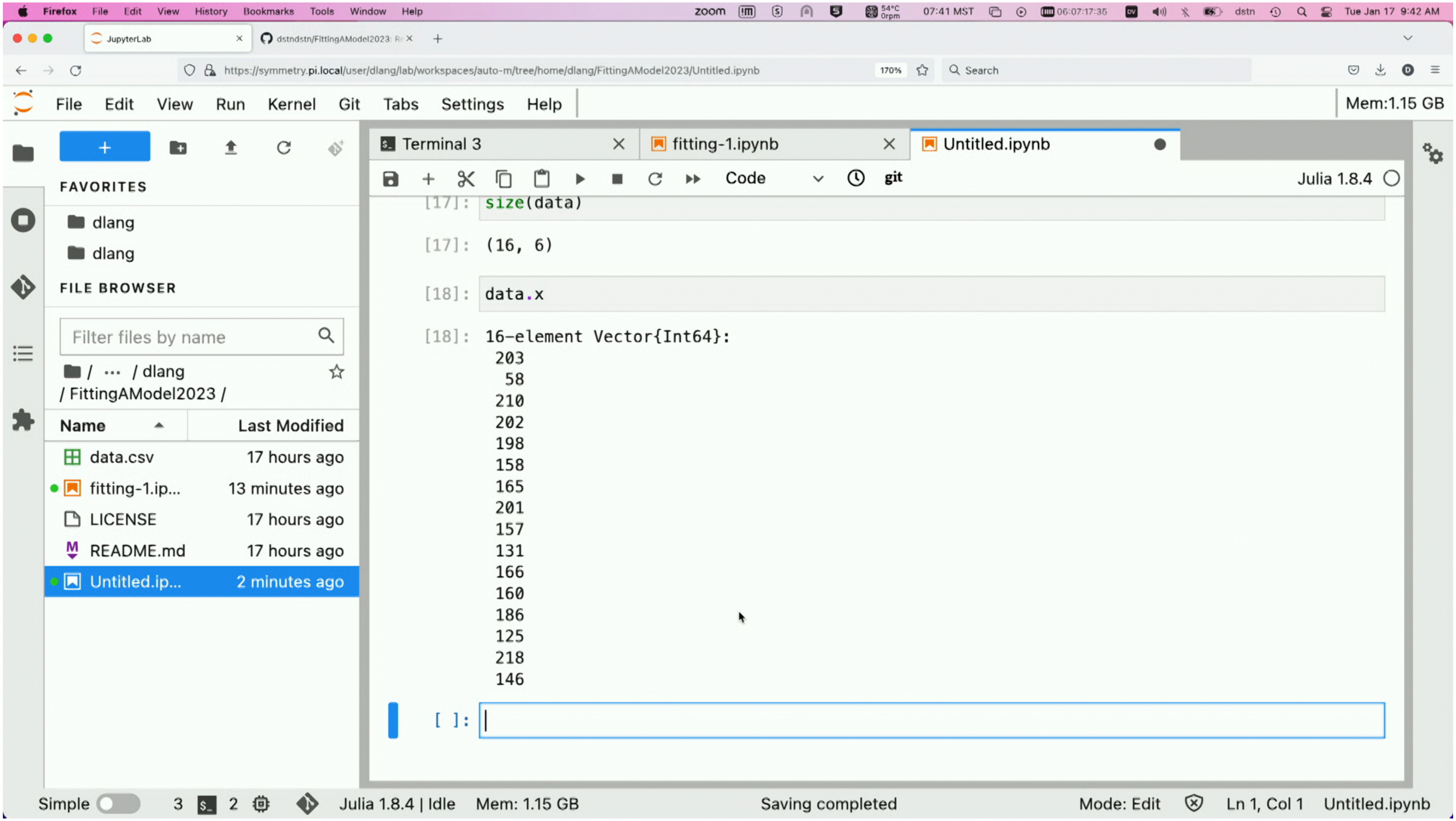
Firefox File Edit View History Bookmarks Tools Window Help
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data.csv 17 hours ago
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[17]: size(data)
[17]: (16, 6)
[18]: data.x
[18]: 16-element Vector{Int64}:
203
58
210
202
198
158
165
201
157
131
166
160
186
125
218
146
[ ]:
Simple
Julia 1.8.4 | Idle
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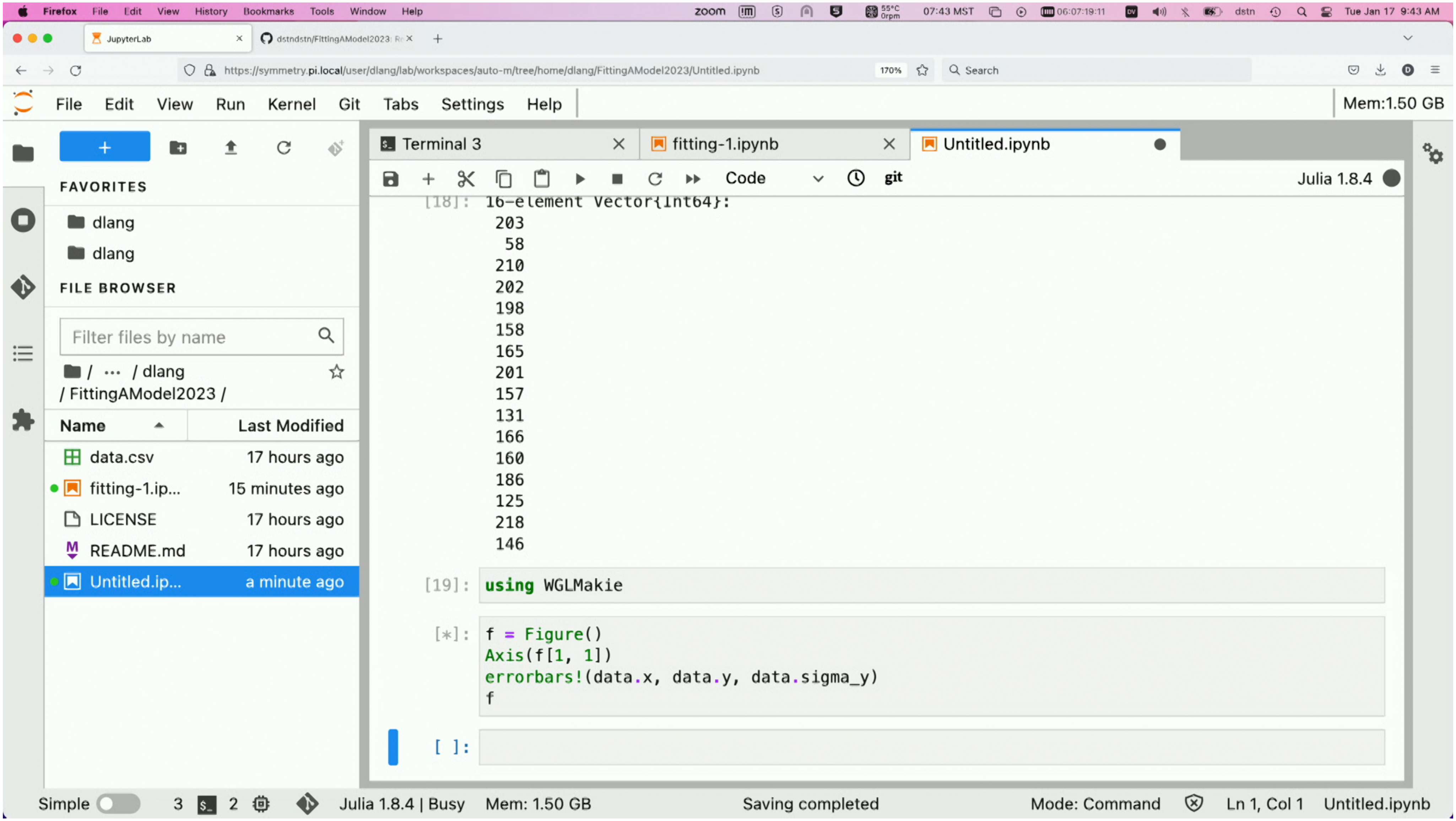
Firefox File Edit View History Bookmarks Tools Window Help
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Code
git
Julia 1.8.4
[18]: 16-element Vector{Int64}:
203
58
210
202
198
158
165
201
157
131
166
160
186
125
218
146
[19]: using WGLMakie
[*]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
f
[ ]:
Simple
Julia 1.8.4 | Busy
Mem: 1.50 GB
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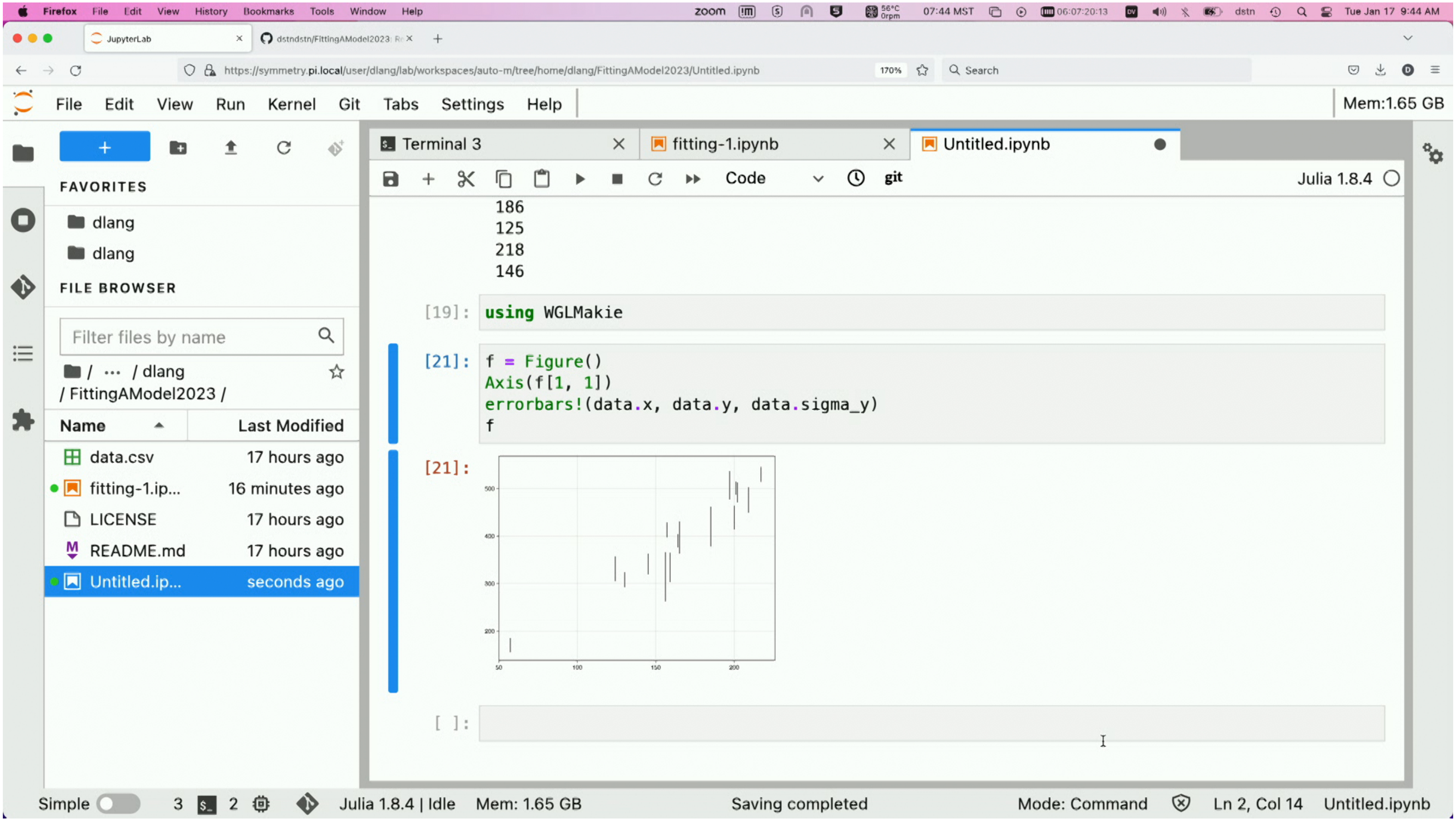
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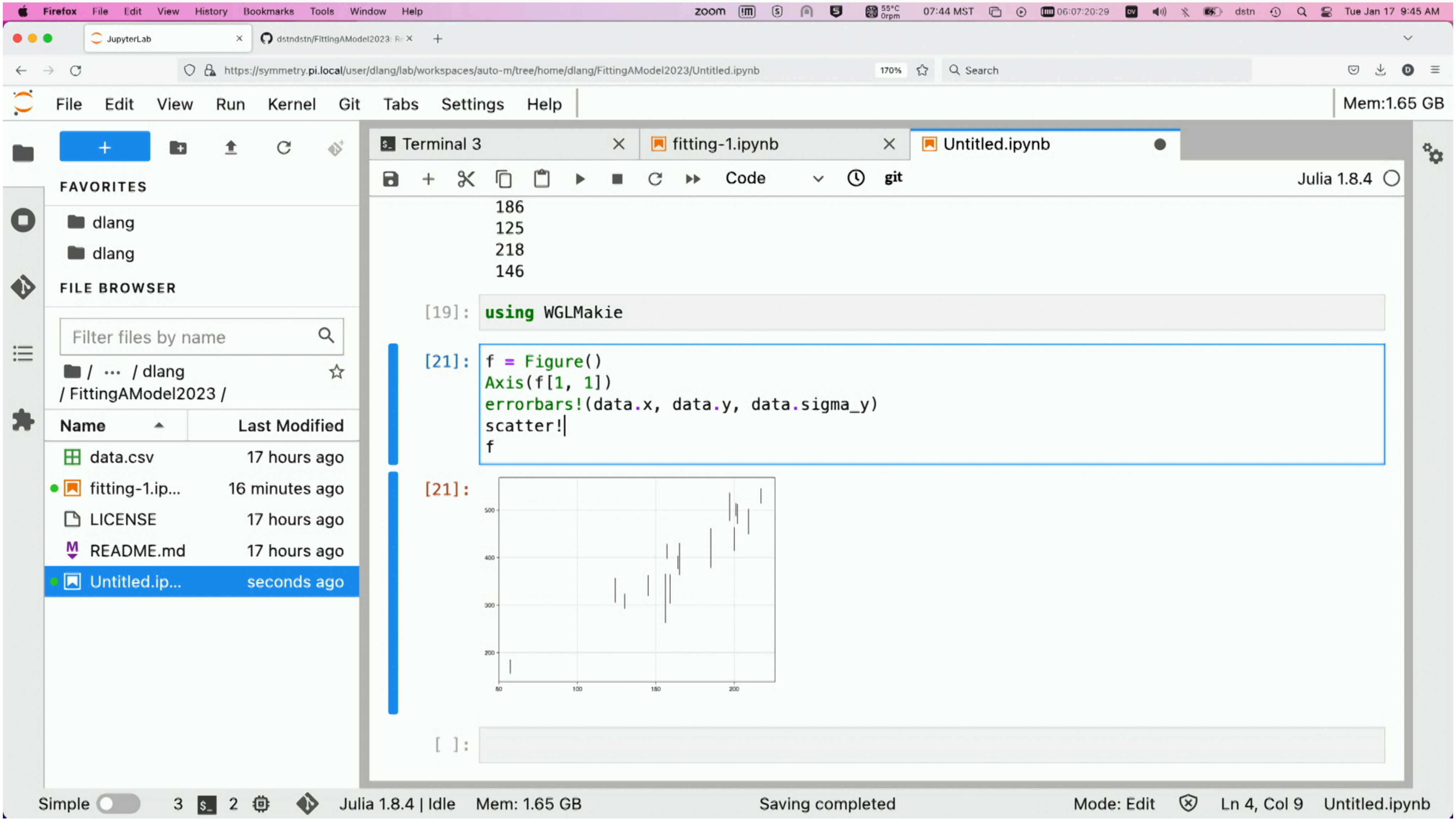
186
125
218
146
[19]: using WGLMakie
[21]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
f
[21]:
[ ]:
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.65 GB Saving completed Mode: Command Ln 2, Col 14 Untitled.ipynb


Firefox File Edit View History Bookmarks Tools Window Help
Tue Jan 17 9:45 AM
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186
125
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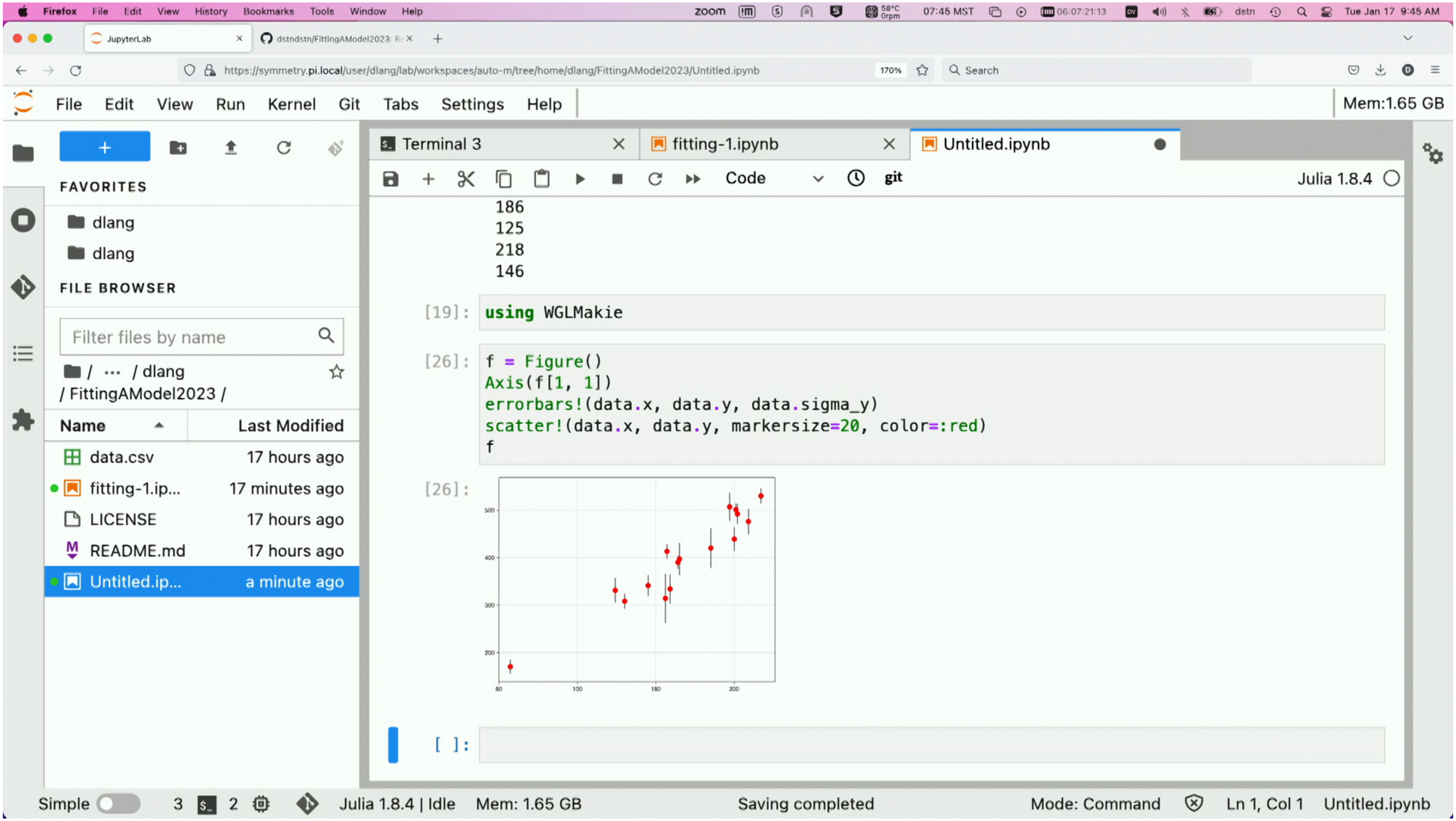
[19]: using WGLMakie
[21]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!
f
[21]:
[ ]:
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.65 GB Saving completed Mode: Edit Ln 4, Col 9 Untitled.ipynb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186
125
218
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[19]: using WGLMakie
[26]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
f
[26]:
[ ]:
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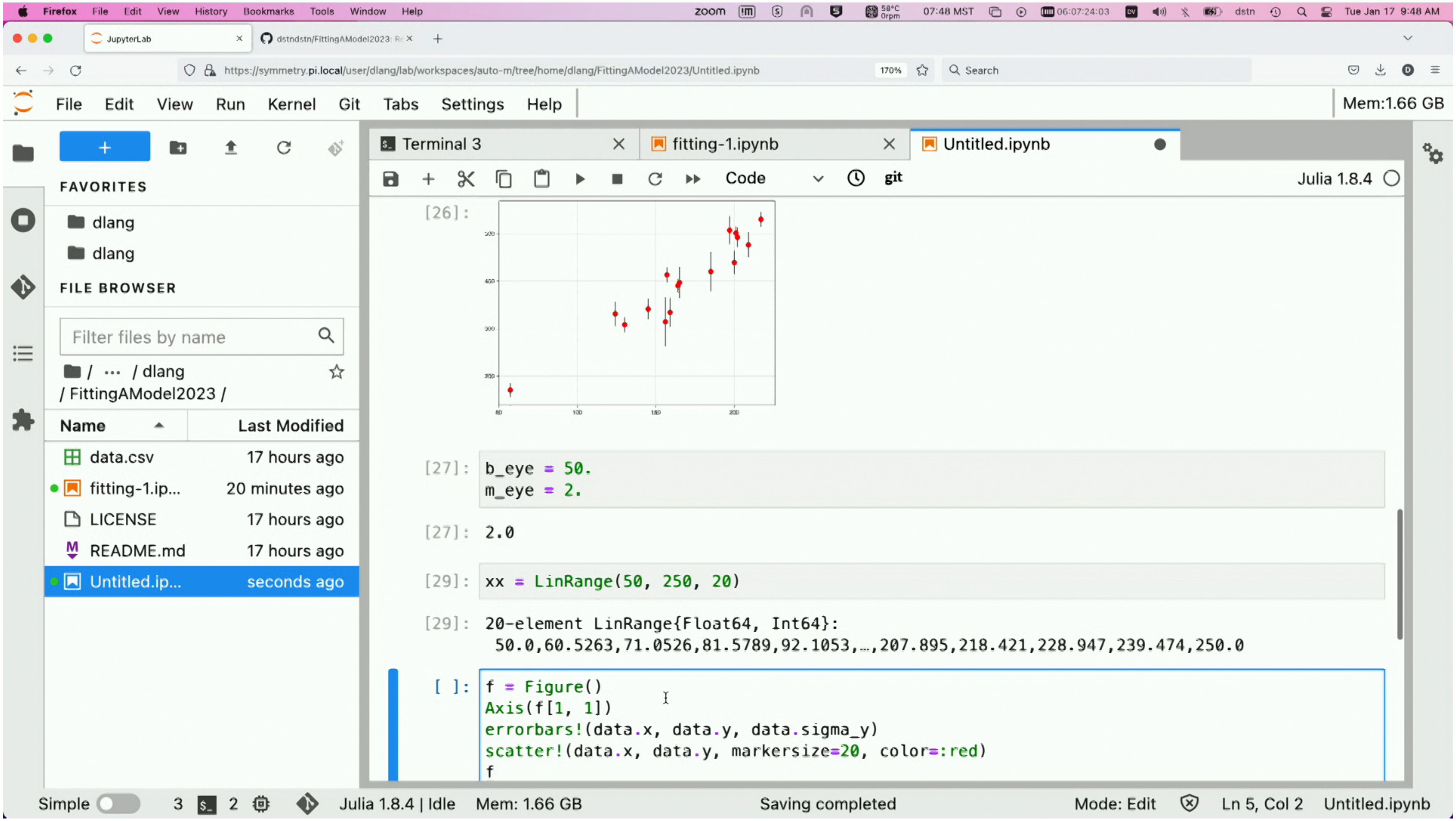

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[27]: b_eye = 50.
m_eye = 2.
[27]: 2.0
[29]: xx = LinRange(50, 250, 20)
[29]: 20-element LinRange{Float64, Int64}:
50.0,60.5263,71.0526,81.5789,92.1053,…,207.895,218.421,228.947,239.474,250.0
[ ]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
f
Julia 1.8.4 | Idle
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Ln 5, Col 2
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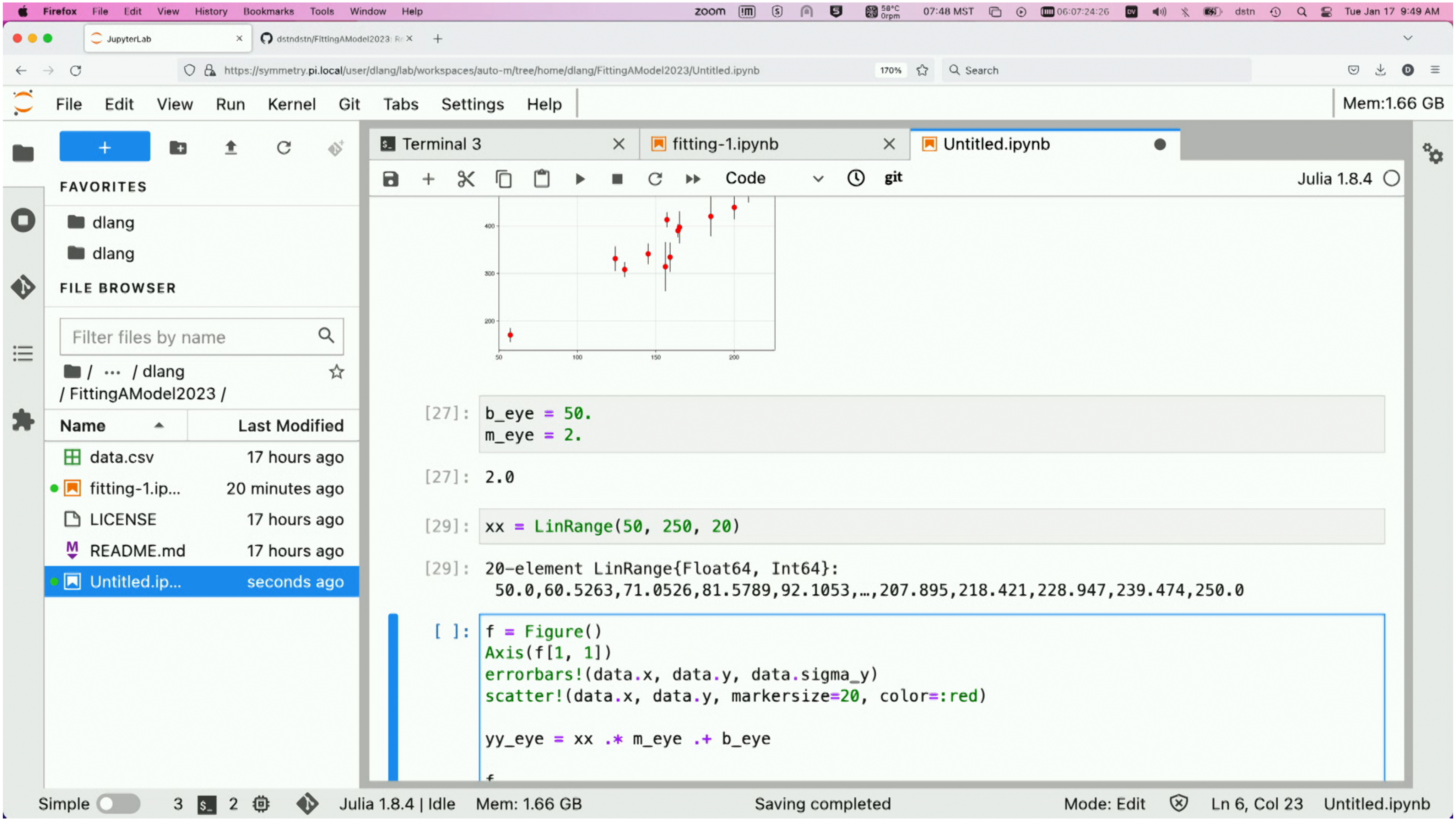
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[27]: b_eye = 50.
m_eye = 2.
[27]: 2.0
[29]: xx = LinRange(50, 250, 20)
[29]: 20-element LinRange{Float64, Int64}:
50.0,60.5263,71.0526,81.5789,92.1053,…,207.895,218.421,228.947,239.474,250.0
[ ]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
yy_eye = xx .* m_eye .+ b_eye
Simple
Julia 1.8.4 | Idle
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Ln 6, Col 23
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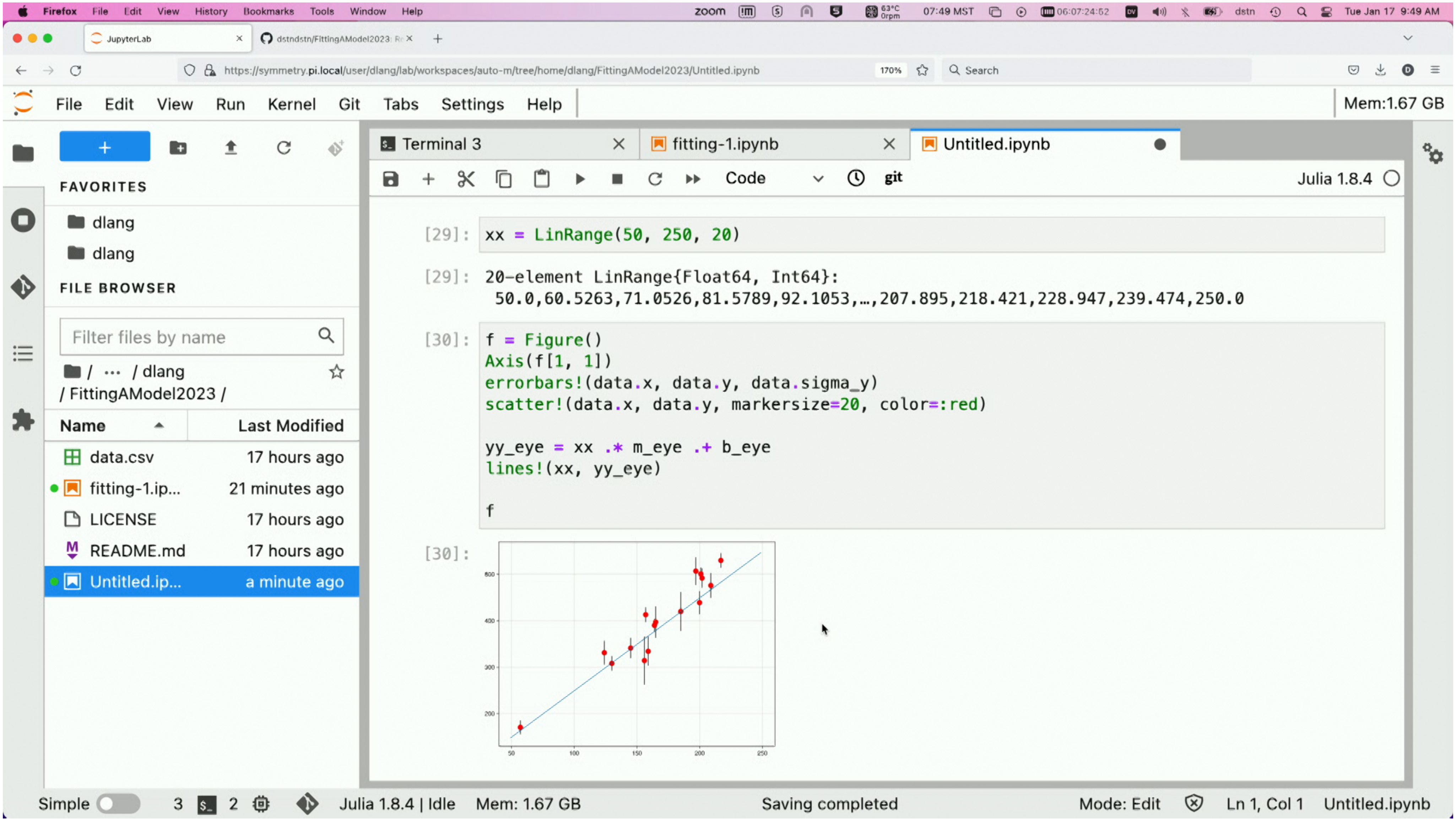
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[29]: xx = LinRange(50, 250, 20)
[29]: 20-element LinRange{Float64, Int64}:
50.0,60.5263,71.0526,81.5789,92.1053,…,207.895,218.421,228.947,239.474,250.0
[30]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye)
f
[30]:
Simple
Julia 1.8.4 | Idle
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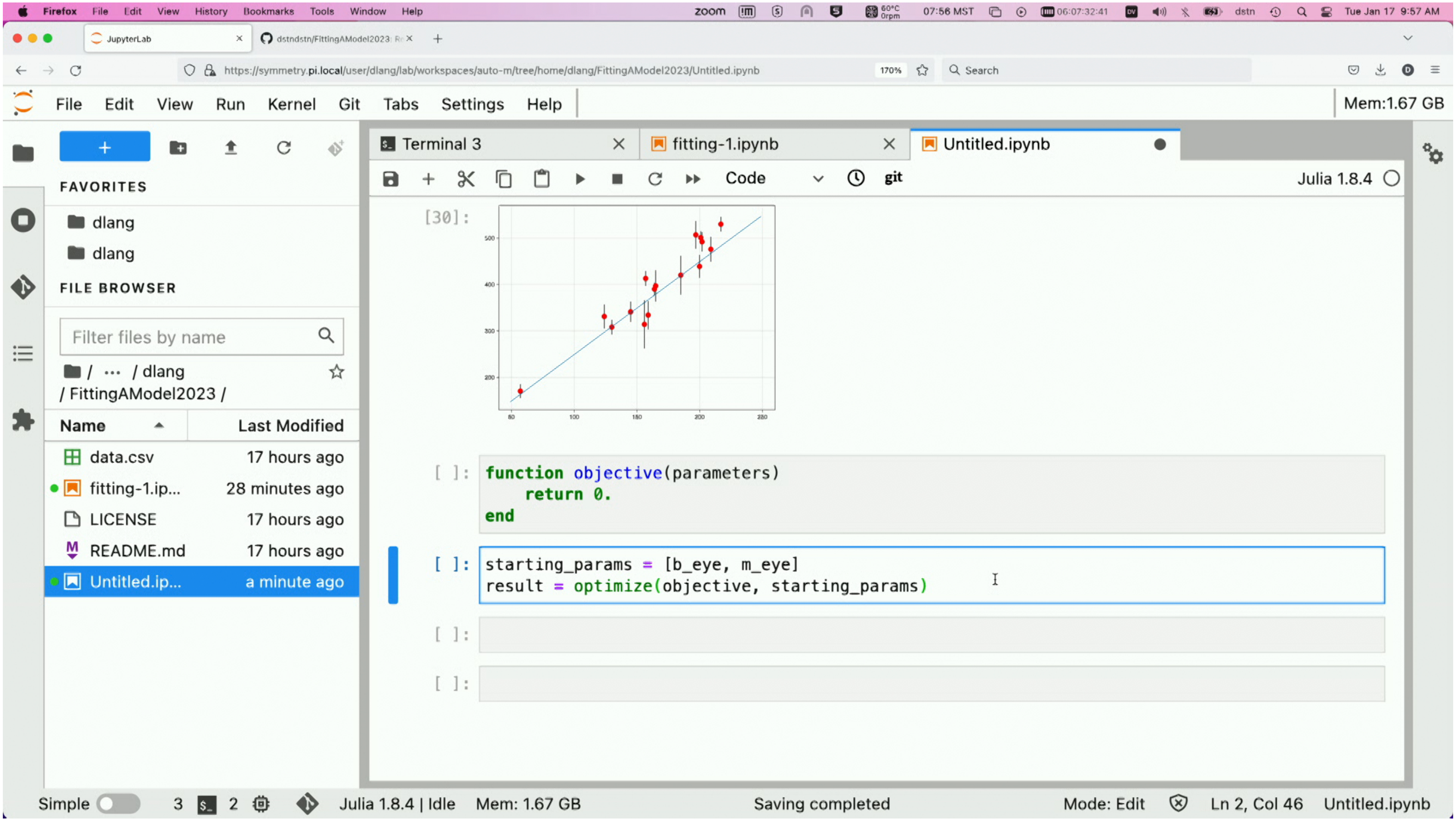
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Code
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Julia 1.8.4
[30]:
[ ]: function objective(parameters)
    return 0.
end
[ ]: starting_params = [b_eye, m_eye]
result = optimize(objective, starting_params)
[ ]:
[ ]:
Simple
Julia 1.8.4 | Idle
Mem: 1.67 GB
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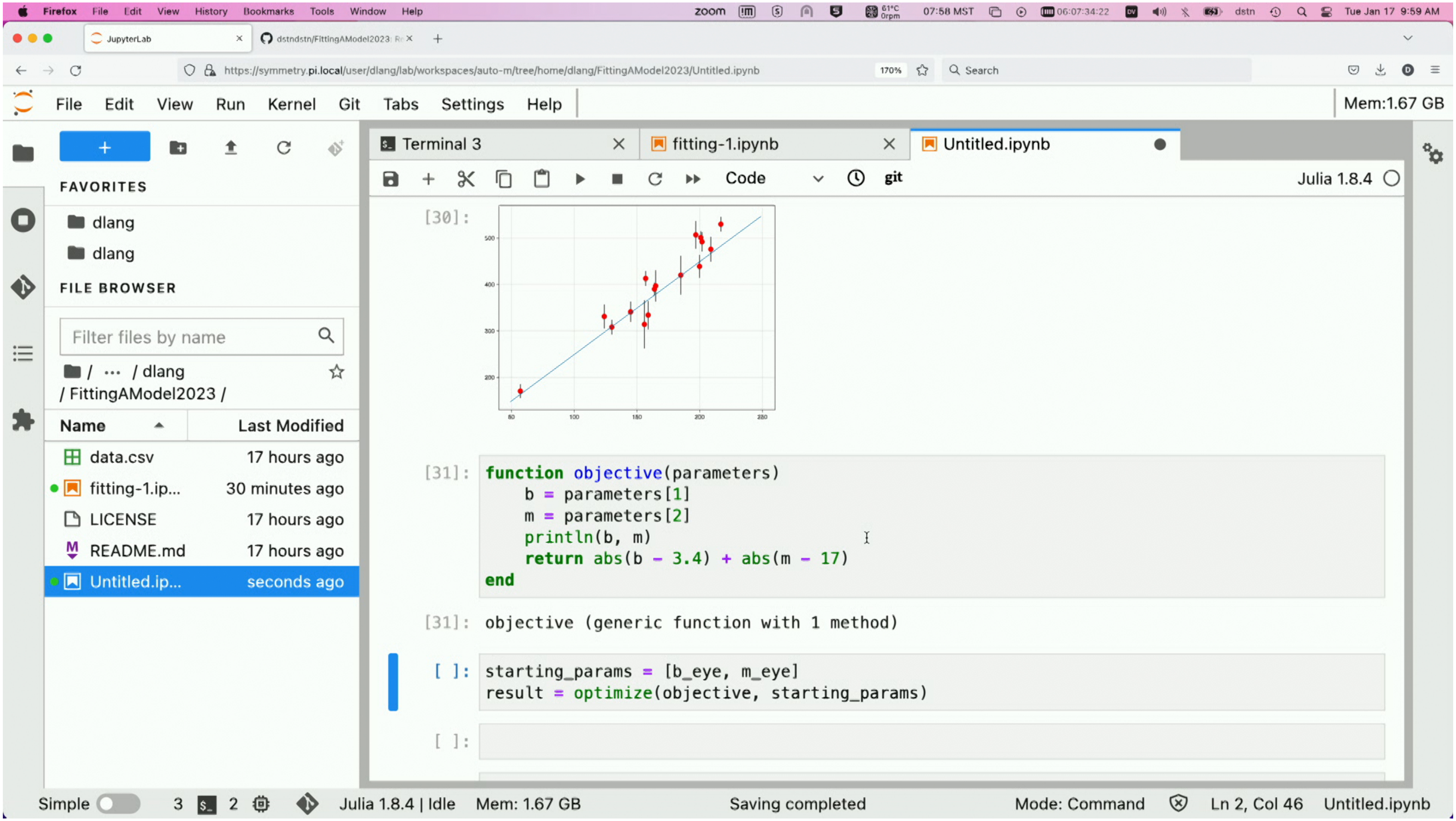
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[30]:
[31]:
function objective(parameters)
    b = parameters[1]
    m = parameters[2]
    println(b, m)
    return abs(b - 3.4) + abs(m - 17)
end
[31]: objective (generic function with 1 method)
[ ]:
starting_params = [b_eye, m_eye]
result = optimize(objective, starting_params)
[ ]:
Simple
Julia 1.8.4 | Idle
Mem: 1.67 GB
Saving completed
Mode: Command
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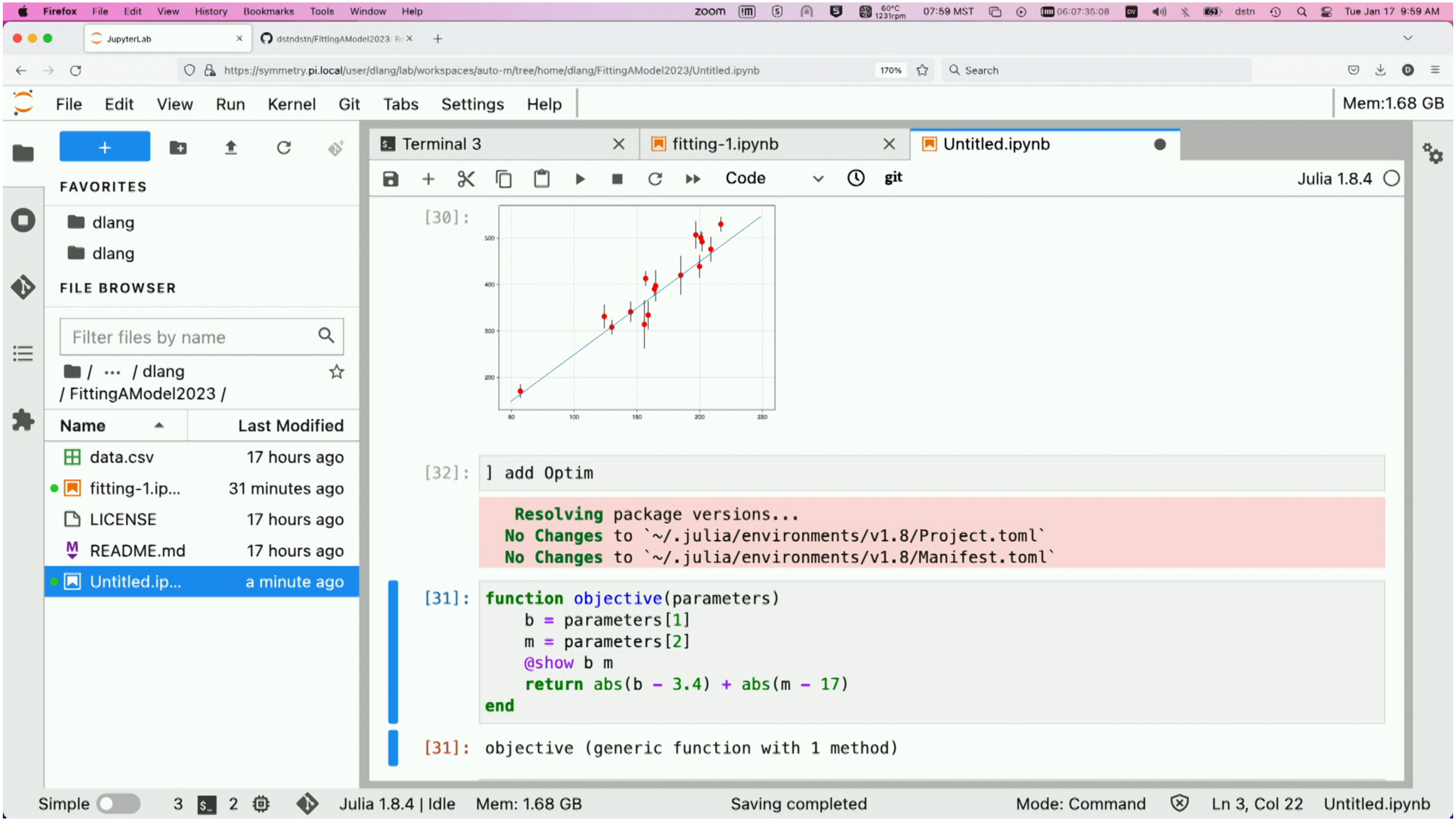
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https://symmetry.pi.local/user/dlang/lab/workspaces/auto-m/tree/home/dlang/FittingAModel2023/Untitled.ipynb
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Terminal 3
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Code
git
Julia 1.8.4
[30]:
[32]:] add Optim
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[31]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b m
return abs(b - 3.4) + abs(m - 17)
end
[31]: objective (generic function with 1 method)
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.68 GB Saving completed Mode: Command Ln 3, Col 22 Untitled.ipynb

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JupyterLab | dstndstn/FittingAModel2023 | Minimizing a function - Optim.jl

https://julianlsolvers.github.io/Optim.jl/stable/#user/minimization/

Optim.jl

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Unconstrained Optimization

To show how the Optim package can be used, we minimize the Rosenbrock function, a classical test problem for numerical optimization. We'll assume that you've already installed the Optim package using Julia's package manager. First, we load Optim and define the Rosenbrock function:

```
using Optim
f(x) = (1.0 - x[1])^2 + 100.0 * (x[2] - x[1]^2)^2
```

Once we've defined this function, we can find the minimizer (the input that minimizes the objective) and the minimum (the value of the objective at the minimizer) using any of our favorite optimization algorithms. With a function defined, we just specify an initial point `x` and call `optimize` with a starting point `x0`:

```
x0 = [0.0, 0.0]
optimize(f, x0)
```

Note: it is important to pass `initial_x` as an array. If your problem is one-dimensional, you have to wrap it in an array. An easy way to do so is to write `optimize(x->f(first(x)), [initial_x])` which make sure the input is an array, but the anonymous function automatically passes the first (and only) element onto your given `f`.

Optim will default to using the Nelder-Mead method in the multivariate case, as we did not provide a gradient. This can also be explicitly specified using:

```
optimize(f, x0, NelderMead())
```

Other solvers are available. Below, we use L-BFGS, a quasi-Newton method that requires a gradient. If we pass `f` alone, Optim will construct an approximate gradient for us using central finite differencing:

```
optimize(f, x0, LBFGS())
```

For better performance and greater precision, you can pass your own gradient function. If your objective is written in all Julia code with no special calls to external (that is non-Julia) libraries, you can also use automatic differentiation, by using the `autodiff` keyword and setting it to `:forward`:

```
optimize(f, x0, LBFGS(); autodiff = :forward)
```

For the Rosenbrock example, the analytical gradient can be shown to be:

```
function g!(G, x)
G[1] = -2.0 * (1.0 - x[1]) - 400.0 * (x[2] - x[1]^2) * x[1]
G[2] = 200.0 * (x[2] - x[1]^2)
end
```

Note, that the functions we're using to calculate the gradient (and later the Hessian `h!`) of the

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https://julianlsolvers.github.io/Optim.jl/stable/#user/minimization/

Optim.jl

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  - Conditional maximum likelihood estimation
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```

Other solvers are available. Below, we use L-BFGS, a quasi-Newton method that requires a gradient. If we pass `f` alone, Optim will construct an approximate gradient for us using central finite differencing:

```
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```

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```
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```

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G[2] = 200.0 * (x[2] - x[1]^2)
end
```

Note, that the functions we're using to calculate the gradient (and later the Hessian `h!`) of the Rosenbrock function mutate a fixed-sized storage array, which is passed as an additional argument called `G` (or `H` for the Hessian) in these examples. By mutating a single array over many iterations, this style of function definition removes the sometimes considerable costs associated with allocating a new array during each call to the `g!` or `h!` functions. If you prefer to have your gradients simply accept an `x`, you can still use `optimize` by setting the `inplace` keyword to `false`:

```
optimize(f, g, x0; inplace = false)
```

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JupyterLab | dstndstn/FittingAModel2023 | Tips and tricks - Optim.jl

https://julianlsolvers.github.io/Optim.jl/stable/#user/tipsandtricks/

Optim.jl

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Dealing with constant parameters

In many applications, there may be factors that are relevant to the function evaluations, but are fixed throughout the optimization. An obvious example is using data in a likelihood function, but it could also be parameters we wish to hold constant.

Consider a squared error loss function that depends on some data `x` and `y`, and parameters `betas`. As far as the solver is concerned, there should only be one input argument to the function we want to minimize, call it `sqerror`.

The problem is that we want to optimize a function `sqerror` that really depends on three inputs, and two of them are constant throughout the optimization procedure. To do this, we need to define the variables `x` and `y`

```
x = [1.0, 2.0, 3.0]
y = 1.0 + 2.0 * x + [-0.3, 0.3, -0.1]
```

We then simply define a function in three variables

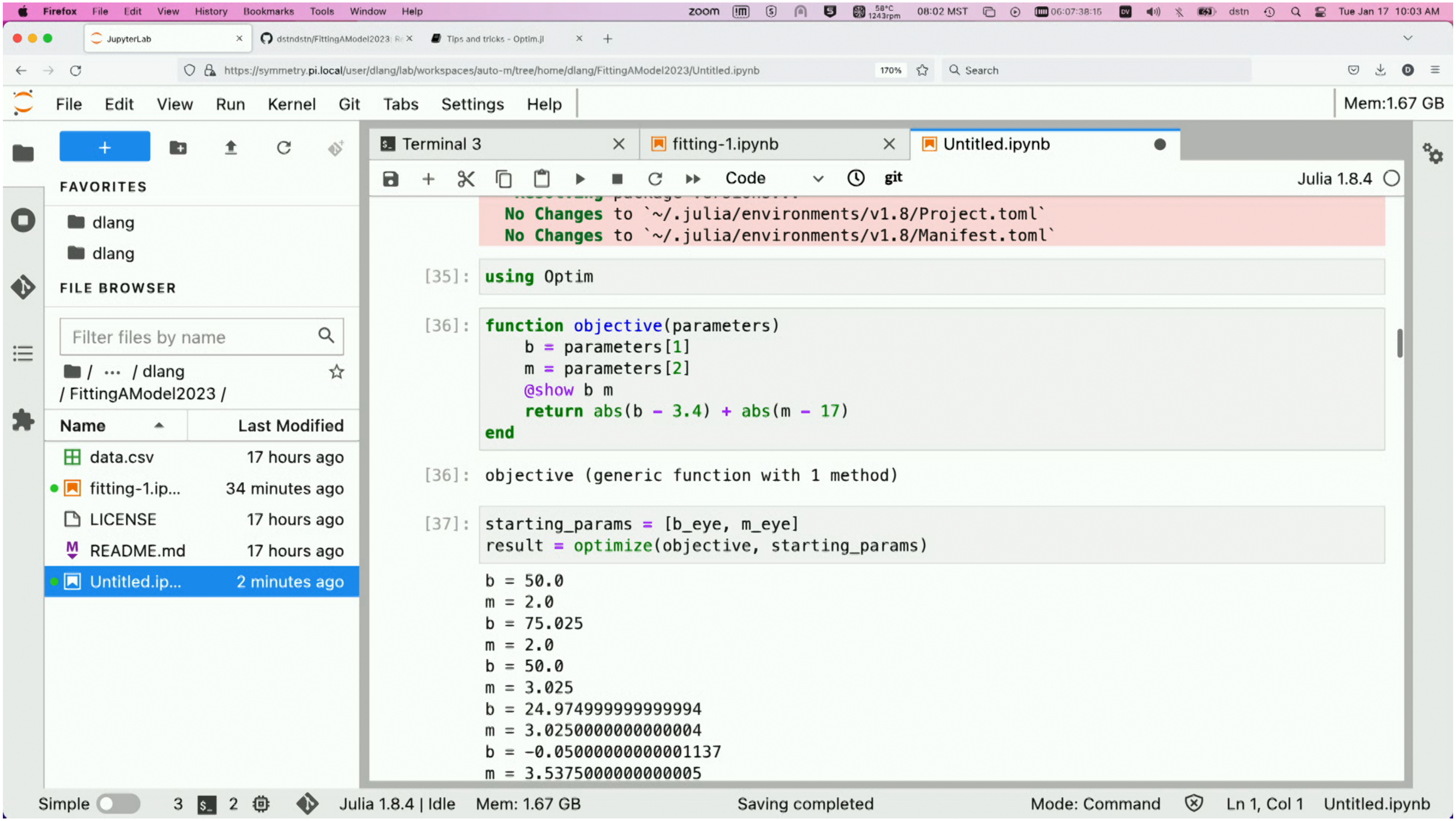
```
function sqerror(betas, X, Y)
    err = 0.0
    for i in 1:length(X)
        pred_i = betas[1] + betas[2] * X[i]
        err += (Y[i] - pred_i)^2
    end
    return err
end
```

and then optimize the following anonymous function

```
res = optimize(b -> sqerror(b, x, y), [0.0, 0.0])
```

Alternatively, we can define a closure `sqerror(betas)` that is aware of the variables we just defined

https://julianlsolvers.github.io/Optim.jl/stable/#examples/generated/maxlikenlm/



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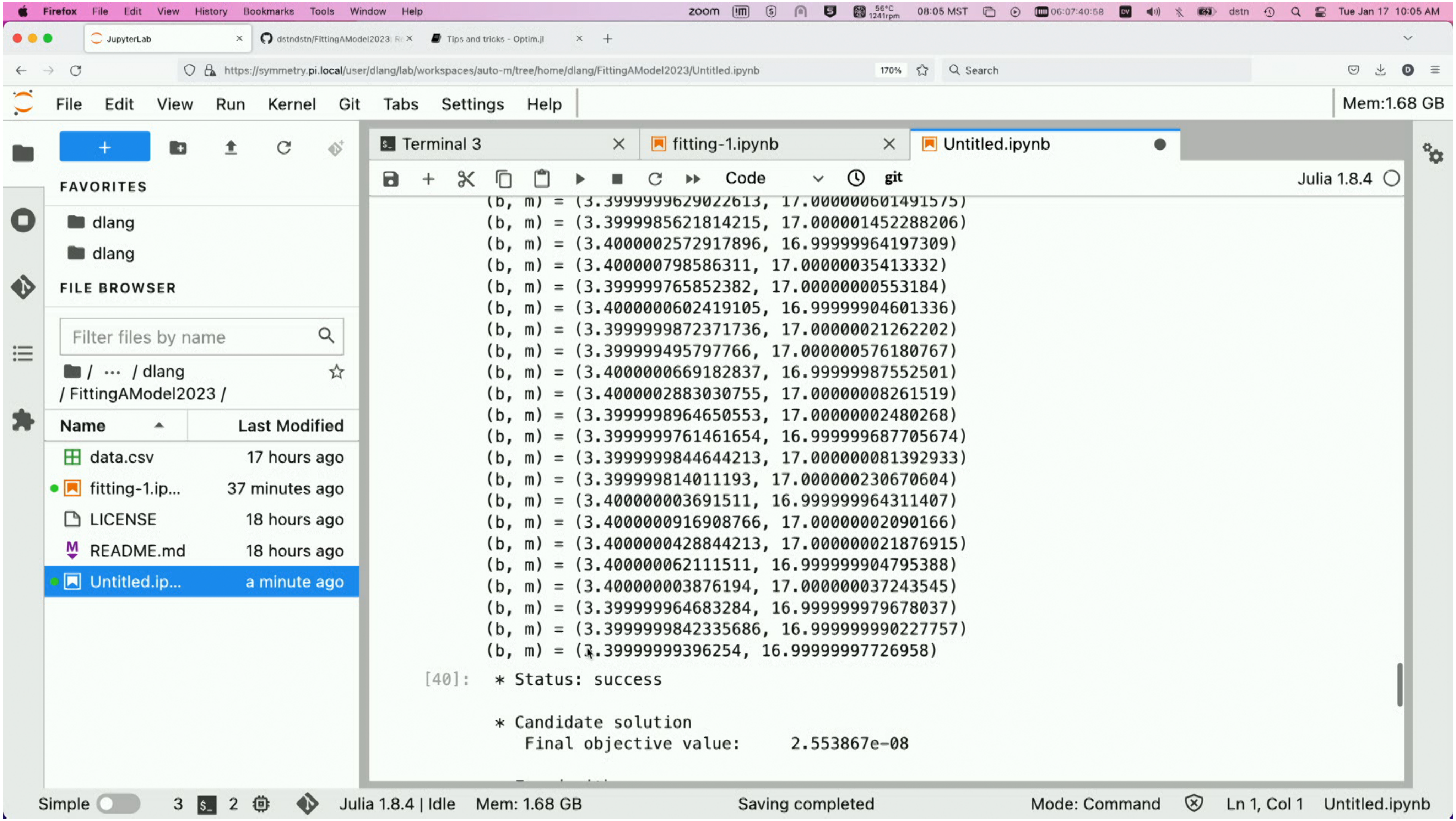
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[35]: using Optim
[36]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b m
return abs(b - 3.4) + abs(m - 17)
end
[36]: objective (generic function with 1 method)
[37]: starting_params = [b_eye, m_eye]
result = optimize(objective, starting_params)
b = 50.0
m = 2.0
b = 75.025
m = 2.0
b = 50.0
m = 3.025
b = 24.974999999999994
m = 3.0250000000000004
b = -0.05000000000001137
m = 3.5375000000000005
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.67 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb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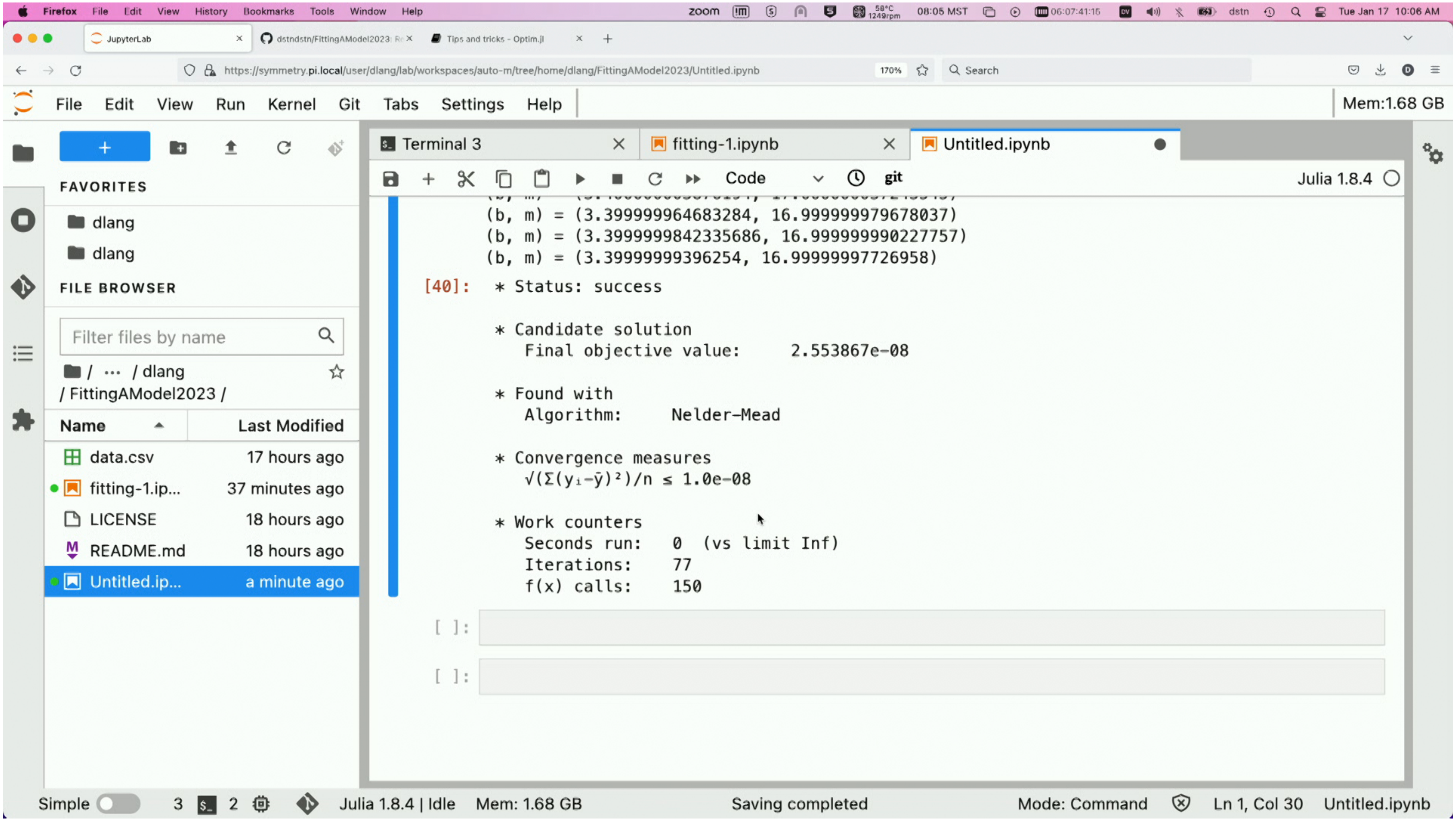
(b, m) = (3.3999985621814215, 17.000001452288206)
(b, m) = (3.4000002572917896, 16.99999964197309)
(b, m) = (3.400000798586311, 17.0000035413332)
(b, m) = (3.399999765852382, 17.00000000553184)
(b, m) = (3.4000000602419105, 16.99999904601336)
(b, m) = (3.3999999872371736, 17.00000021262202)
(b, m) = (3.399999495797766, 17.000000576180767)
(b, m) = (3.4000000669182837, 16.99999987552501)
(b, m) = (3.4000002883030755, 17.00000008261519)
(b, m) = (3.3999998964650553, 17.00000002480268)
(b, m) = (3.3999999761461654, 16.999999687705674)
(b, m) = (3.3999999844644213, 17.000000081392933)
(b, m) = (3.399999814011193, 17.000000230670604)
(b, m) = (3.400000003691511, 16.999999964311407)
(b, m) = (3.4000000916908766, 17.00000002090166)
(b, m) = (3.4000000428844213, 17.000000021876915)
(b, m) = (3.400000062111511, 16.999999904795388)
(b, m) = (3.400000003876194, 17.000000037243545)
(b, m) = (3.399999964683284, 16.999999979678037)
(b, m) = (3.3999999842335686, 16.999999990227757)
(b, m) = (3.39999999396254, 16.99999997726958)
[40]: * Status: success
* Candidate solution
Final objective value: 2.553867e-08
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.68 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb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Tips and tricks - Optim.jl
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(b, m) = (3.399999964683284, 16.999999979678037)
(b, m) = (3.3999999842335686, 16.999999990227757)
(b, m) = (3.39999999396254, 16.99999997726958)
[40]: * Status: success
* Candidate solution
Final objective value: 2.553867e-08
* Found with
Algorithm: Nelder-Mead
* Convergence measures
√(Σ(yᵢ-ȳ)²)/n ≤ 1.0e-08
* Work counters
Seconds run: 0 (vs limit Inf)
Iterations: 77
f(x) calls: 150
[ ]:
[ ]:
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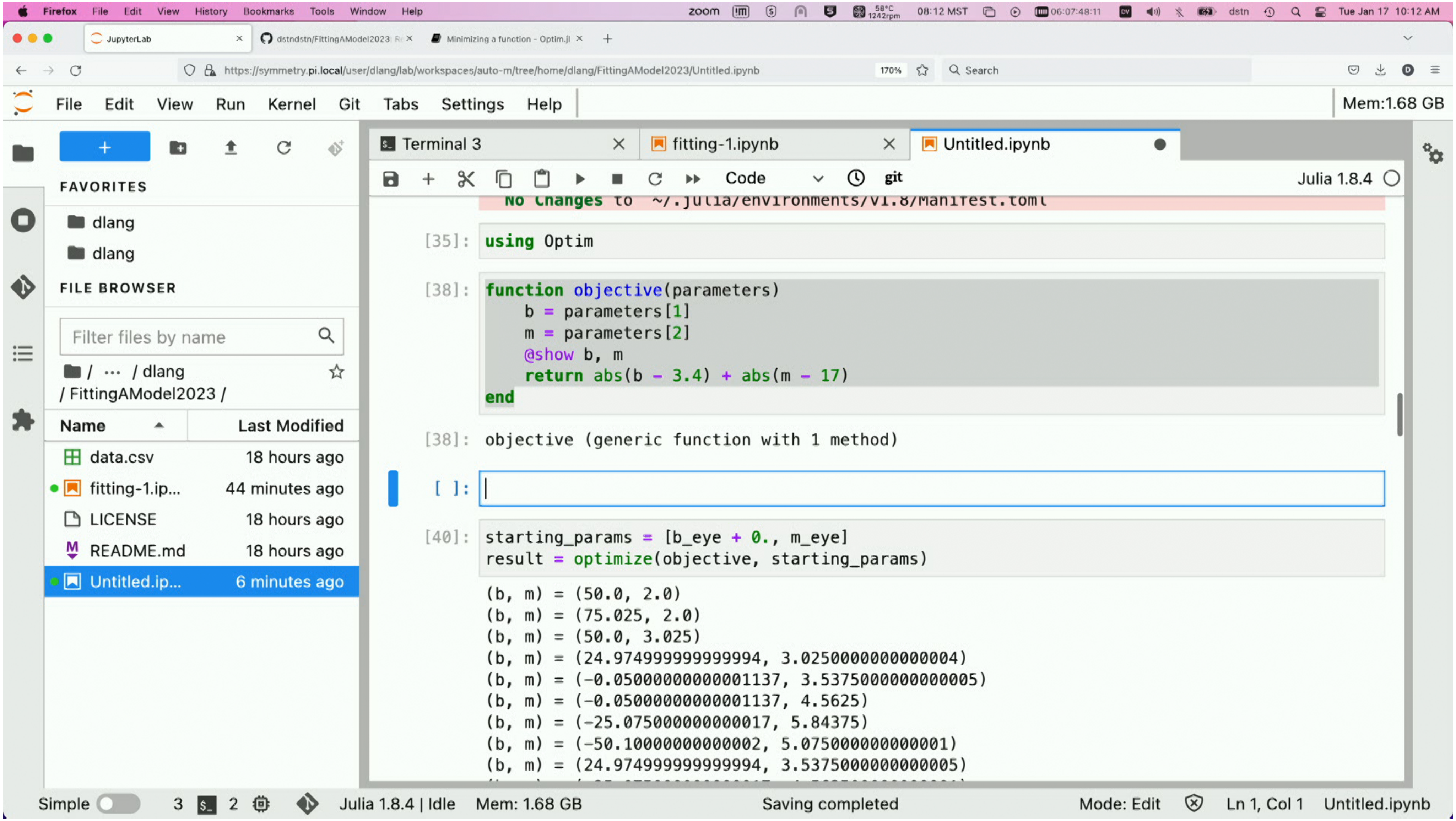

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[35]: using Optim
[38]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b, m
return abs(b - 3.4) + abs(m - 17)
end
[38]: objective (generic function with 1 method)
[ ]:
[40]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective, starting_params)
(b, m) = (50.0, 2.0)
(b, m) = (75.025, 2.0)
(b, m) = (50.0, 3.025)
(b, m) = (24.974999999999994, 3.0250000000000004)
(b, m) = (-0.05000000000001137, 3.5375000000000005)
(b, m) = (-0.05000000000001137, 4.5625)
(b, m) = (-25.075000000000017, 5.84375)
(b, m) = (-50.10000000000002, 5.075000000000001)
(b, m) = (24.974999999999994, 3.5375000000000005)
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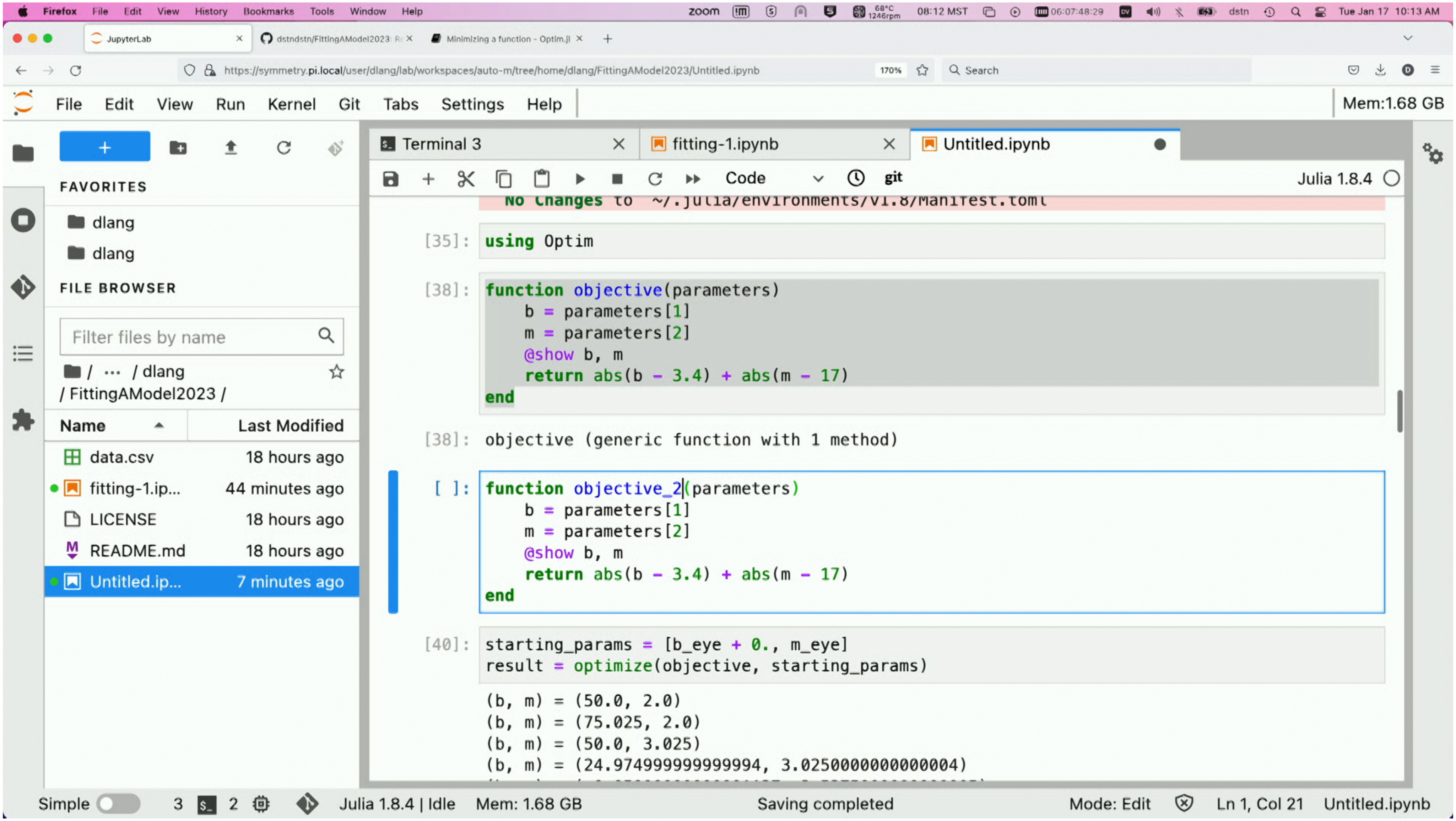
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[35]: using Optim
[38]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b, m
return abs(b - 3.4) + abs(m - 17)
end
[38]: objective (generic function with 1 method)
[ ]: function objective_2(parameters)
b = parameters[1]
m = parameters[2]
@show b, m
return abs(b - 3.4) + abs(m - 17)
end
[40]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective, starting_params)
(b, m) = (50.0, 2.0)
(b, m) = (75.025, 2.0)
(b, m) = (50.0, 3.025)
(b, m) = (24.974999999999994, 3.0250000000000004)
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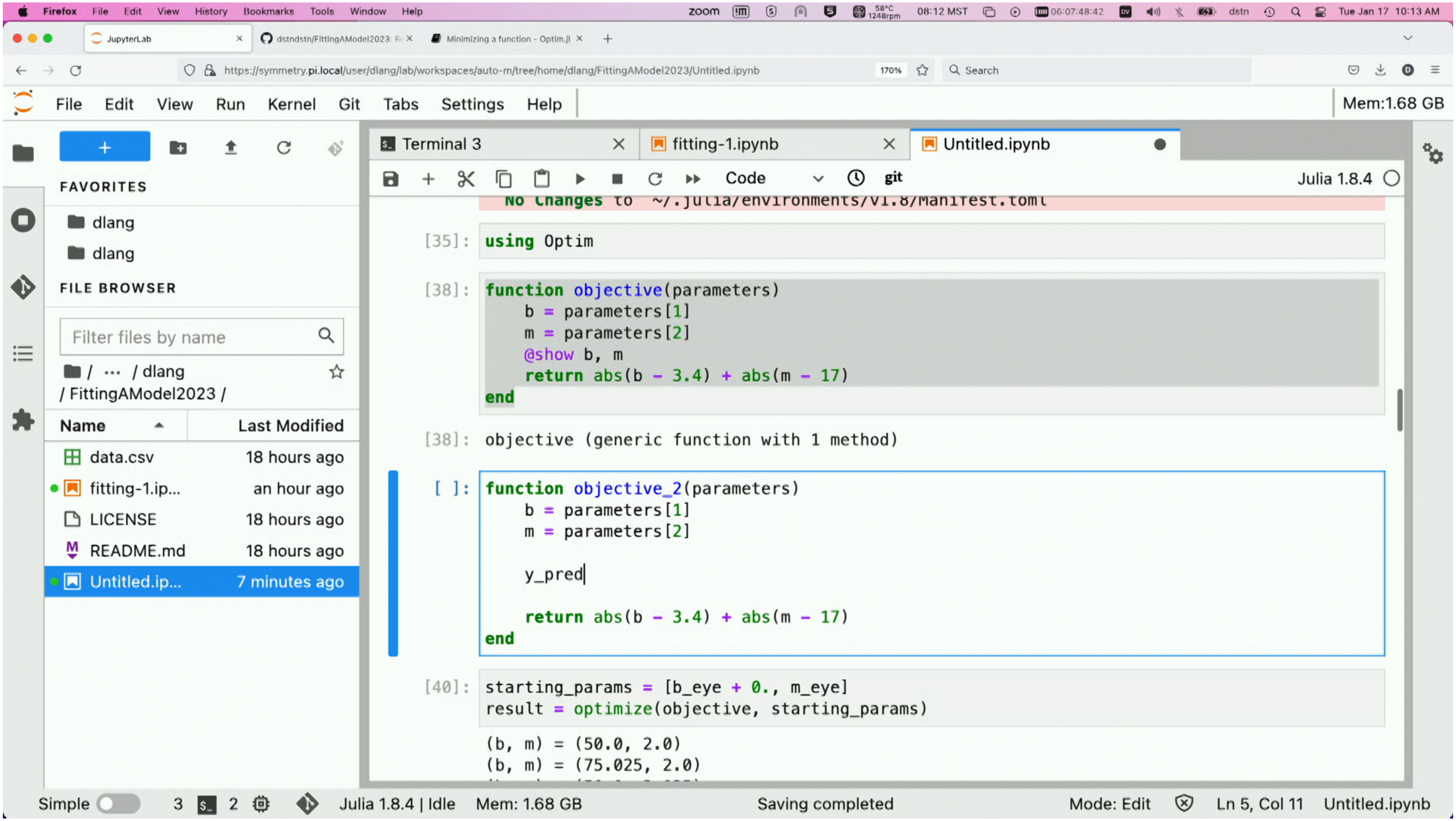
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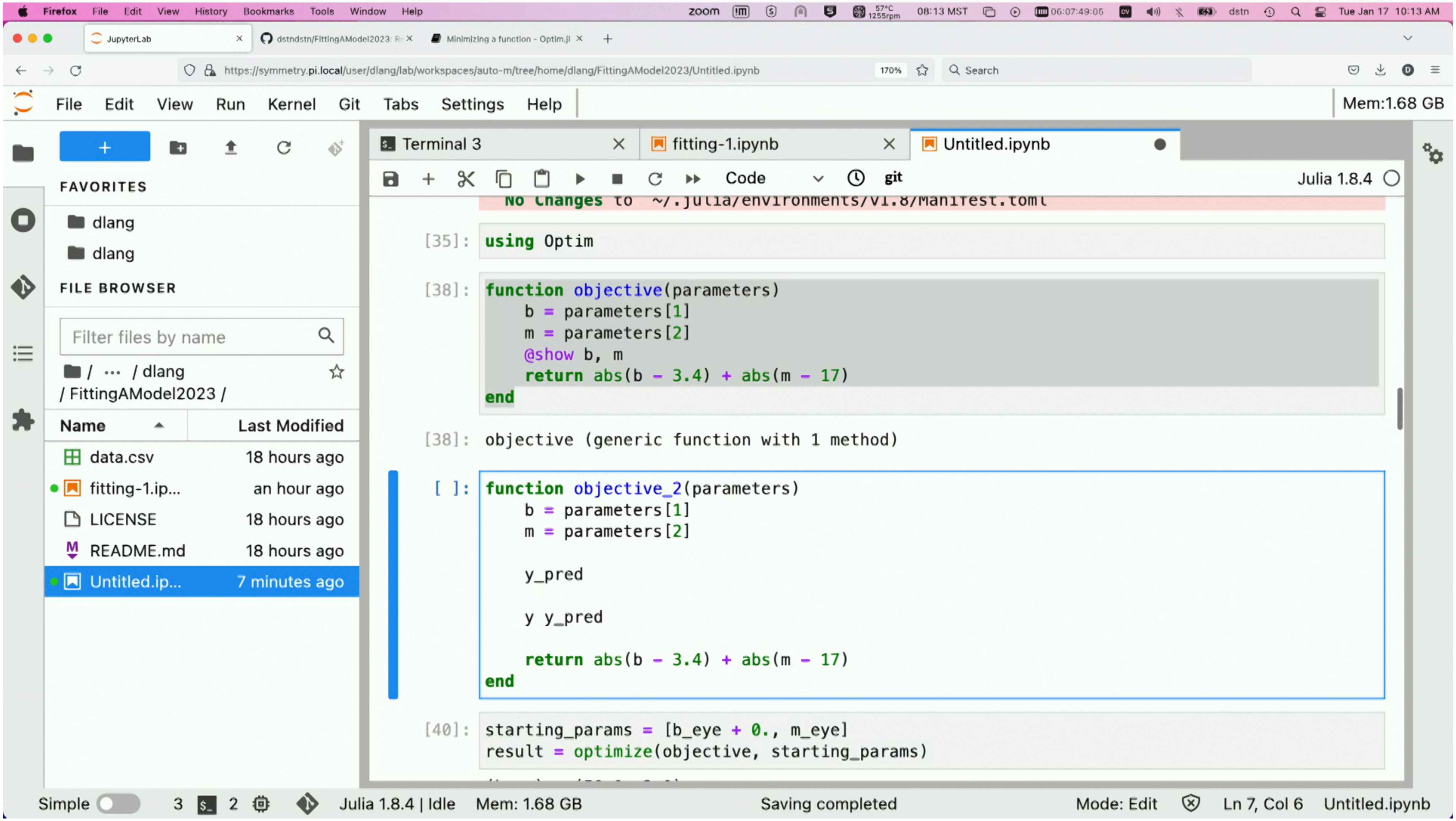
[35]: using Optim
[38]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b, m
return abs(b - 3.4) + abs(m - 17)
end
[38]: objective (generic function with 1 method)
[ ]: function objective_2(parameters)
b = parameters[1]
m = parameters[2]
y_pred
return abs(b - 3.4) + abs(m - 17)
end
[40]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective, starting_params)
(b, m) = (50.0, 2.0)
(b, m) = (75.025, 2.0)
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.68 GB Saving completed Mode: Edit Ln 5, Col 11 Untitled.ipynb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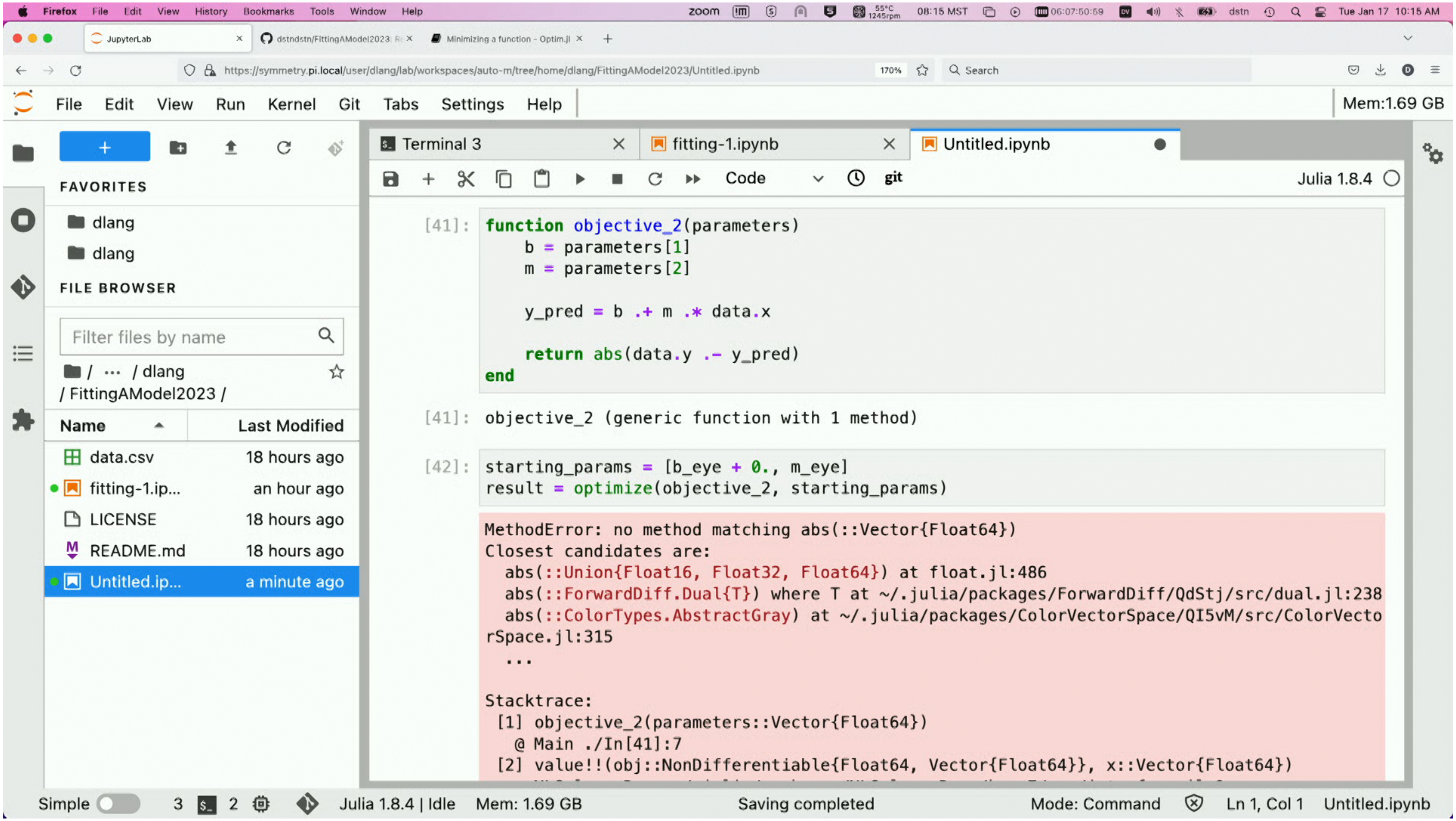
No changes to ~/.julia/environments/v1.8/Manifest.toml
[35]: using Optim
[38]: function objective(parameters)
b = parameters[1]
m = parameters[2]
@show b, m
return abs(b - 3.4) + abs(m - 17)
end
[38]: objective (generic function with 1 method)
[ ]: function objective_2(parameters)
b = parameters[1]
m = parameters[2]
y_pred
y y_pred
return abs(b - 3.4) + abs(m - 17)
end
[40]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective, starting_params)
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.68 GB Saving completed Mode: Edit Ln 7, Col 6 Untitled.ipynb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Minimizing a function - Optim.jl
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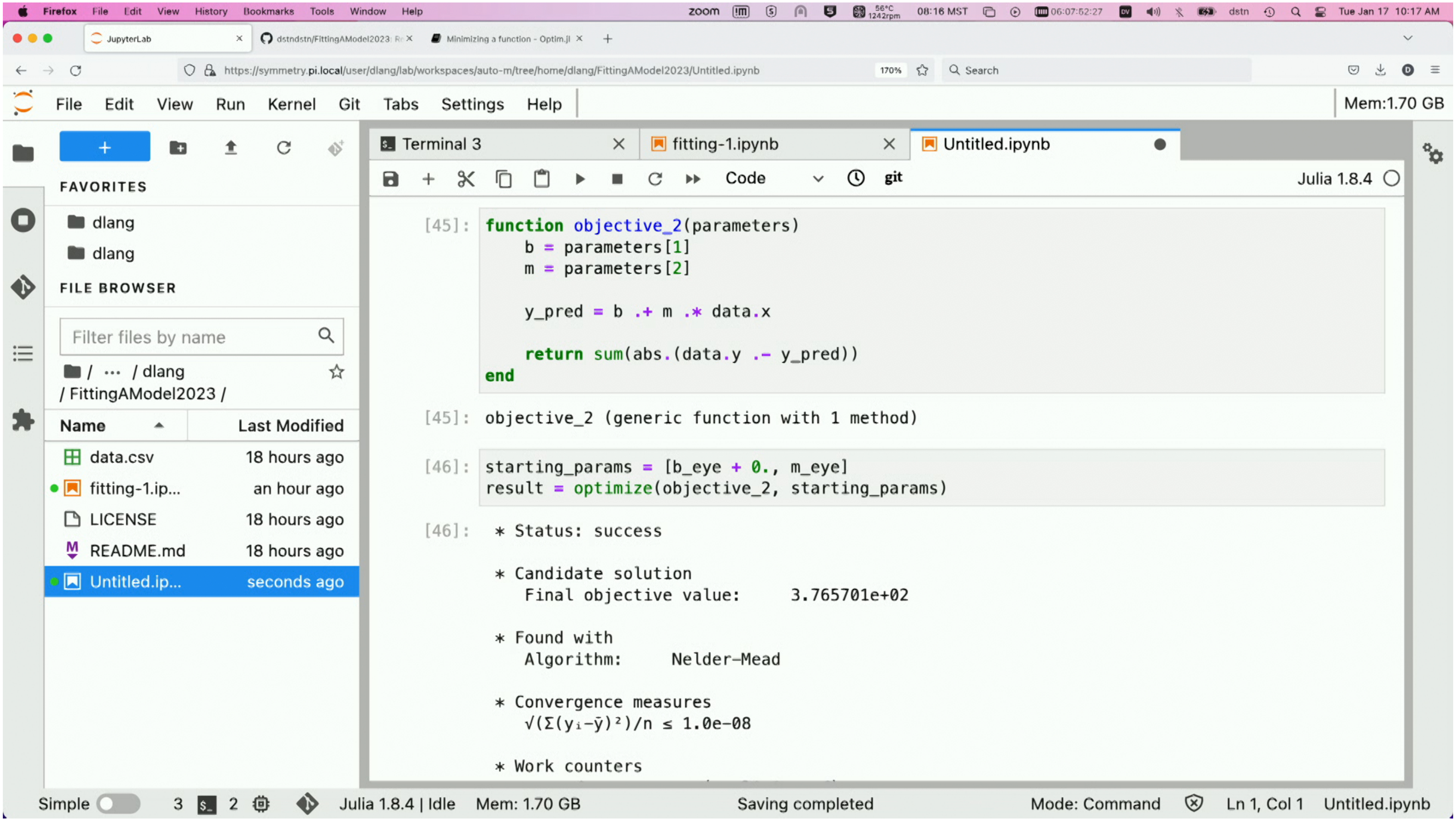
[41]:
function objective_2(parameters)
    b = parameters[1]
    m = parameters[2]
    y_pred = b .+ m .* data.x
    return abs(data.y .- y_pred)
end
[41]: objective_2 (generic function with 1 method)
[42]:
starting_params = [b_eye + 0., m_eye]
result = optimize(objective_2, starting_params)
MethodError: no method matching abs(::Vector{Float64})
Closest candidates are:
  abs(::Union{Float16, Float32, Float64}) at float.jl:486
  abs(::ForwardDiff.Dual{T}) where T at ~/.julia/packages/ForwardDiff/QdStj/src/dual.jl:238
  abs(::ColorTypes.AbstractGray) at ~/.julia/packages/ColorVectorSpace/QI5vM/src/ColorVectorSpace.jl:315
  ...
Stacktrace:
 [1] objective_2(parameters::Vector{Float64})
   @ Main ./In[41]:7
 [2] value!!(obj::NonDifferentiable{Float64, Vector{Float64}}, x::Vector{Float64})
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.69 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb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Julia 1.8.4
[45]: function objective_2(parameters)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* data.x
return sum(abs.(data.y .- y_pred))
end
[45]: objective_2 (generic function with 1 method)
[46]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective_2, starting_params)
[46]: * Status: success
* Candidate solution
Final objective value: 3.765701e+02
* Found with
Algorithm: Nelder-Mead
* Convergence measures
√(Σ(yᵢ-ȳ)²)/n ≤ 1.0e-08
* Work counters
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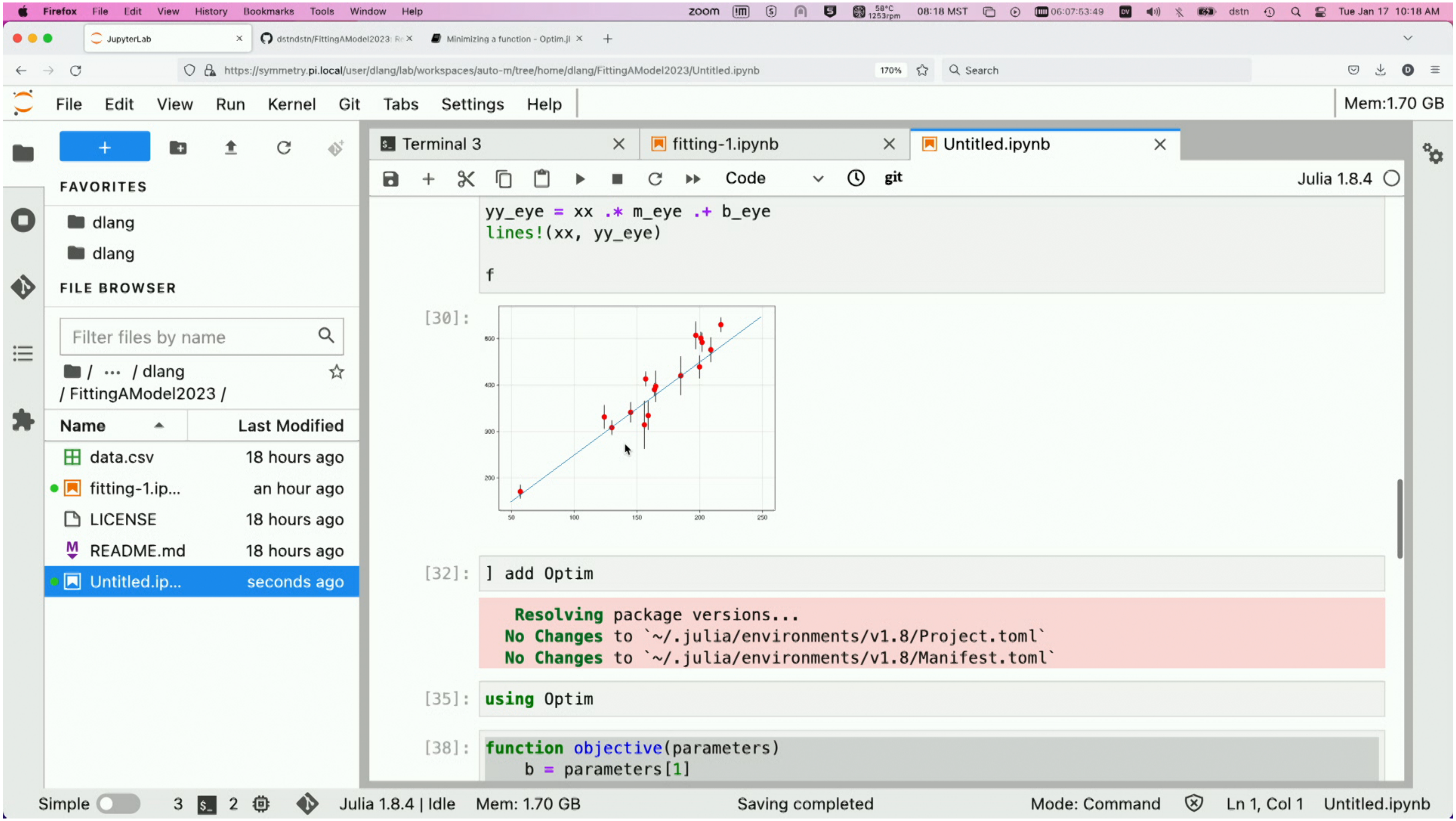
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Minimizing a function - Optim.jl
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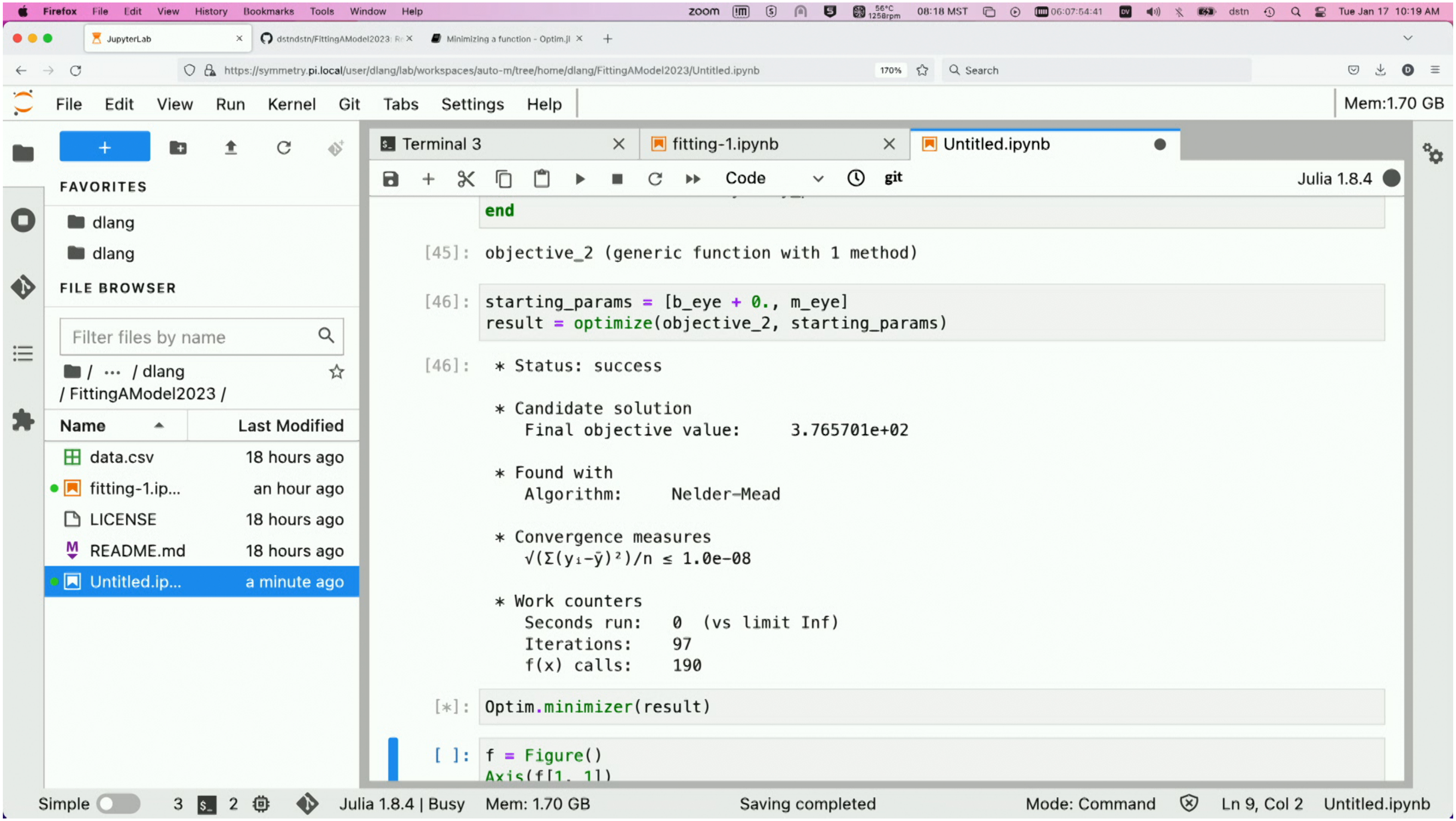
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye)
f
[30]:
[32]:] add Optim
Resolving package versions...
No Changes to `~/.julia/environments/v1.8/Project.toml`
No Changes to `~/.julia/environments/v1.8/Manifest.toml`
[35]: using Optim
[38]: function objective(parameters)
b = parameters[1]
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.70 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb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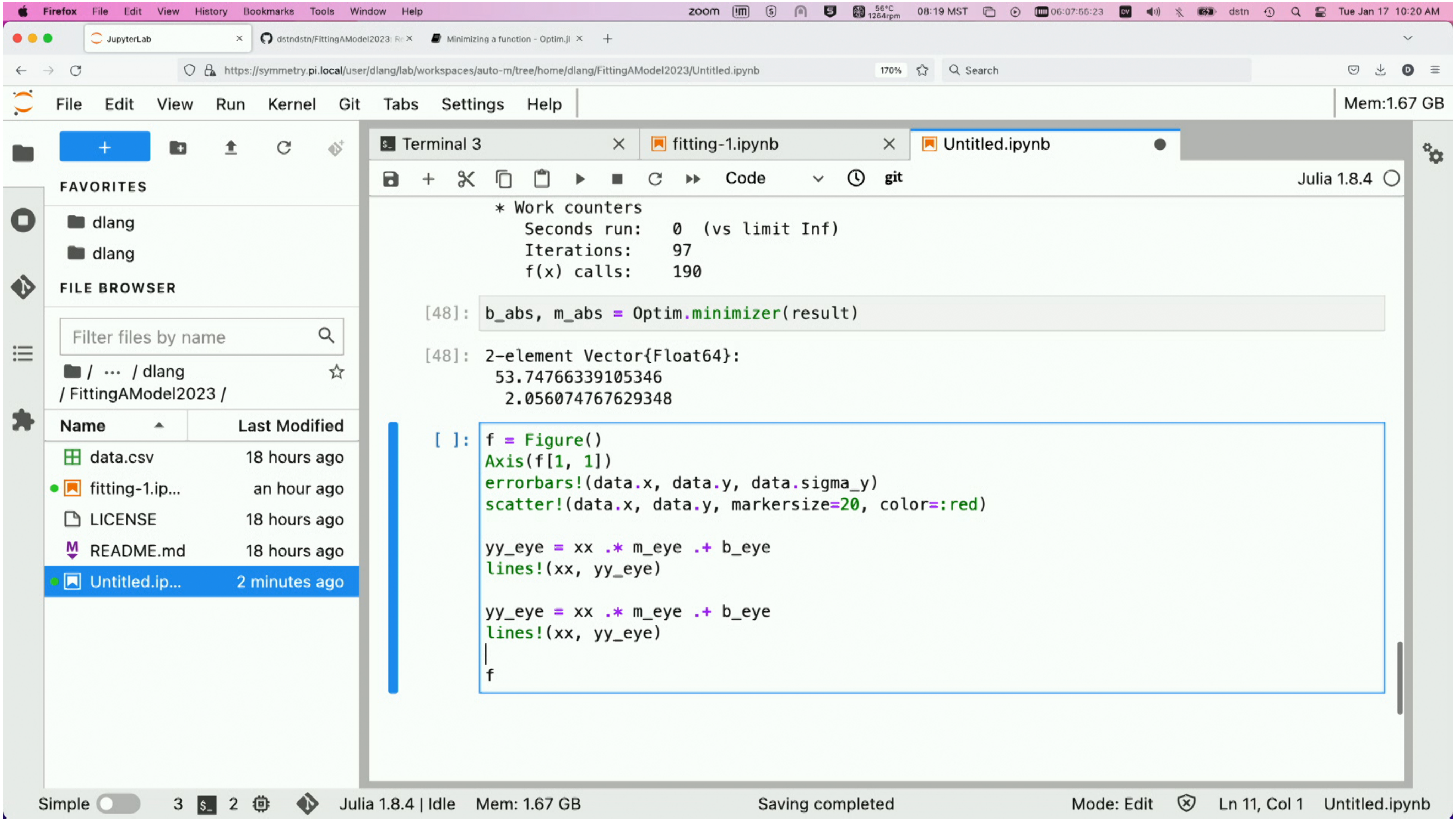
end
[45]: objective_2 (generic function with 1 method)
[46]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective_2, starting_params)
[46]: * Status: success
* Candidate solution
Final objective value: 3.765701e+02
* Found with
Algorithm: Nelder-Mead
* Convergence measures
√(Σ(yᵢ-ȳ)²)/n ≤ 1.0e-08
* Work counters
Seconds run: 0 (vs limit Inf)
Iterations: 97
f(x) calls: 190
[*]: Optim.minimizer(result)
[ ]: f = Figure()
Simple 3 2 Julia 1.8.4 | Busy Mem: 1.70 GB Saving completed Mode: Command Ln 9, Col 2 Untitled.ipynb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Untitled.ip... 2 minutes ago
* Work counters
Seconds run: 0 (vs limit Inf)
Iterations: 97
f(x) calls: 190
[48]: b_abs, m_abs = Optim.minimizer(result)
[48]: 2-element Vector{Float64}:
53.74766339105346
2.056074767629348
[ ]: f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye)
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye)
f
Simple
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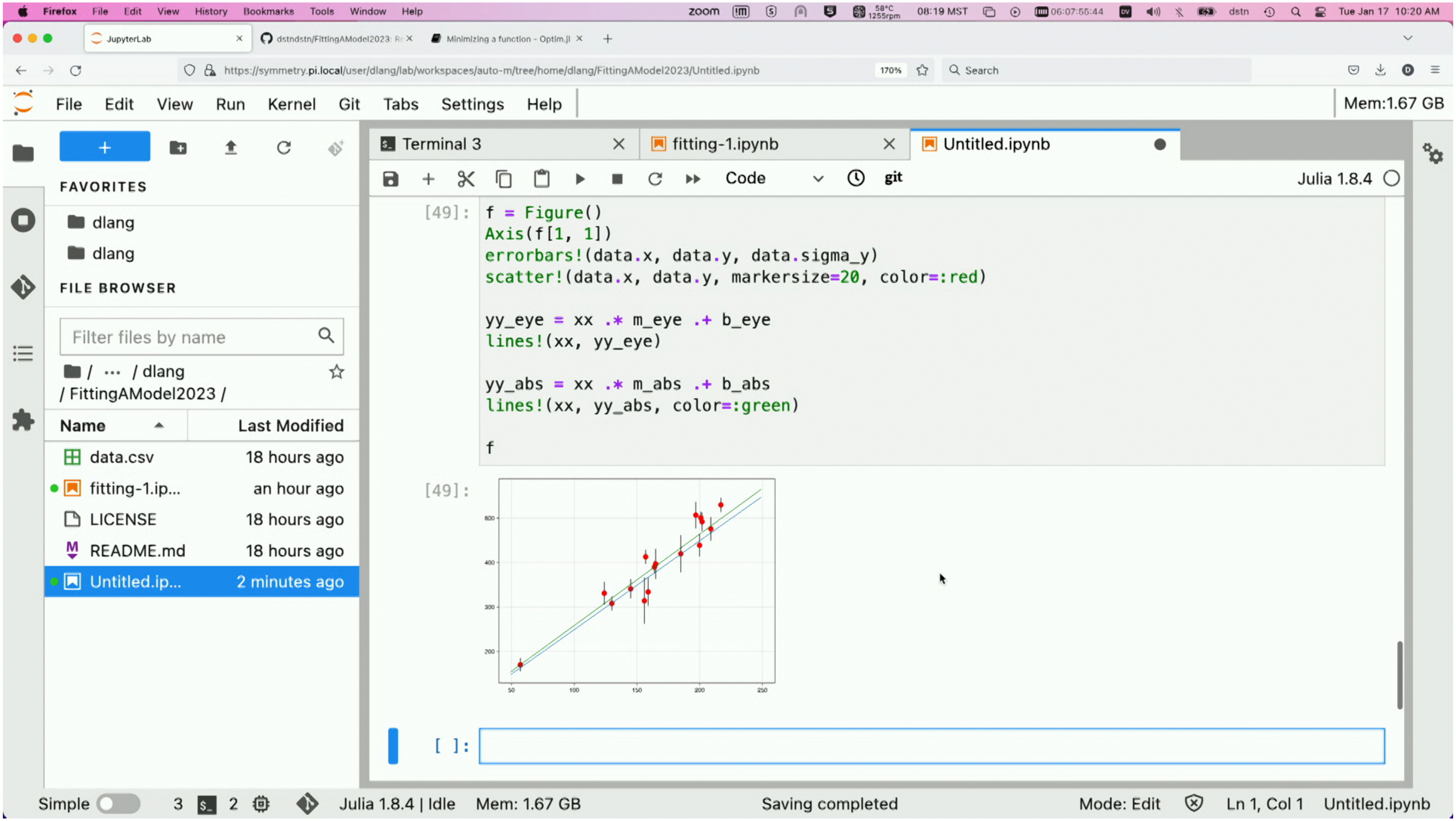
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Julia 1.8.4
[49]:
f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye)
yy_abs = xx .* m_abs .+ b_abs
lines!(xx, yy_abs, color=:green)
f
[49]:
[ ]:
Simple
Julia 1.8.4 | Idle
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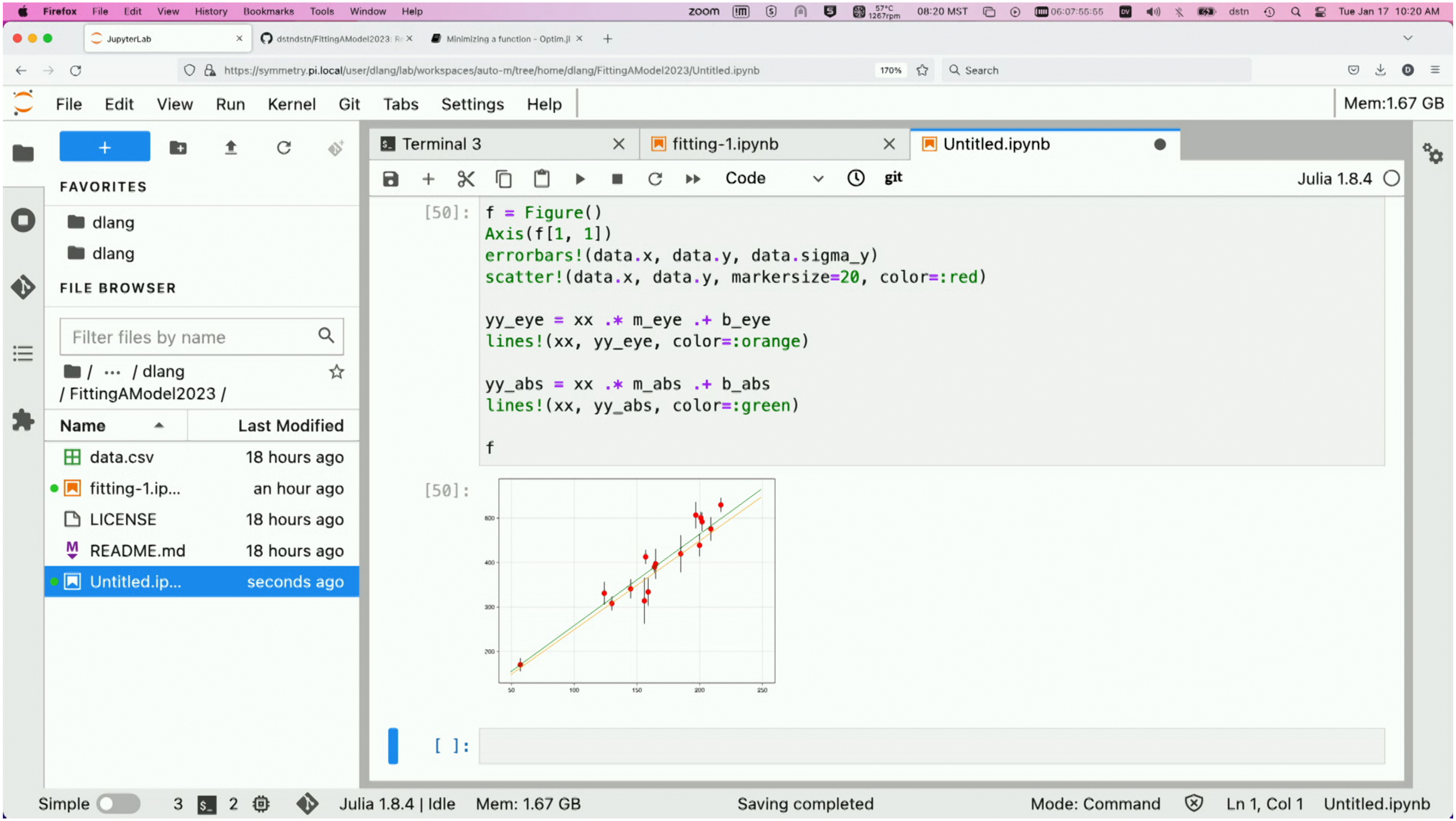
File Edit View Run Kernel Git Tabs Settings Help
Mem:1.67 GB
Terminal 3
fitting-1.ipynb
Untitled.ipynb
FAVORITES
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dlang
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Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
Code
git
Julia 1.8.4
[50]:
f = Figure()
Axis(f[1, 1])
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)
yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye, color=:orange)
yy_abs = xx .* m_abs .+ b_abs
lines!(xx, yy_abs, color=:green)
f
[50]:
[ ]:
Simple
Julia 1.8.4 | Idle
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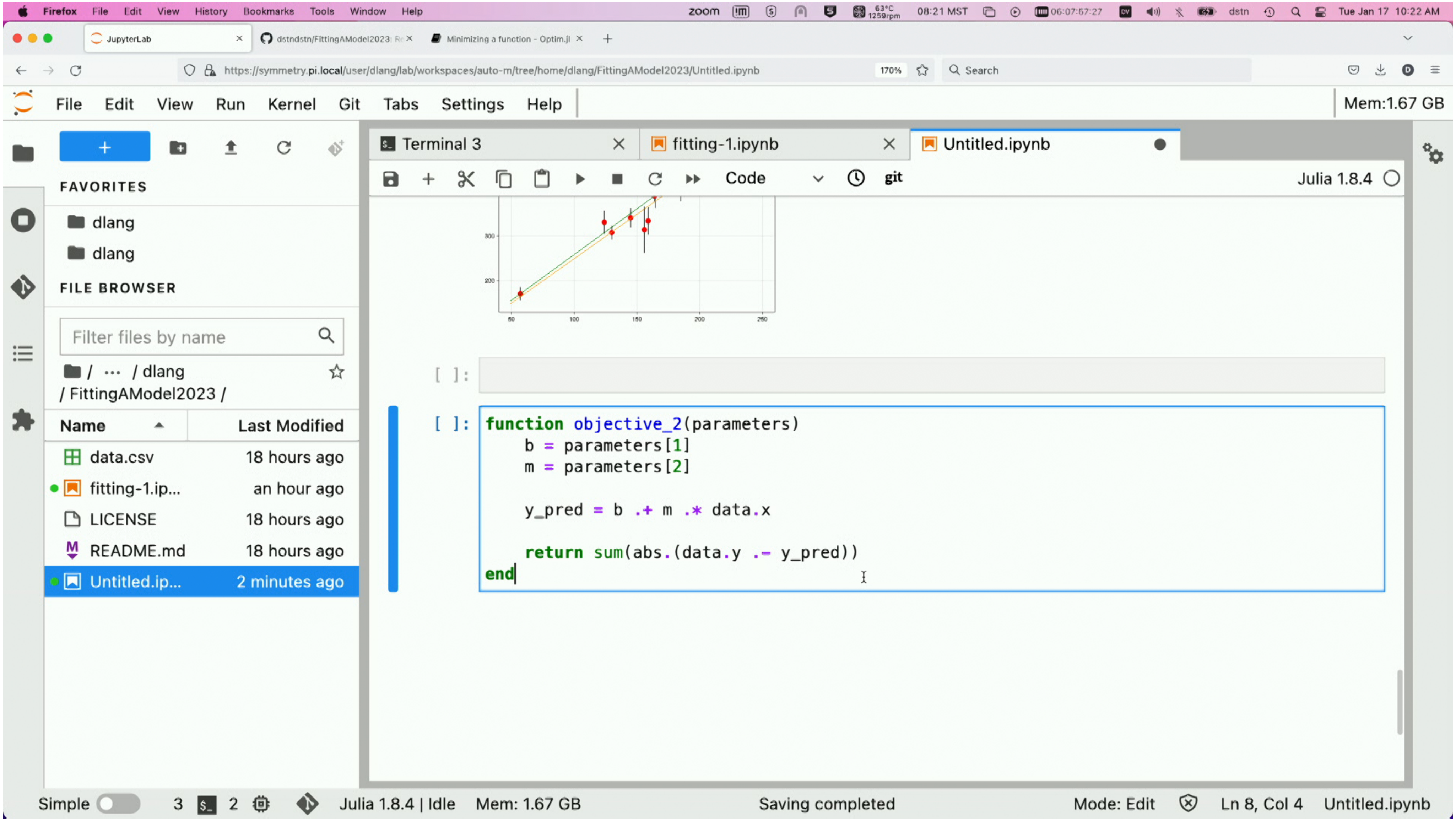
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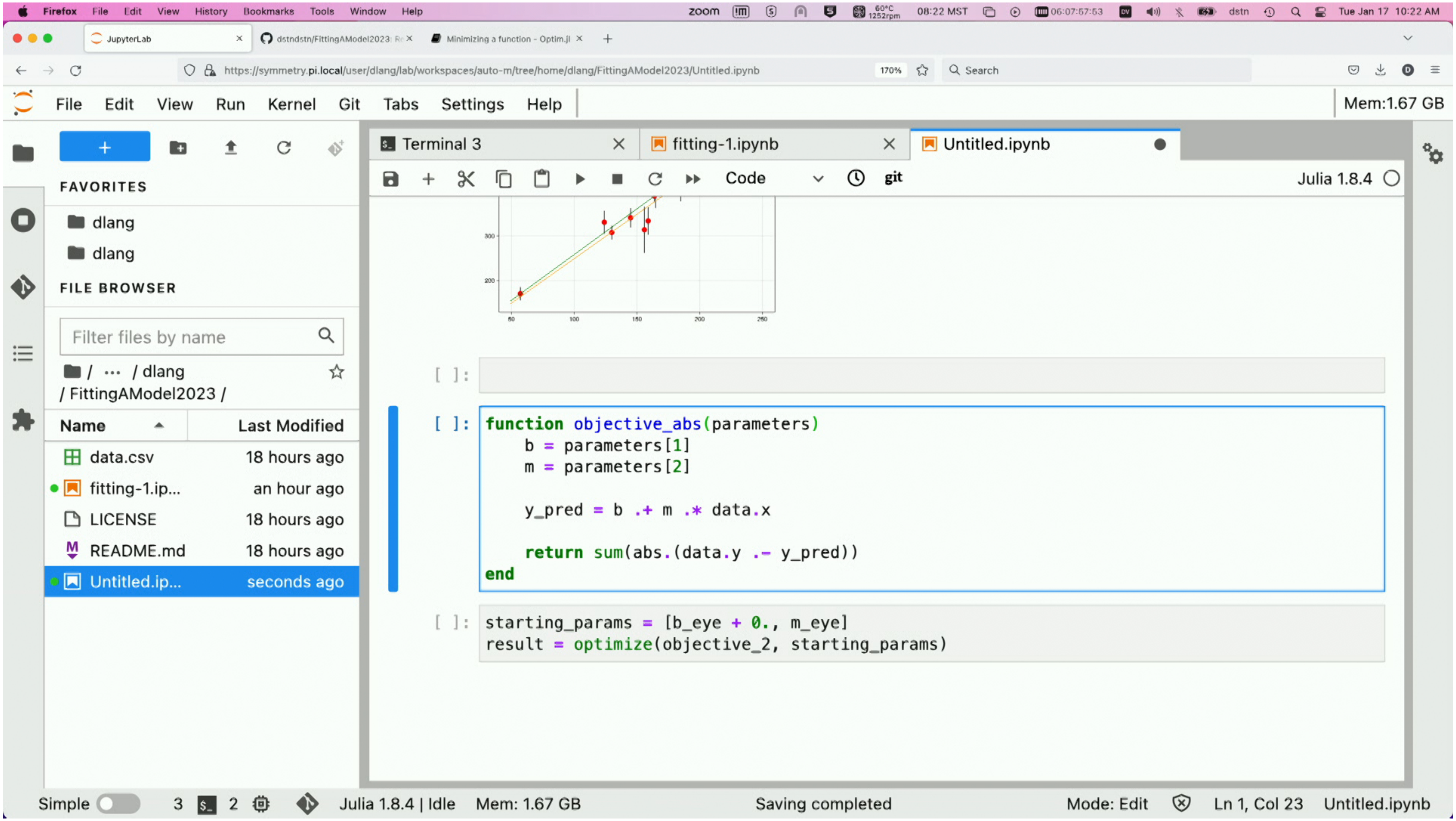
Name Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... 2 minutes ago
Terminal 3
fitting-1.ipynb
Untitled.ipynb
Code
git
Julia 1.8.4
[ ]:
[ ]:
function objective_2(parameters)
    b = parameters[1]
    m = parameters[2]
    y_pred = b .+ m .* data.x
    return sum(abs.(data.y .- y_pred))
end
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.67 GB Saving completed Mode: Edit Ln 8, Col 4 Untitled.ipynb



Firefox File Edit View History Bookmarks Tools Window Help
Tue Jan 17 10:22 AM
JupyterLab
Minimizing a function - Optim.jl
https://symmetry.pi.local/user/dlang/lab/workspaces/auto-m/tree/home/dlang/FittingAModel2023/Untitled.ipynb
File Edit View Run Kernel Git Tabs Settings Help
Mem:1.67 GB
Terminal 3
fitting-1.ipynb
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Code
git
Julia 1.8.4
FAVORITES
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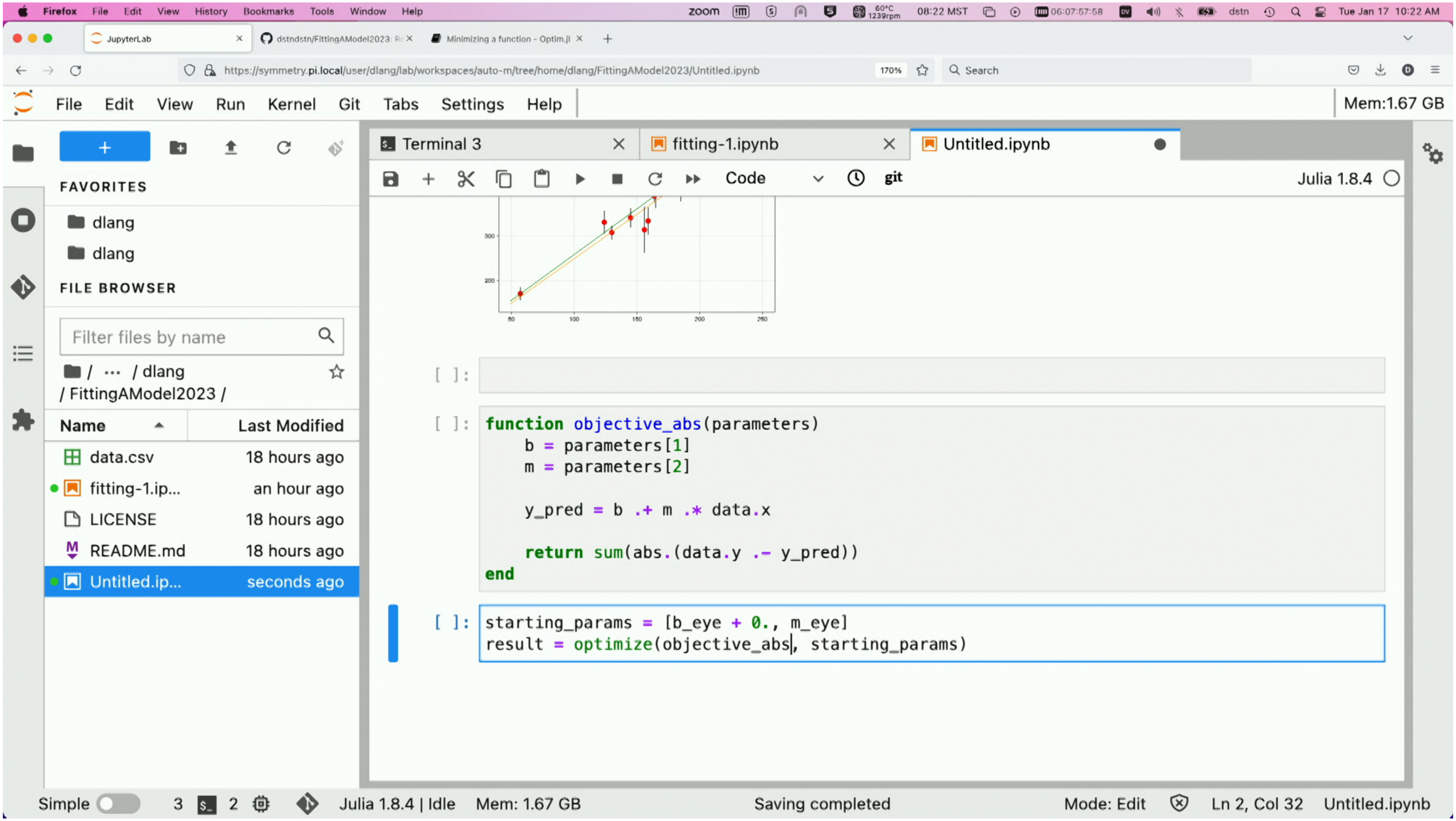
Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
[ ]:
[ ]: function objective_abs(parameters)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* data.x
return sum(abs.(data.y .- y_pred))
end
[ ]: starting_params = [b_eye + 0., m_eye]
result = optimize(objective_2, starting_params)
Simple
Julia 1.8.4 | Idle
Mem: 1.67 GB
Saving completed
Mode: Edit
Ln 1, Col 23
Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Mem:1.67 GB
Terminal 3
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Name
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data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
[ ]:
[ ]:
function objective_abs(parameters)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* data.x
return sum(abs.(data.y .- y_pred))
end
[ ]:
starting_params = [b_eye + 0., m_eye]
result = optimize(objective_abs, starting_params)
Simple
Julia 1.8.4 | Idle
Mem: 1.67 GB
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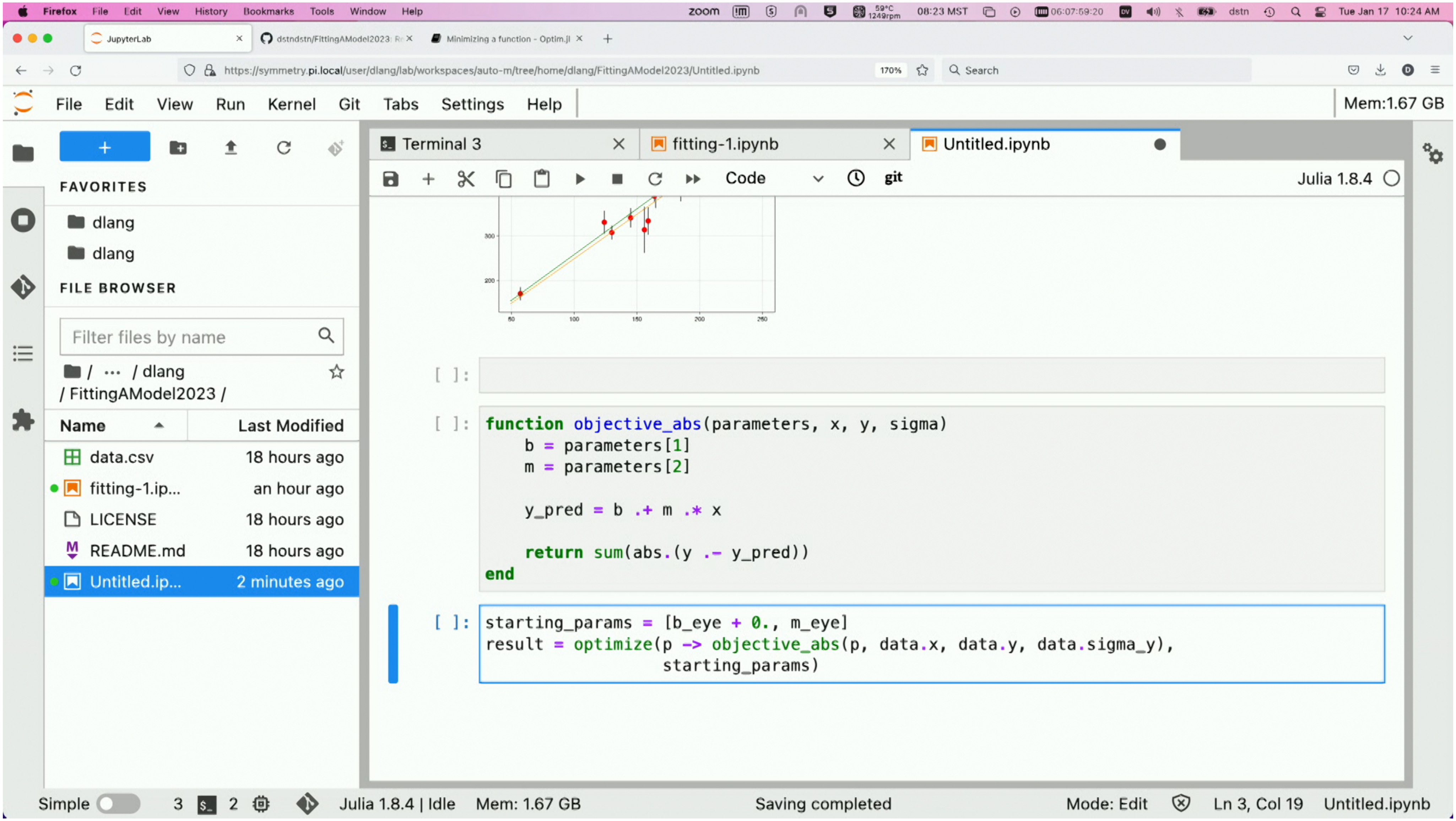
Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
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Code
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Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... 2 minutes ago
[ ]:
[ ]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return sum(abs.(y .- y_pred))
end
[ ]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
Simple
Julia 1.8.4 | Idle
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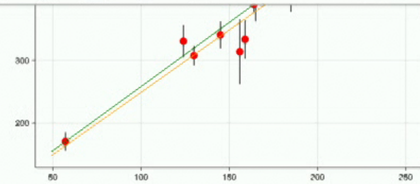


```
[ ]:
```

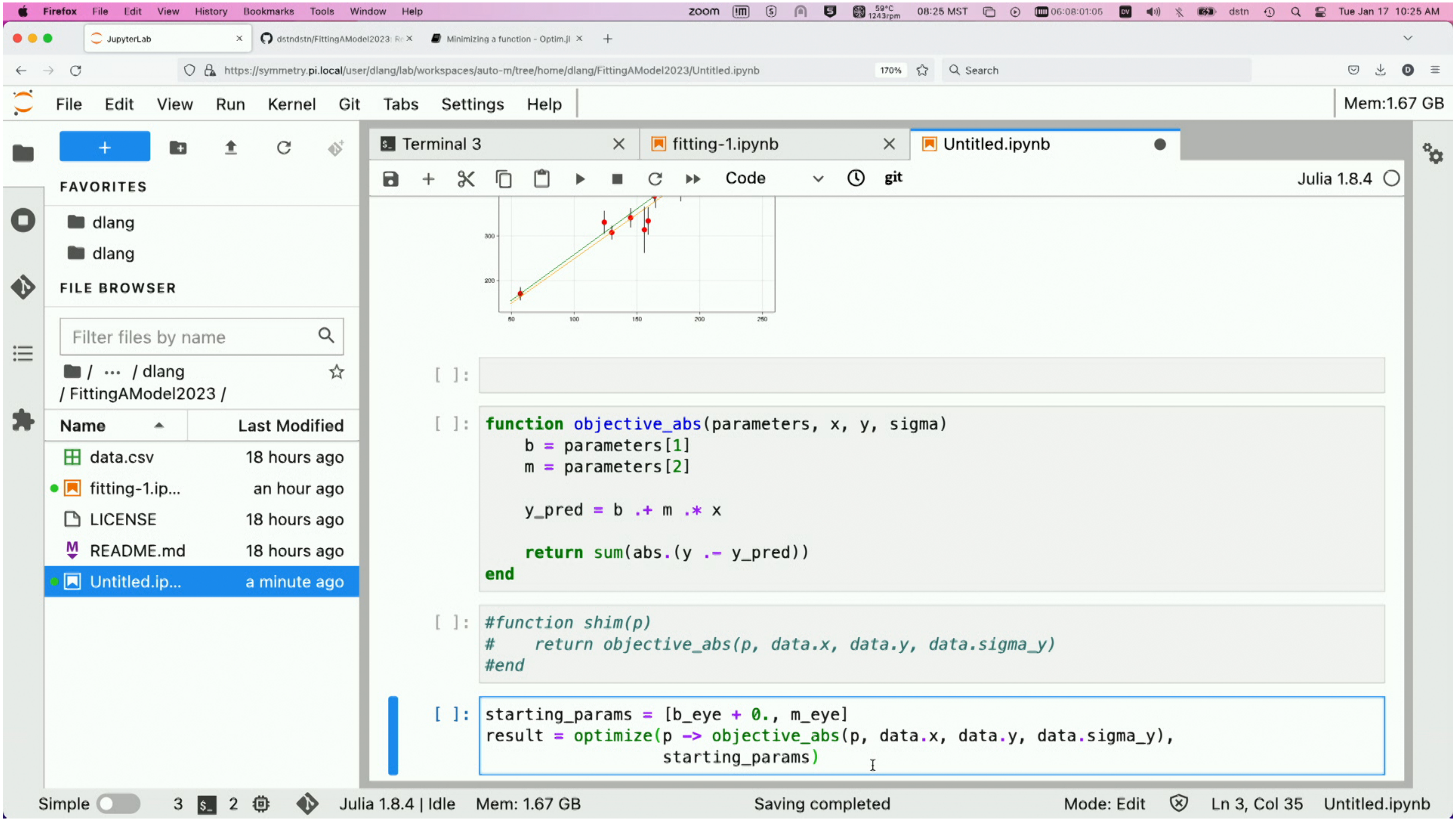
```julia
function objective_abs(parameters, x, y, sigma)
    b = parameters[1]
    m = parameters[2]

    y_pred = b .+ m .* x

    return sum(abs.(y .- y_pred))
end
```

```julia
function shim(p)
    return objective_abs(p, data.x, data.y, data.sigma_y)
end
```

```julia
starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
                  starting_params)
```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Code
git
Julia 1.8.4
FAVORITES
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Name
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data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... a minute ago
[ ]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return sum(abs.(y .- y_pred))
end
[ ]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[ ]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
Simple
Julia 1.8.4 | Idle
Mem: 1.67 GB
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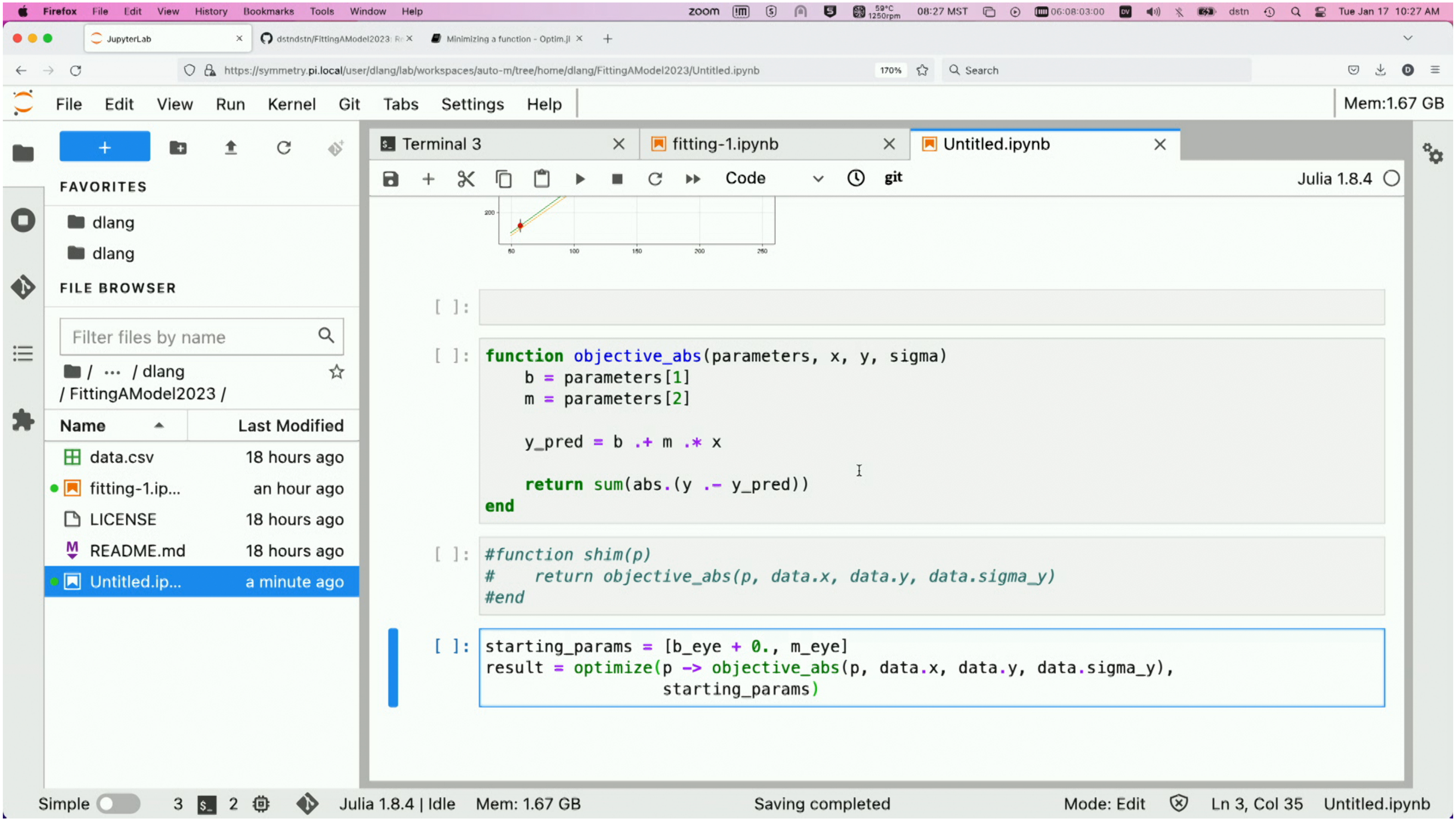
Ln 3, Col 35
Untitled.ipynb



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Terminal 3
fitting-1.ipynb
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Code
git
Julia 1.8.4
FAVORITES
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Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
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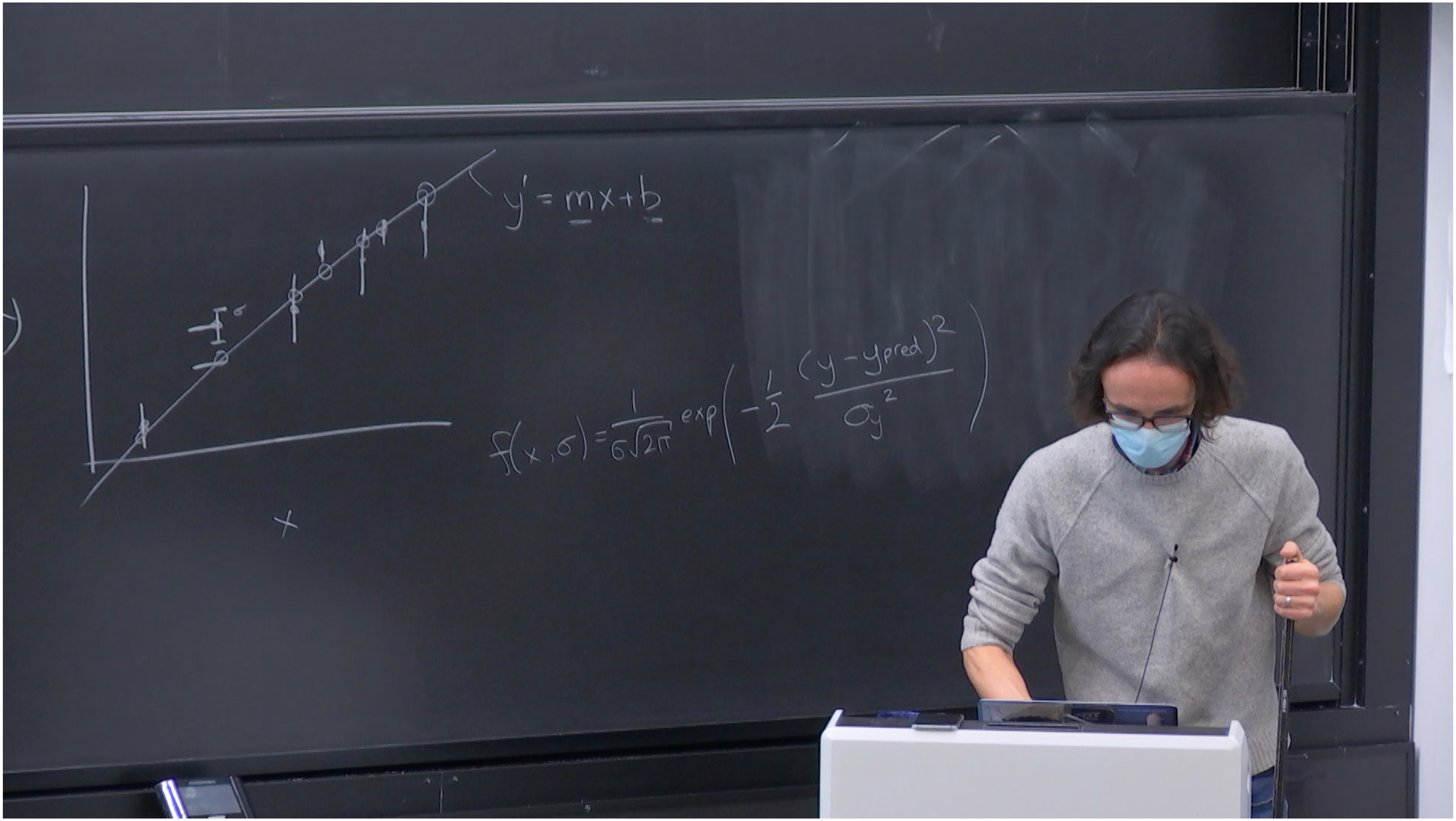
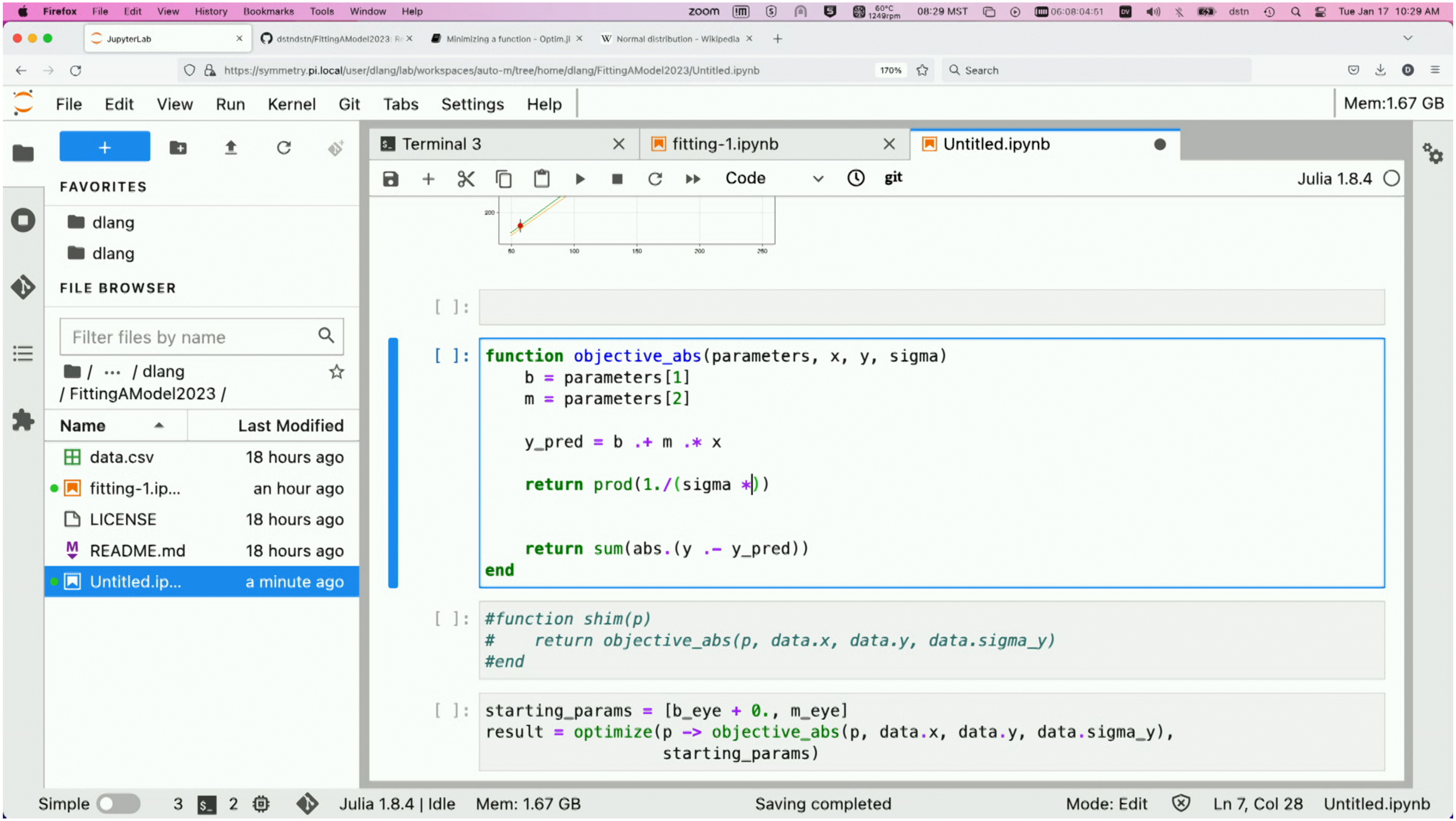
[ ]:
[ ]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return sum(abs.(y .- y_pred))
end
[ ]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[ ]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.67 GB Saving completed Mode: Edit Ln 3, Col 35 Untitled.ipynb


y' = mx + b
f(x, σ) = 1/(σ√2π) exp(−1/2 (y − y_pred)²/σ_y²)
σ
x



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[ ]:
```
function objective_abs(parameters, x, y, sigma)
    b = parameters[1]
    m = parameters[2]

    y_pred = b .+ m .* x

    return prod(1./(sigma *))


    return sum(abs.(y .- y_pred))
end
```
[ ]:
```
#function shim(p)
#    return objective_abs(p, data.x, data.y, data.sigma_y)
#end
```
[ ]:
```
starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
                  starting_params)
```
Julia 1.8.4 | Idle
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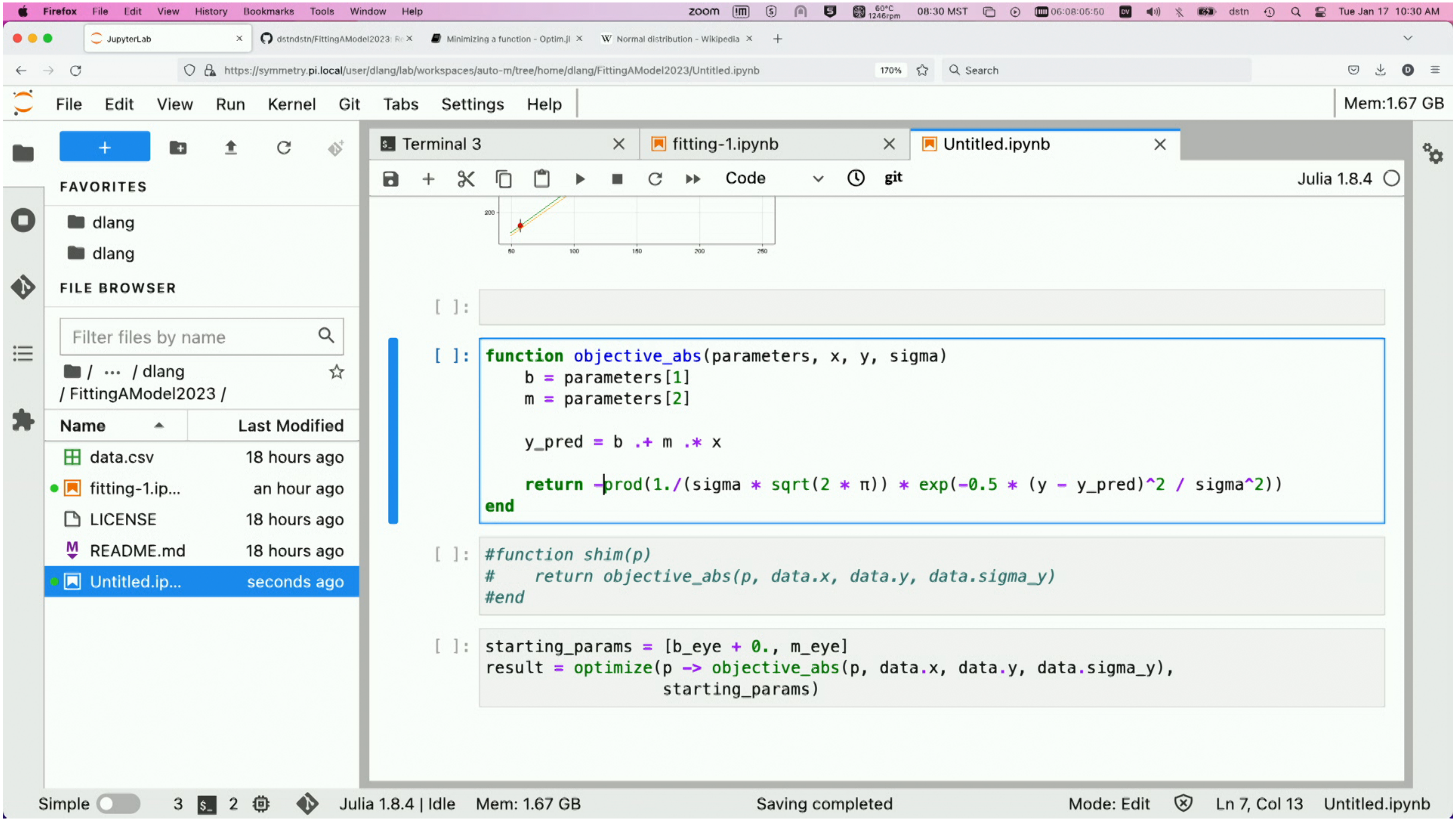
Ln 7, Col 28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Code
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Julia 1.8.4
FAVORITES
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Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
[ ]:
[ ]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return -prod(1./(sigma * sqrt(2 * π)) * exp(-0.5 * (y - y_pred)^2 / sigma^2))
end
[ ]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[ ]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
Simple
Julia 1.8.4 | Idle
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Ln 7, Col 13
Untitled.ipynb

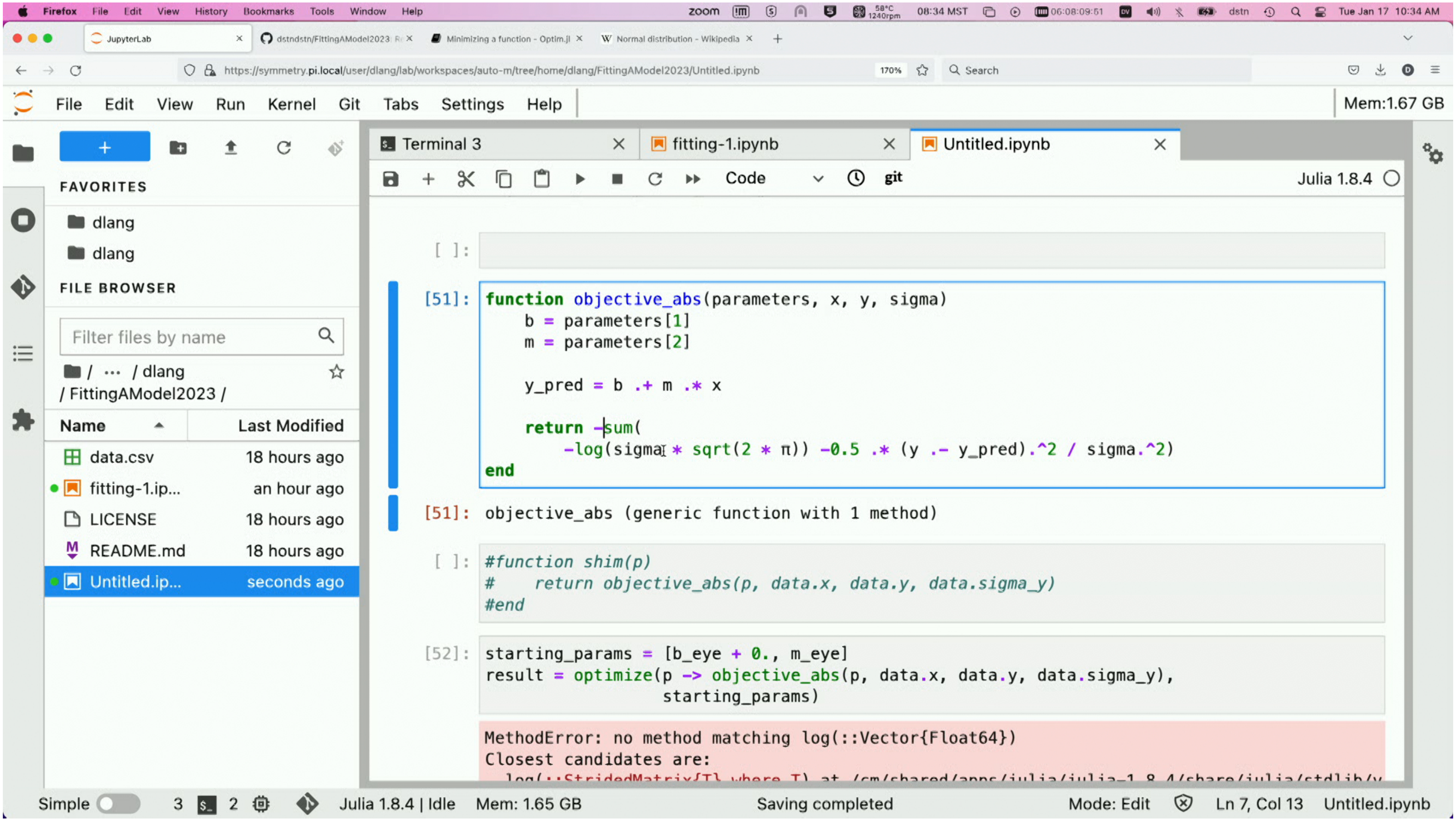
```
[51]: function objective_abs(parameters, x, y, sigma)
          b = parameters[1]
          m = parameters[2]

          y_pred = b .+ m .* x

          return -sum(-log(sigma * sqrt(2 * π)) -0.5 .* (y .- y_pred).^2 / sigma.^2)
      end
```

```
[51]: objective_abs (generic function with 1 method)
```

```
[ ]: #function shim(p)
     #    return objective_abs(p, data.x, data.y, data.sigma_y)
     #end
```

```
[52]: starting_params = [b_eye + 0., m_eye]
      result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
                        starting_params)
```

```
MethodError: no method matching log(::Vector{Float64})
Closest candidates are:
  log(::StridedMatrix{T} where T) at /cm/shared/apps/julia/julia-1.8.4/share/julia/stdlib/v
1.8/LinearAlgebra/src/dense.jl:774
```


File Edit View Run Kernel Git Tabs Settings Help
Mem:1.67 GB
Terminal 3
fitting-1.ipynb
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git
Julia 1.8.4
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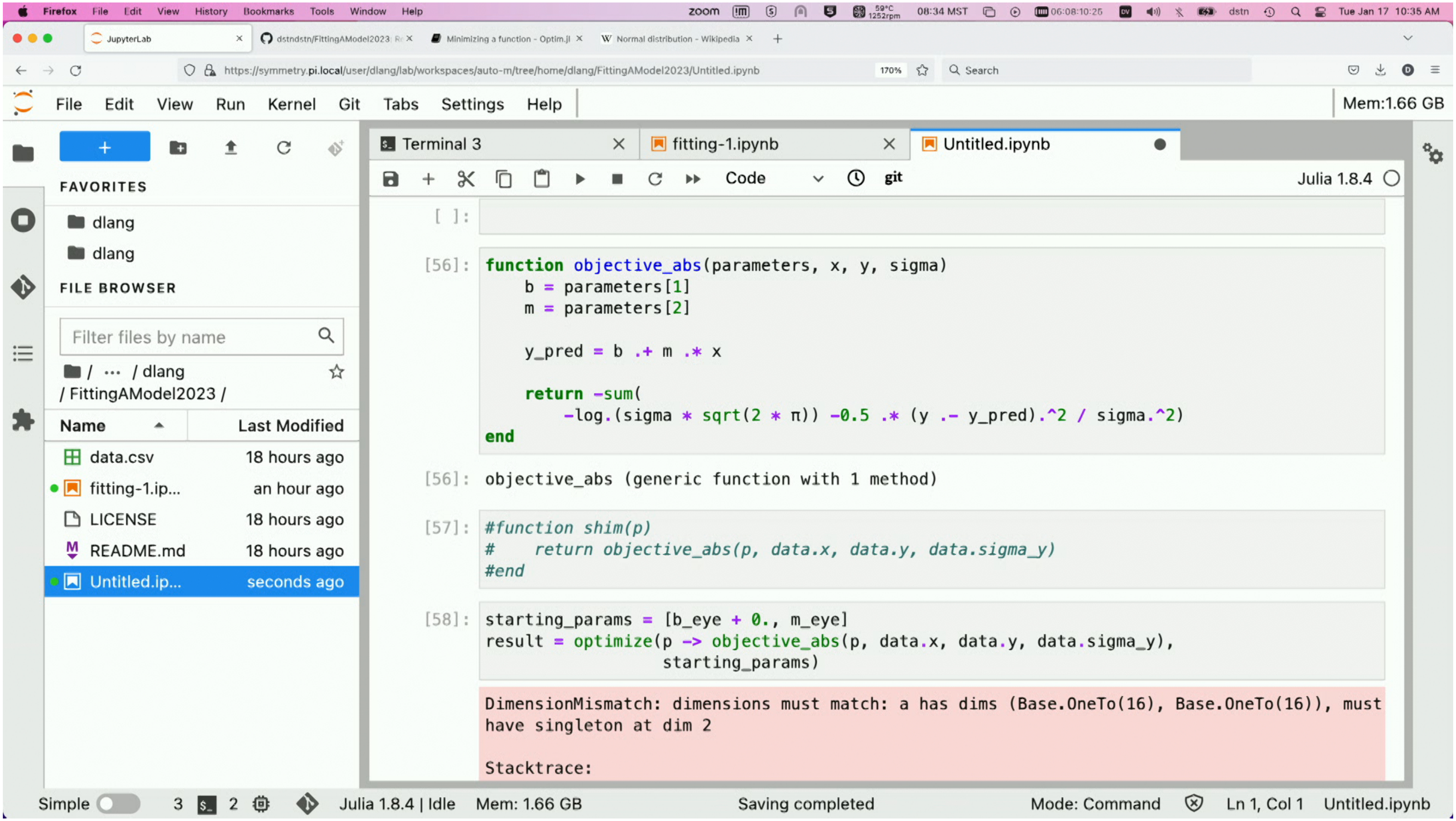
Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
[ ]:
[51]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return -sum(
-log(sigma * sqrt(2 * π)) -0.5 .* (y .- y_pred).^2 / sigma.^2)
end
[51]: objective_abs (generic function with 1 method)
[ ]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[52]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
MethodError: no method matching log(::Vector{Float64})
Closest candidates are:
Simple
Julia 1.8.4 | Idle
Mem: 1.65 GB
Saving completed
Mode: Edit
Ln 7, Col 13
Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
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Julia 1.8.4
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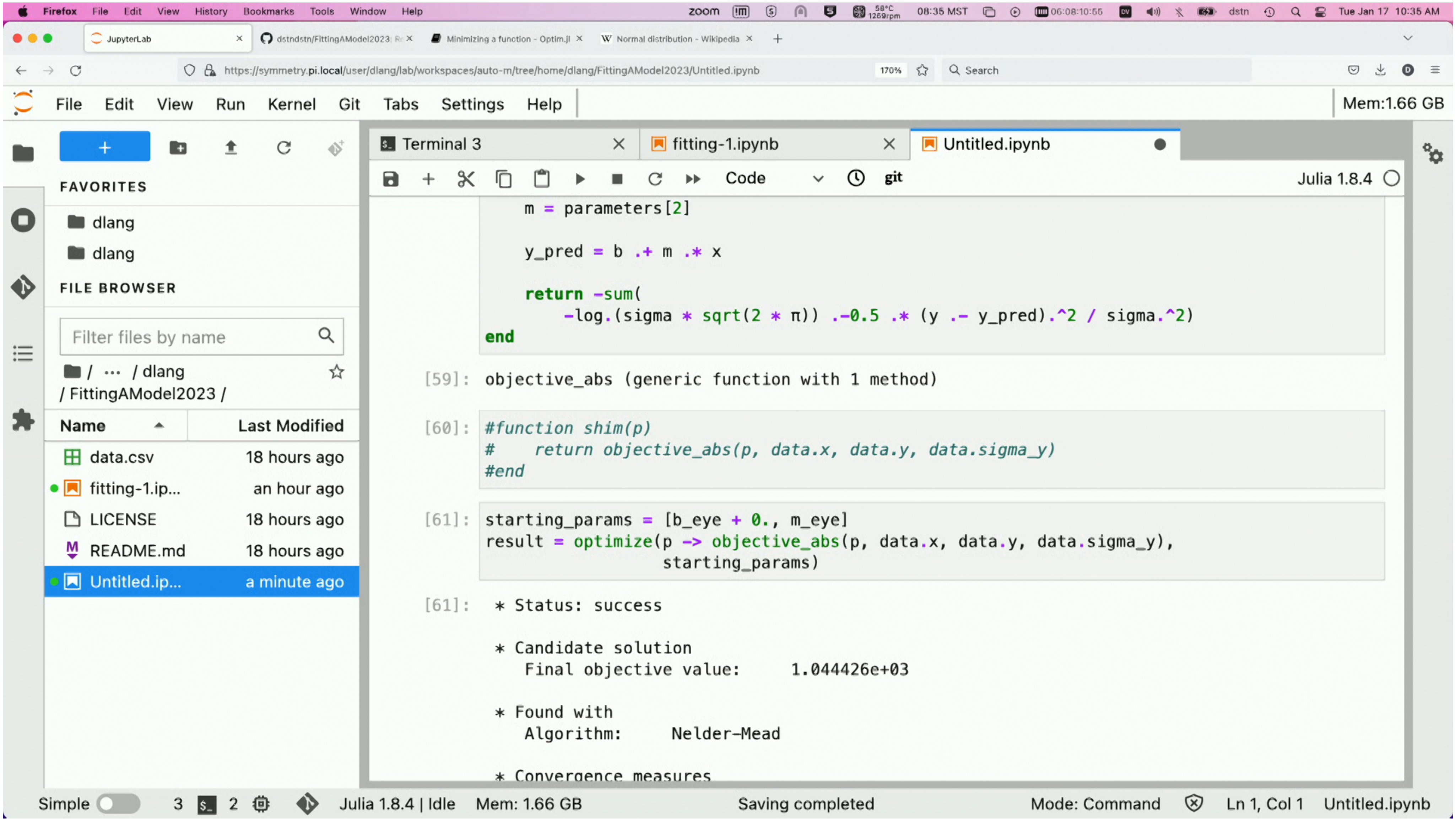
Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... seconds ago
[ ]:
[56]:
function objective_abs(parameters, x, y, sigma)
    b = parameters[1]
    m = parameters[2]
    y_pred = b .+ m .* x
    return -sum(
        -log.(sigma * sqrt(2 * π)) -0.5 .* (y .- y_pred).^2 / sigma.^2)
end
[56]: objective_abs (generic function with 1 method)
[57]:
#function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[58]:
starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
                  starting_params)
DimensionMismatch: dimensions must match: a has dims (Base.OneTo(16), Base.OneTo(16)), must have singleton at dim 2
Stacktrace:
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.66 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Mem:1.66 GB
Terminal 3
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Code
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FAVORITES
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Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... a minute ago
m = parameters[2]
y_pred = b .+ m .* x
return -sum(
-log.(sigma * sqrt(2 * π)) .-0.5 .* (y .- y_pred).^2 / sigma.^2)
end
[59]: objective_abs (generic function with 1 method)
[60]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[61]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
[61]: * Status: success
* Candidate solution
Final objective value: 1.044426e+03
* Found with
Algorithm: Nelder-Mead
* Convergence measures
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.66 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb

Firefox File Edit View History Bookmarks Tools Window Help

JupyterLab | dstndstn/FittingAModel2023 | Minimizing a function - Optim.jl | Normal distribution - Wikipedia

https://symmetry.pi.local/user/dlang/lab/workspaces/auto-m/tree/home/dlang/FittingAModel2023/Untitled.ipynb

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FAVORITES
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- dlang

FILE BROWSER

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Name	Last Modified
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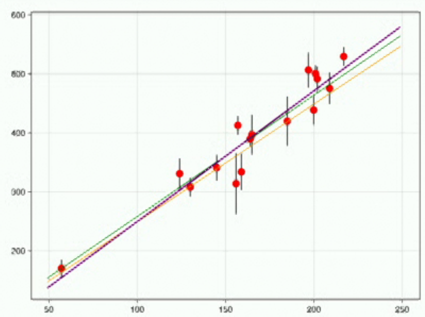
fitting-1.ip...	an hour ago
LICENSE	18 hours ago
README.md	18 hours ago
Untitled.ip...	seconds ago

Terminal 3 | fitting-1.ipynb | Untitled.ipynb

Code | git | Julia 1.8.4

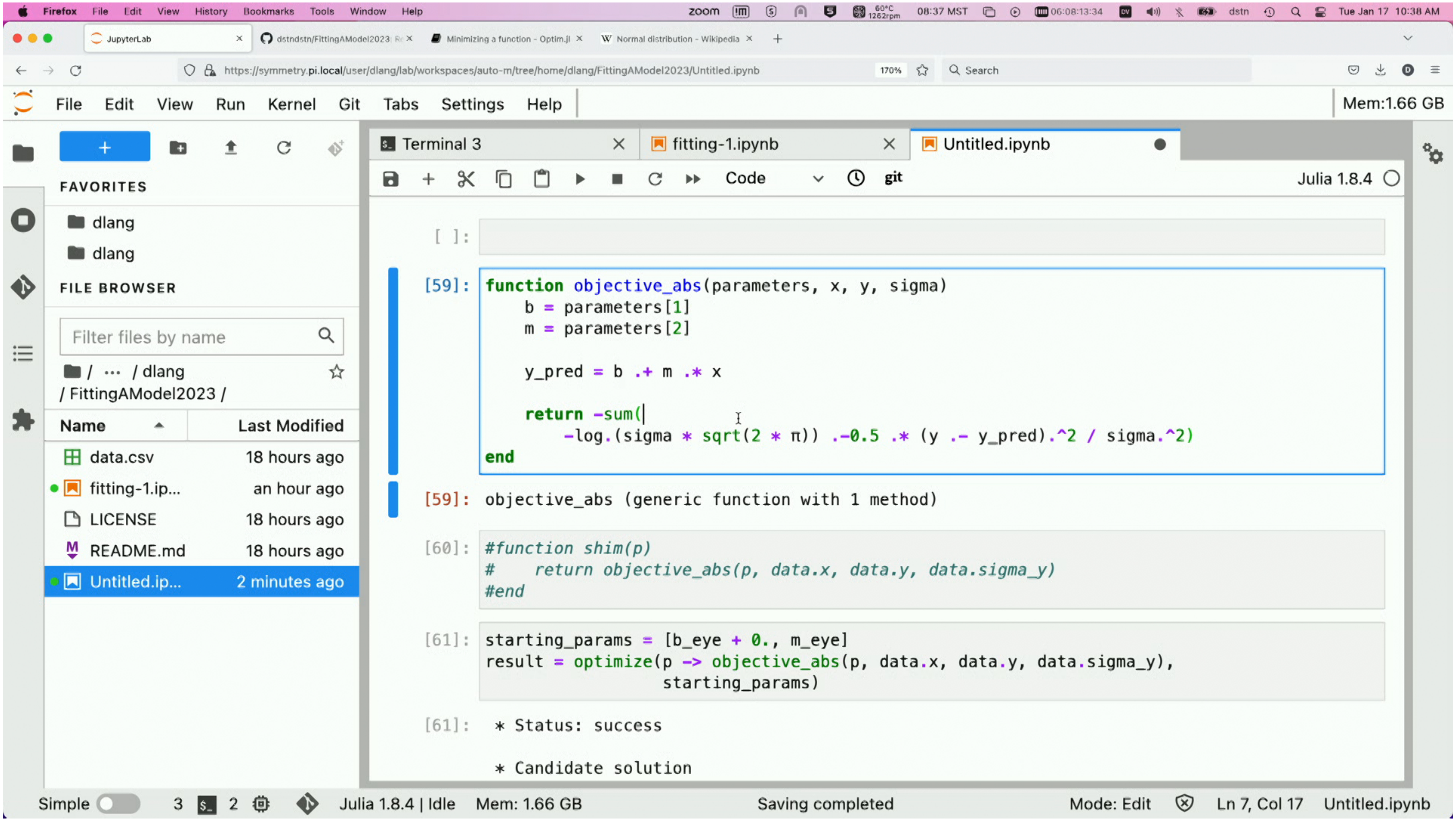
```julia
errorbars!(data.x, data.y, data.sigma_y)
scatter!(data.x, data.y, markersize=20, color=:red)

yy_eye = xx .* m_eye .+ b_eye
lines!(xx, yy_eye, color=:orange)

yy_abs = xx .* m_abs .+ b_abs
lines!(xx, yy_abs, color=:green)

yy_gauss = xx .* m_gauss .+ b_gauss
lines!(xx, yy_gauss, color=:purple, linewidth=3)

f
```

[64]:



[ ]:

Simple 3 2 Julia 1.8.4 | Idle Mem: 1.66 GB Saving completed Mode: Command Ln 1, Col 1 Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Mem:1.66 GB
Terminal 3
fitting-1.ipynb
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Code
git
Julia 1.8.4
FAVORITES
dlang
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FILE BROWSER
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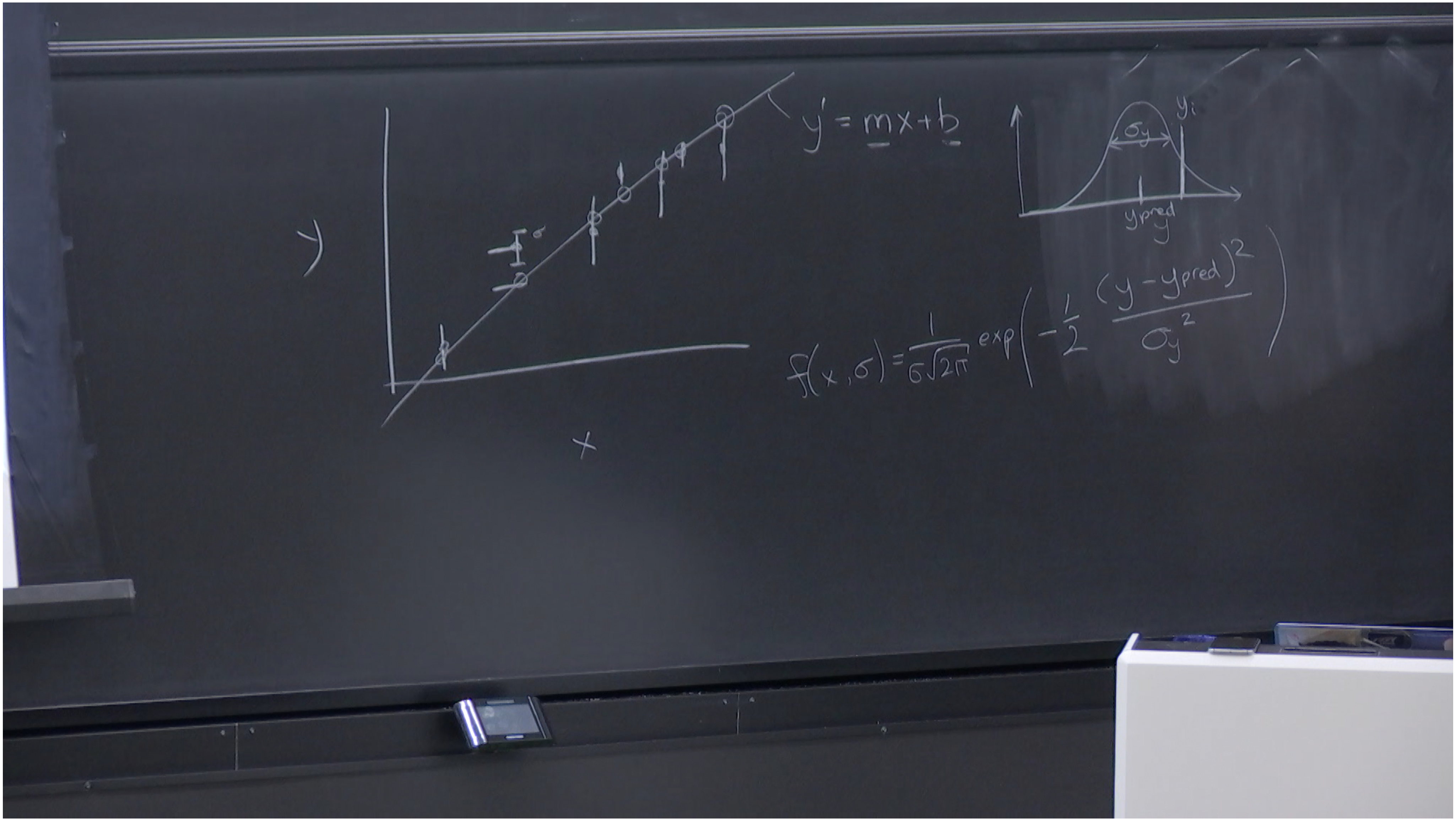
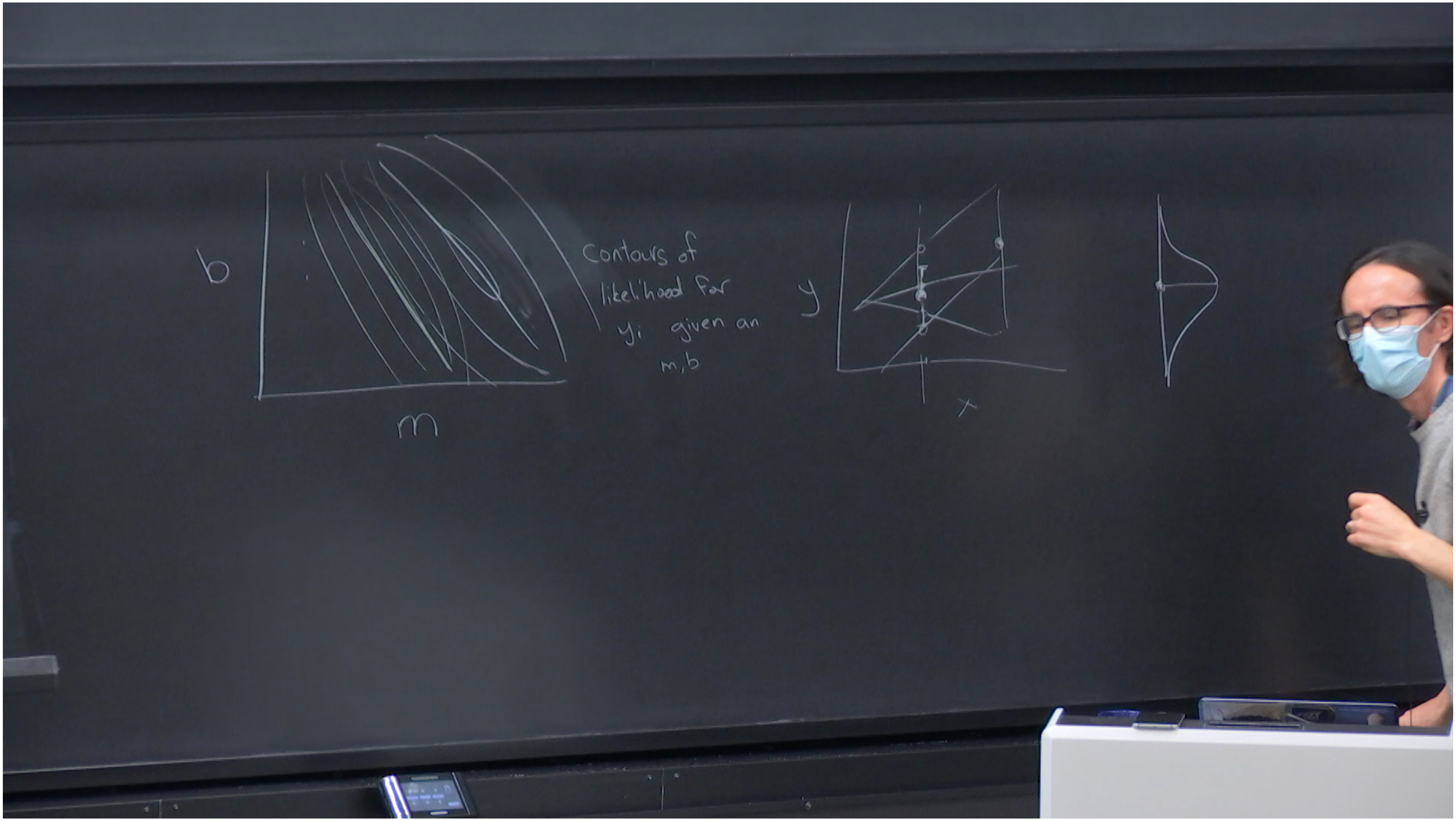
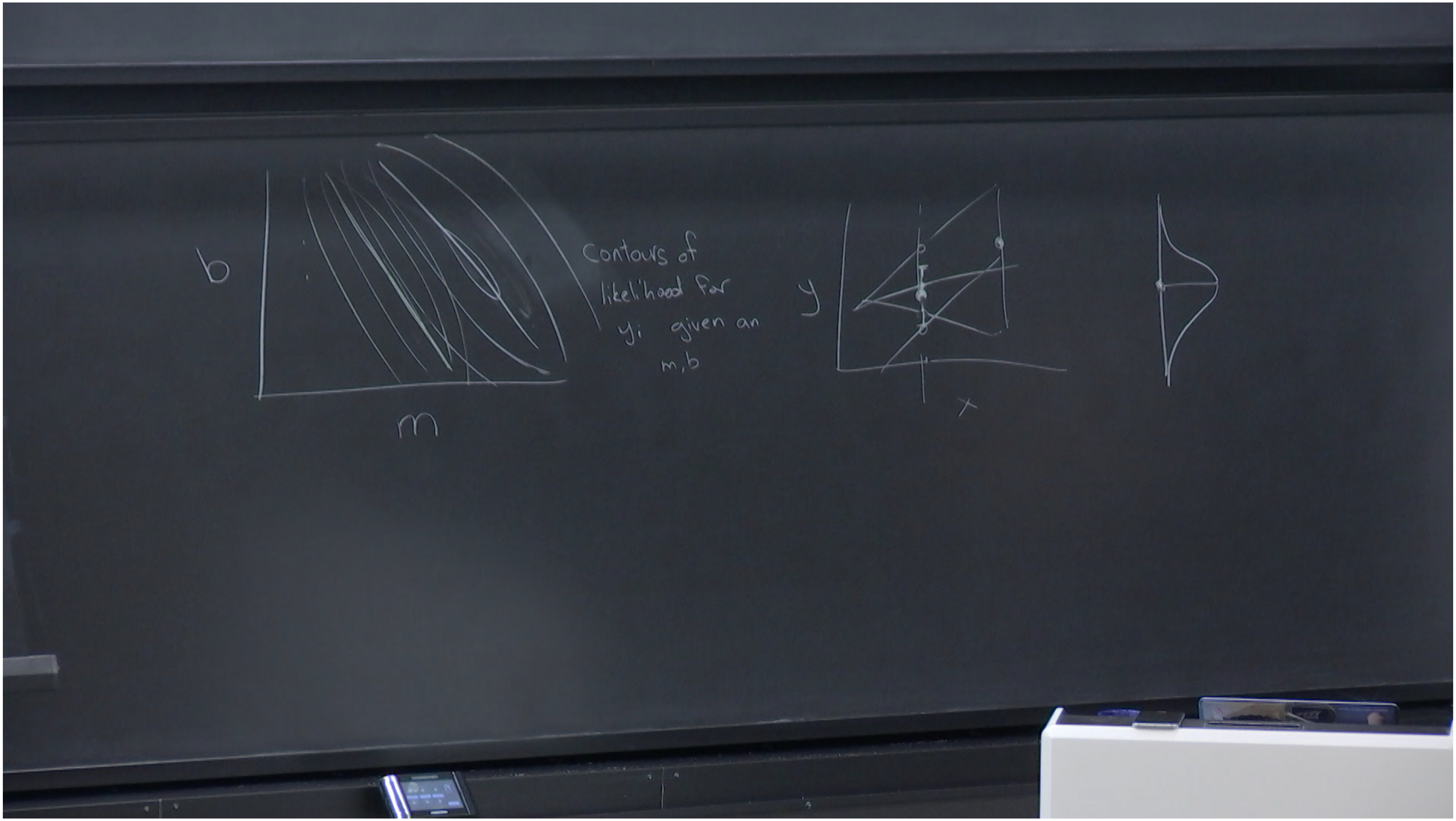
/ ··· / dlang
/ FittingAModel2023 /
Name
Last Modified
data.csv 18 hours ago
fitting-1.ip... an hour ago
LICENSE 18 hours ago
README.md 18 hours ago
Untitled.ip... 2 minutes ago
[ ]:
[59]: function objective_abs(parameters, x, y, sigma)
b = parameters[1]
m = parameters[2]
y_pred = b .+ m .* x
return -sum(
-log.(sigma * sqrt(2 * π)) .-0.5 .* (y .- y_pred).^2 / sigma.^2)
end
[59]: objective_abs (generic function with 1 method)
[60]: #function shim(p)
return objective_abs(p, data.x, data.y, data.sigma_y)
#end
[61]: starting_params = [b_eye + 0., m_eye]
result = optimize(p -> objective_abs(p, data.x, data.y, data.sigma_y),
starting_params)
[61]: * Status: success
* Candidate solution
Simple 3 2 Julia 1.8.4 | Idle Mem: 1.66 GB Saving completed Mode: Edit Ln 7, Col 17 Untitled.ipynb



y
x
σ
$y' = mx + b$
y_i
σ_y
y_{pred}
y
$f(x,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(y - y_{pred})^2}{\sigma_y^2}\right)$


b
m
Contours of
likelihood for
yi given an
m,b
y
x


b
m
Contours of
likelihood for
yi given an
m,b
y
x