Title: Lecture - Numerical Methods, PHYS 777

Speakers: Erik Schnetter, Dustin Lang

Collection/Series: Numerical Methods (Core), PHYS 777-, January 6 - February 5, 2025

Subject: Other

Date: January 14, 2025 - 11:30 AM

URL: https://pirsa.org/25010056

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Preview Code Blame 80 lines (80 loc) · 1.53 KB Raw

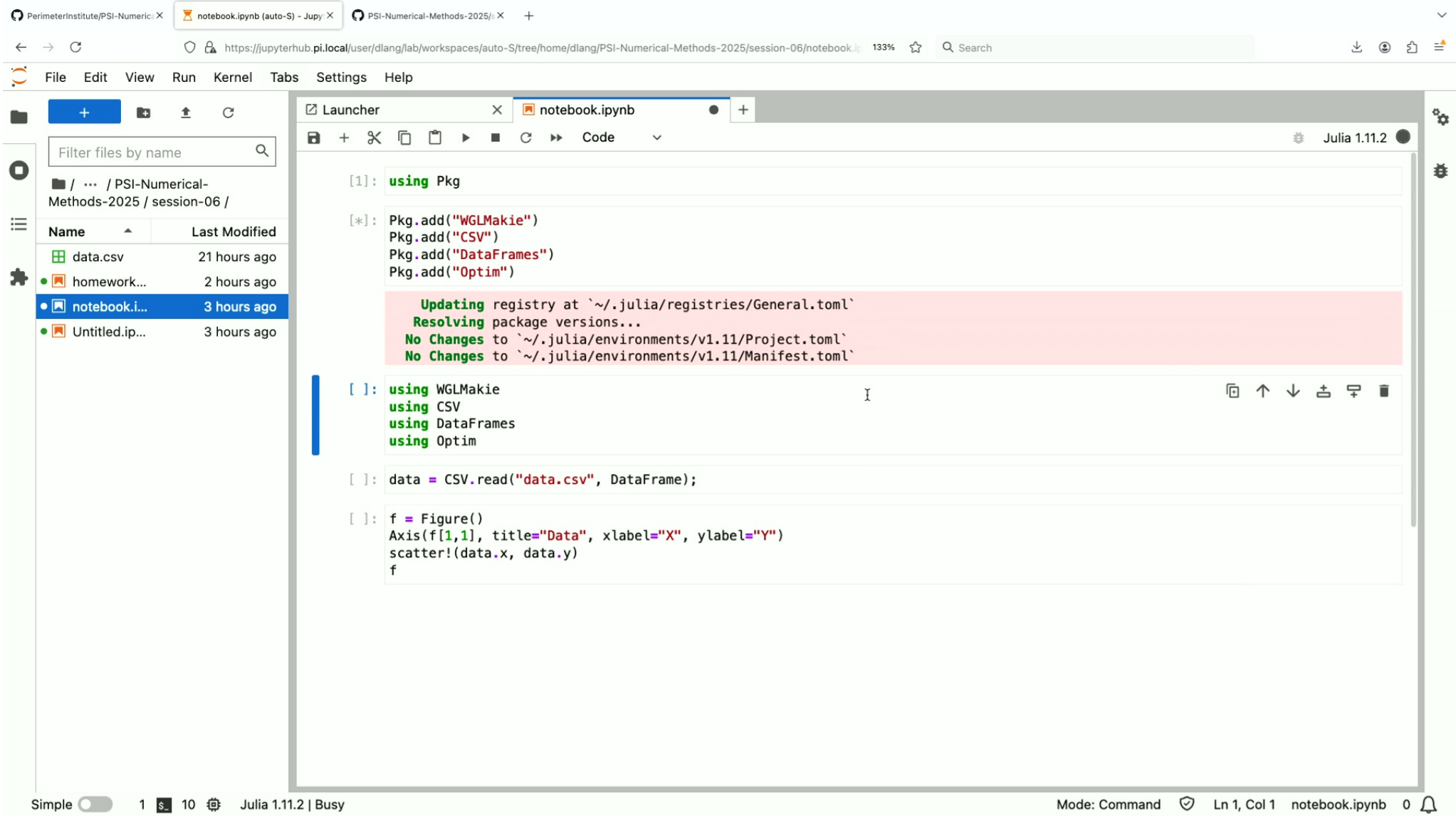
In [ ]:
```
using Pkg
```

In [ ]:
```
Pkg.add("WGLMakie")
Pkg.add("CSV")
Pkg.add("DataFrames")
Pkg.add("Optim")
```

In [ ]:
```
using WGLMakie
using CSV
using DataFrames
using Optim
```

In [ ]:
```
data = CSV.read("data.csv", DataFrame);
```

In [ ]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
f
```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Code
Julia 1.11.2
[1]: using Pkg
[*]: Pkg.add("WGLMakie")
Pkg.add("CSV")
Pkg.add("DataFrames")
Pkg.add("Optim")
Updating registry at `~/.julia/registries/General.toml`
Resolving package versions...
No Changes to `~/.julia/environments/v1.11/Project.toml`
No Changes to `~/.julia/environments/v1.11/Manifest.toml`
[ ]: using WGLMakie
using CSV
using DataFrames
using Optim
[ ]: data = CSV.read("data.csv", DataFrame);
[ ]: f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
f
Simple
1
10
Julia 1.11.2 | Busy
Mode: Command
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notebook.ipynb
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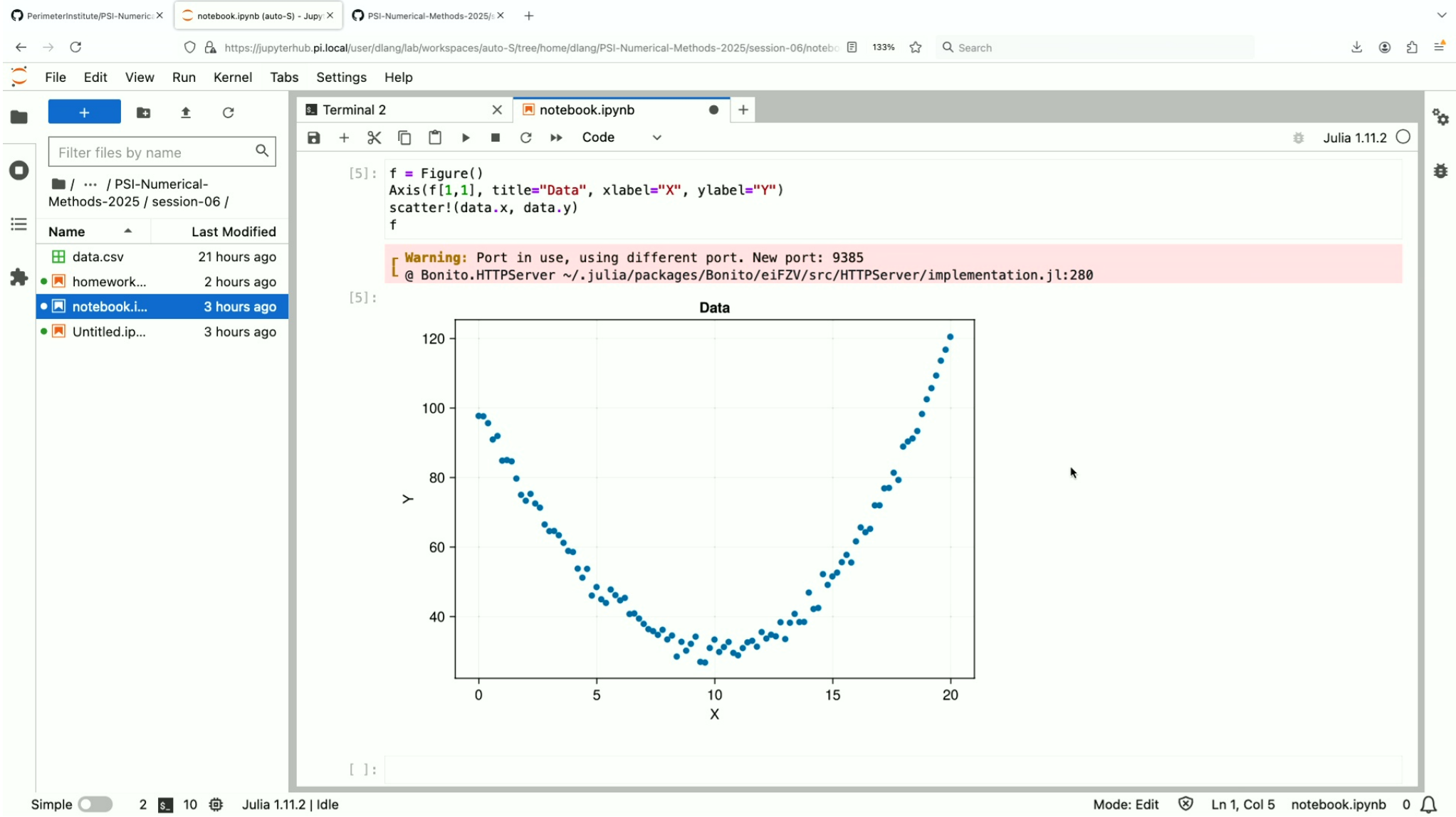
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Terminal 2
notebook.ipynb
Code
Julia 1.11.2
[5]:
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
f
Warning: Port in use, using different port. New port: 9385
@ Bonito.HTTPServer ~/.julia/packages/Bonito/eiFZV/src/HTTPServer/implementation.jl:280
[5]:
Data
120
100
80
60
40
Y
0
5
10
15
20
X
[ ]:
Simple
2
10
Julia 1.11.2 | Idle
Mode: Edit
Ln 1, Col 5
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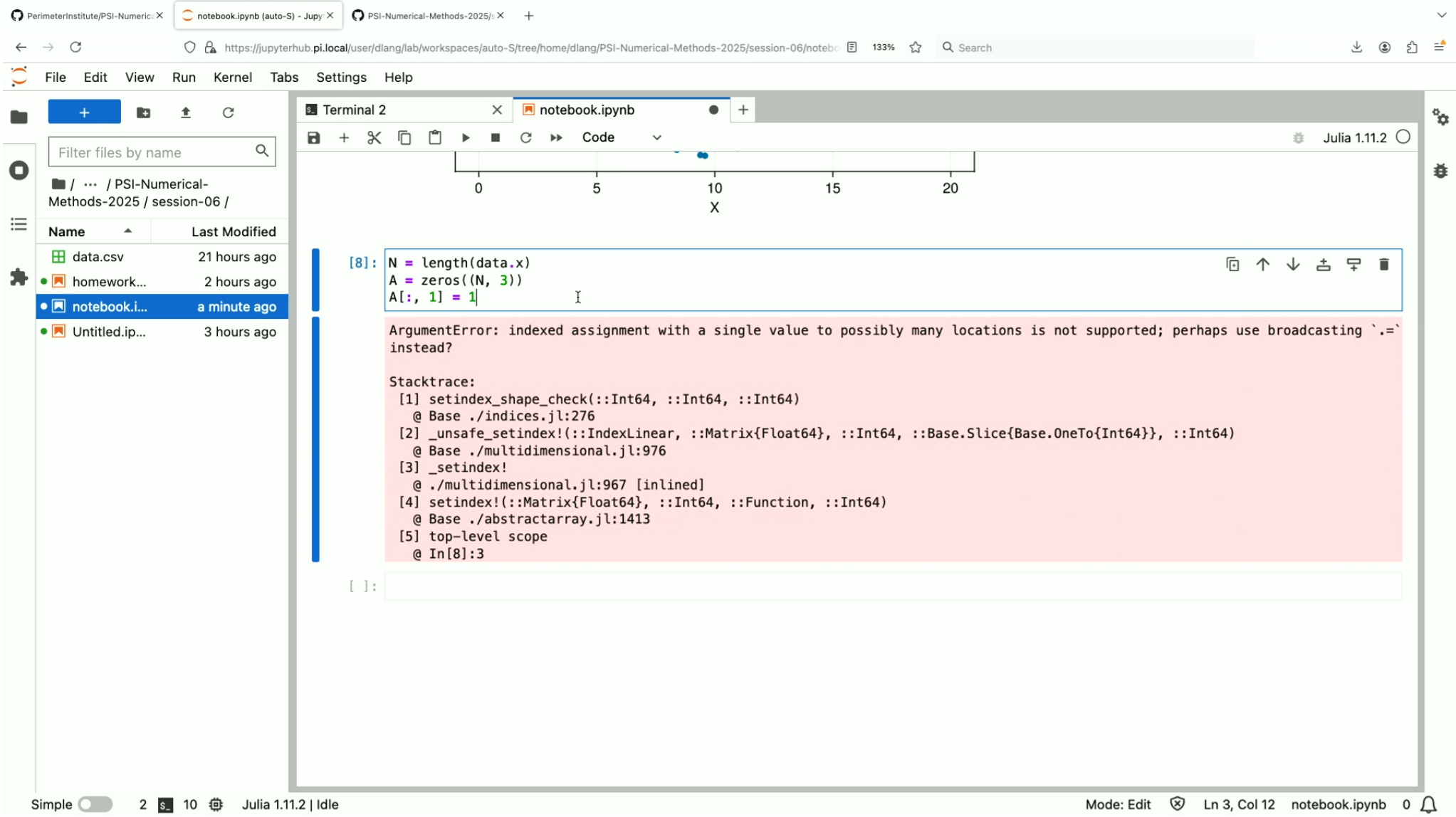
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Code
Julia 1.11.2
0 5 10 15 20
X
[8]:
N = length(data.x)
A = zeros((N, 3))
A[:, 1] = 1
ArgumentError: indexed assignment with a single value to possibly many locations is not supported; perhaps use broadcasting `.=` instead?
Stacktrace:
[1] setindex_shape_check(::Int64, ::Int64, ::Int64)
@ Base ./indices.jl:276
[2] _unsafe_setindex!(::IndexLinear, ::Matrix{Float64}, ::Int64, ::Base.Slice{Base.OneTo{Int64}}, ::Int64)
@ Base ./multidimensional.jl:976
[3] _setindex!
@ ./multidimensional.jl:967 [inlined]
[4] setindex!(::Matrix{Float64}, ::Int64, ::Function, ::Int64)
@ Base ./abstractarray.jl:1413
[5] top-level scope
@ In[8]:3
[ ]:
Simple
2 10
Julia 1.11.2 | Idle
Mode: Edit
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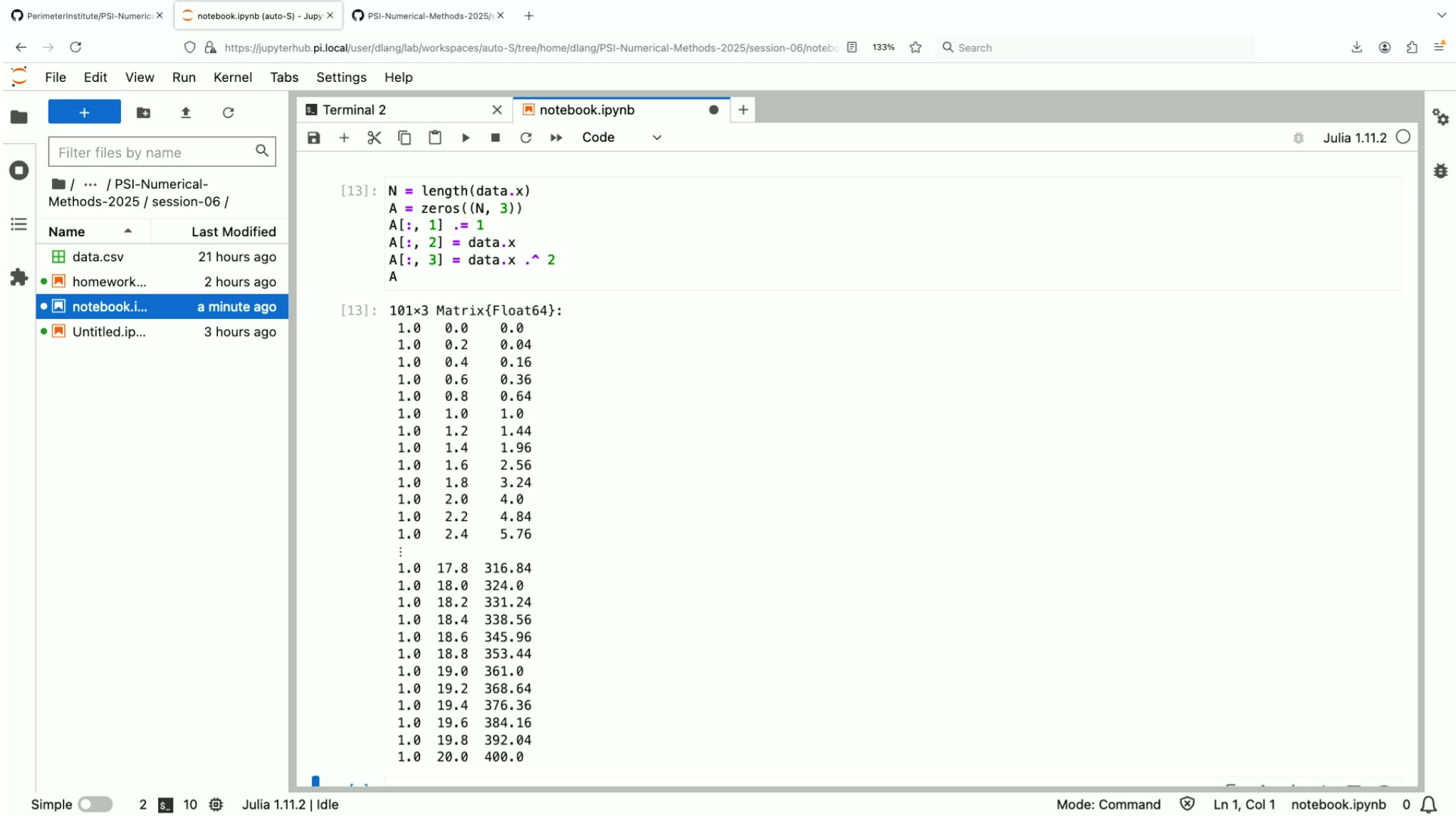
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Code
Julia 1.11.2
[13]:
N = length(data.x)
A = zeros((N, 3))
A[:, 1] .= 1
A[:, 2] = data.x
A[:, 3] = data.x .^ 2
A
[13]:
101×3 Matrix{Float64}:
1.0 0.0 0.0
1.0 0.2 0.04
1.0 0.4 0.16
1.0 0.6 0.36
1.0 0.8 0.64
1.0 1.0 1.0
1.0 1.2 1.44
1.0 1.4 1.96
1.0 1.6 2.56
1.0 1.8 3.24
1.0 2.0 4.0
1.0 2.2 4.84
1.0 2.4 5.76
1.0 17.8 316.84
1.0 18.0 324.0
1.0 18.2 331.24
1.0 18.4 338.56
1.0 18.6 345.96
1.0 18.8 353.44
1.0 19.0 361.0
1.0 19.2 368.64
1.0 19.4 376.36
1.0 19.6 384.16
1.0 19.8 392.04
1.0 20.0 400.0
Simple
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Julia 1.11.2 | Idle
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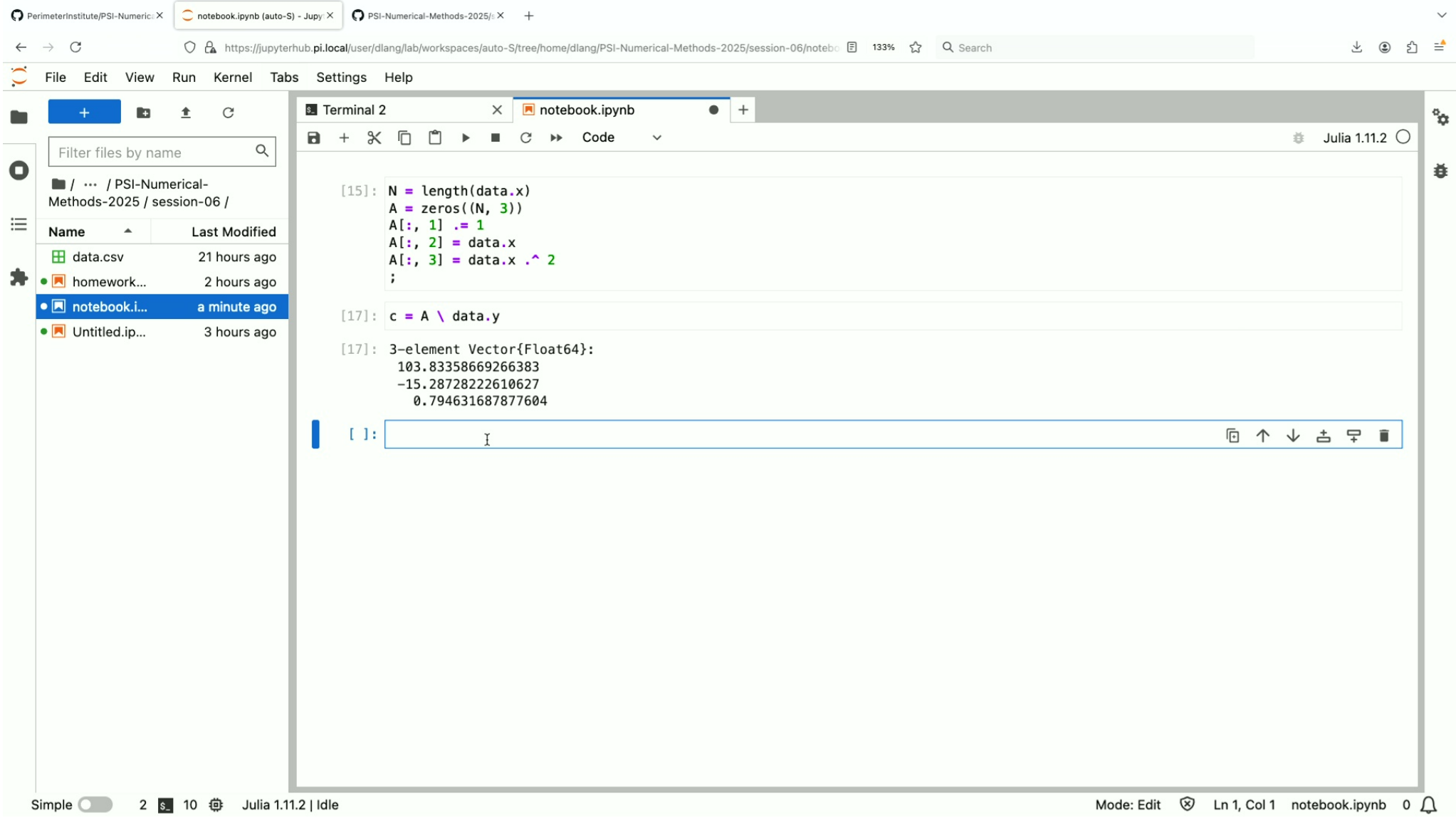
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Code
Julia 1.11.2
[15]:
N = length(data.x)
A = zeros((N, 3))
A[:, 1] .= 1
A[:, 2] = data.x
A[:, 3] = data.x .^ 2
;
[17]:
c = A \ data.y
[17]:
3-element Vector{Float64}:
103.83358669266383
-15.28728222610627
0.794631687877604
[ ]:
Simple
2
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Julia 1.11.2 | Idle
Mode: Edit
Ln 1, Col 1
notebook.ipynb
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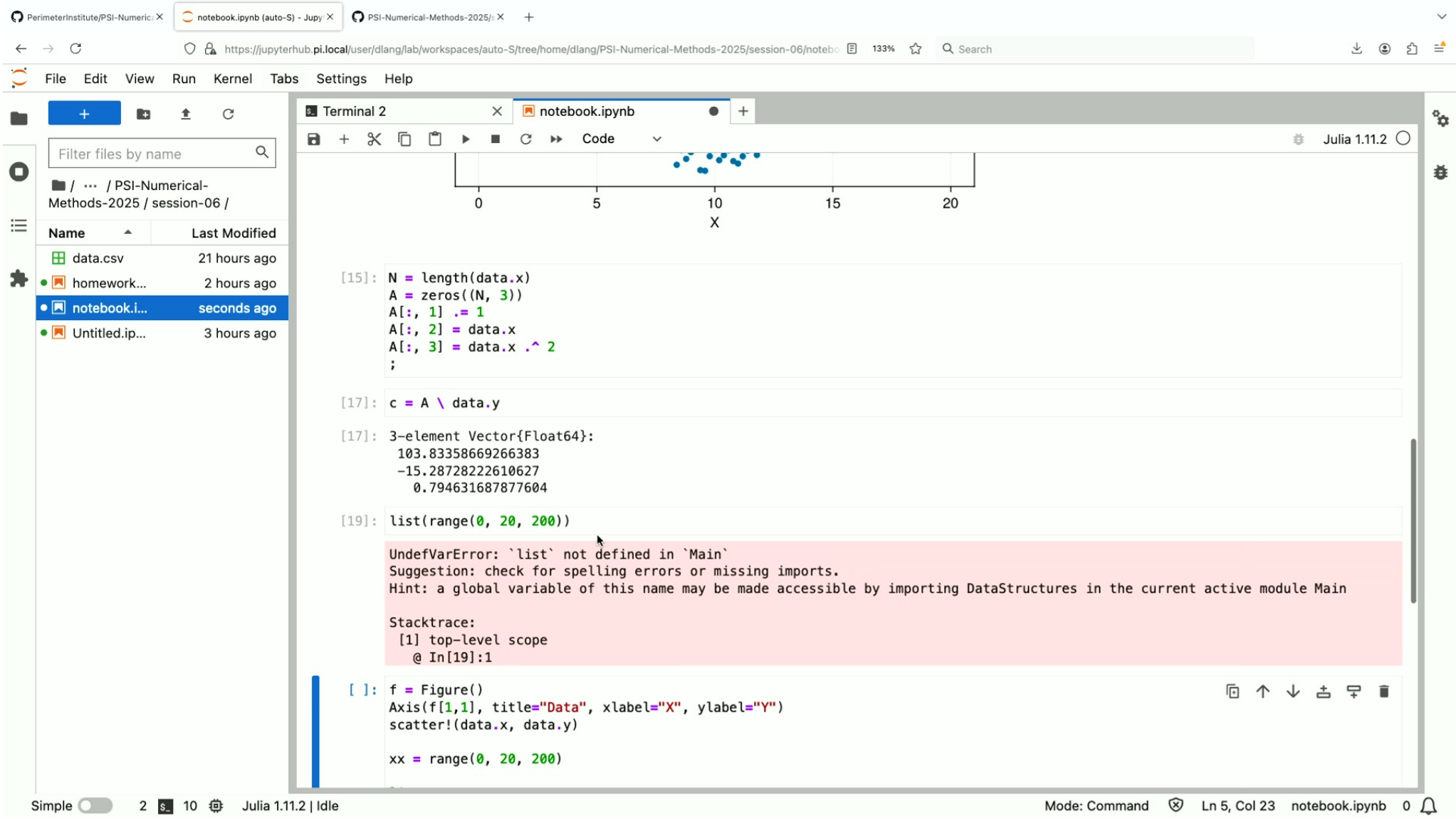
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Code
Julia 1.11.2
0 5 10 15 20
X
[15]:
N = length(data.x)
A = zeros((N, 3))
A[:, 1] .= 1
A[:, 2] = data.x
A[:, 3] = data.x .^ 2
;
[17]:
c = A \ data.y
[17]:
3-element Vector{Float64}:
103.83358669266383
-15.28728222610627
0.794631687877604
[19]:
list(range(0, 20, 200))
UndefVarError: `list` not defined in `Main`
Suggestion: check for spelling errors or missing imports.
Hint: a global variable of this name may be made accessible by importing DataStructures in the current active module Main
Stacktrace:
[1] top-level scope
@ In[19]:1
[ ]:
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
xx = range(0, 20, 200)
Simple
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Julia 1.11.2 | Idle
Mode: Command
Ln 5, Col 23
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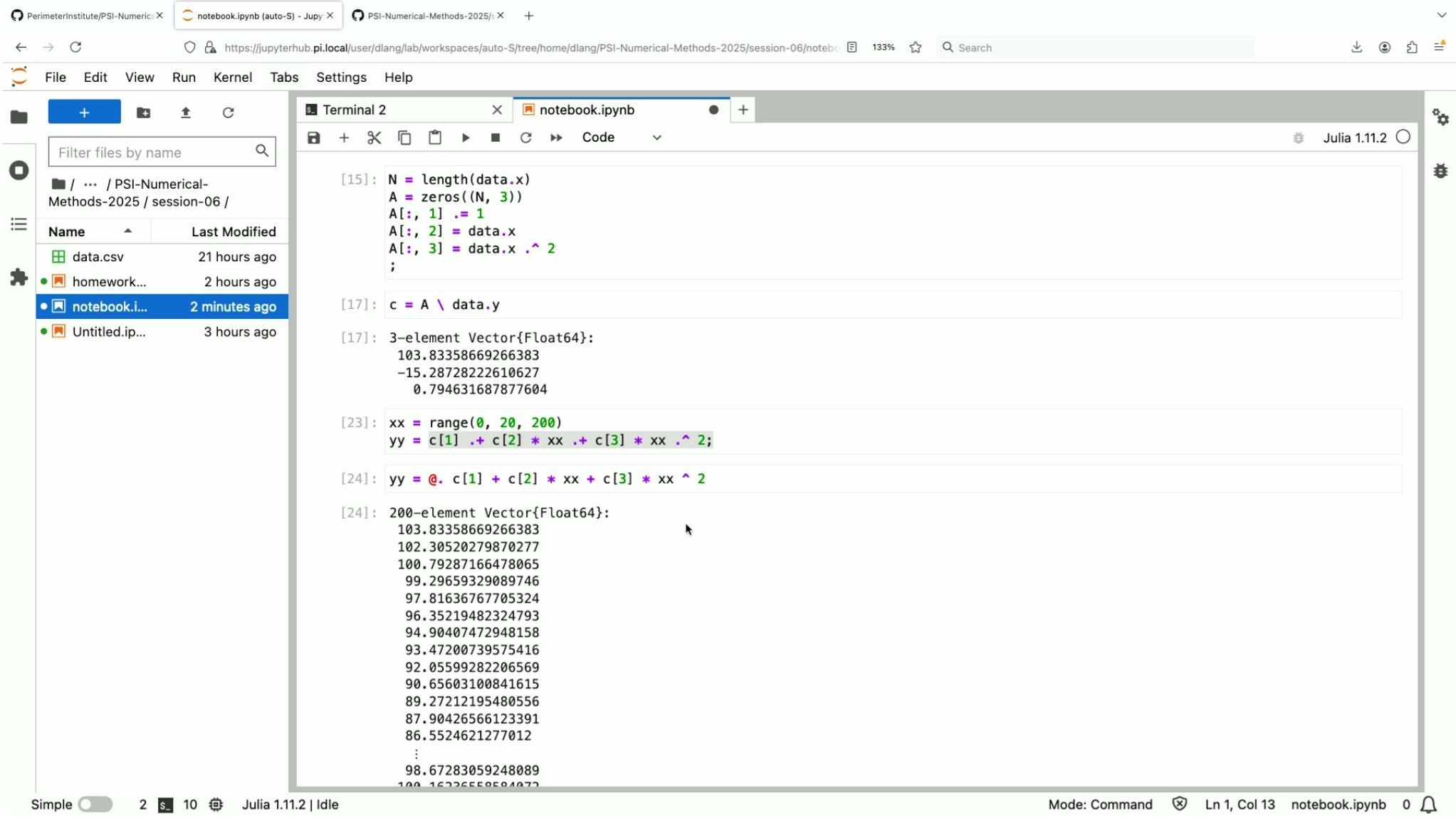
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notebook.ipynb
Code
Julia 1.11.2
[15]:
N = length(data.x)
A = zeros((N, 3))
A[:, 1] .= 1
A[:, 2] = data.x
A[:, 3] = data.x .^ 2
;
[17]:
c = A \ data.y
[17]:
3-element Vector{Float64}:
103.83358669266383
-15.28728222610627
0.794631687877604
[23]:
xx = range(0, 20, 200)
yy = c[1] .+ c[2] * xx .+ c[3] * xx .^ 2;
[24]:
yy = @. c[1] + c[2] * xx + c[3] * xx ^ 2
[24]:
200-element Vector{Float64}:
103.83358669266383
102.30520279870277
100.79287166478065
99.29659329089746
97.81636767705324
96.35219482324793
94.90407472948158
93.47200739575416
92.05599282206569
90.65603100841615
89.27212195480556
87.90426566123391
86.5524621277012
98.67283059248089
Simple
2
10
Julia 1.11.2 | Idle
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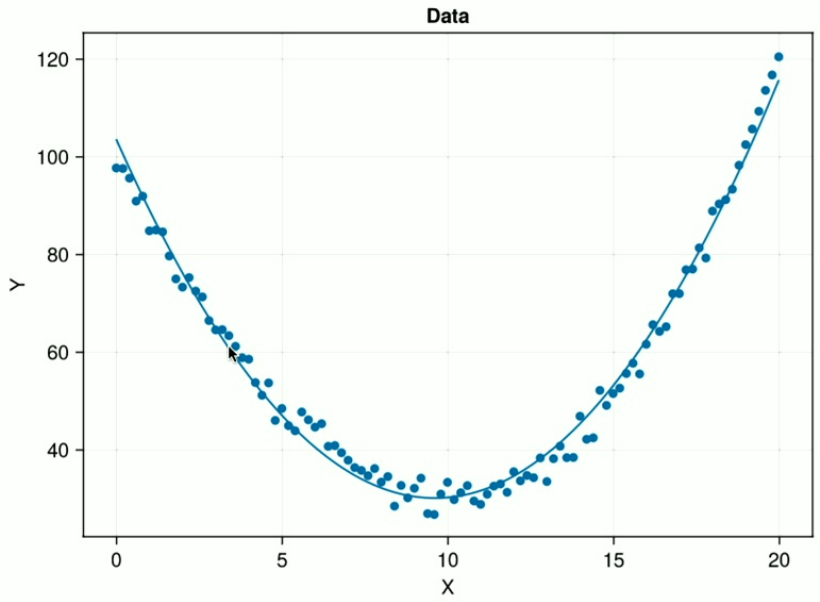
Terminal 2 | notebook.ipynb

Code Julia 1.11.2

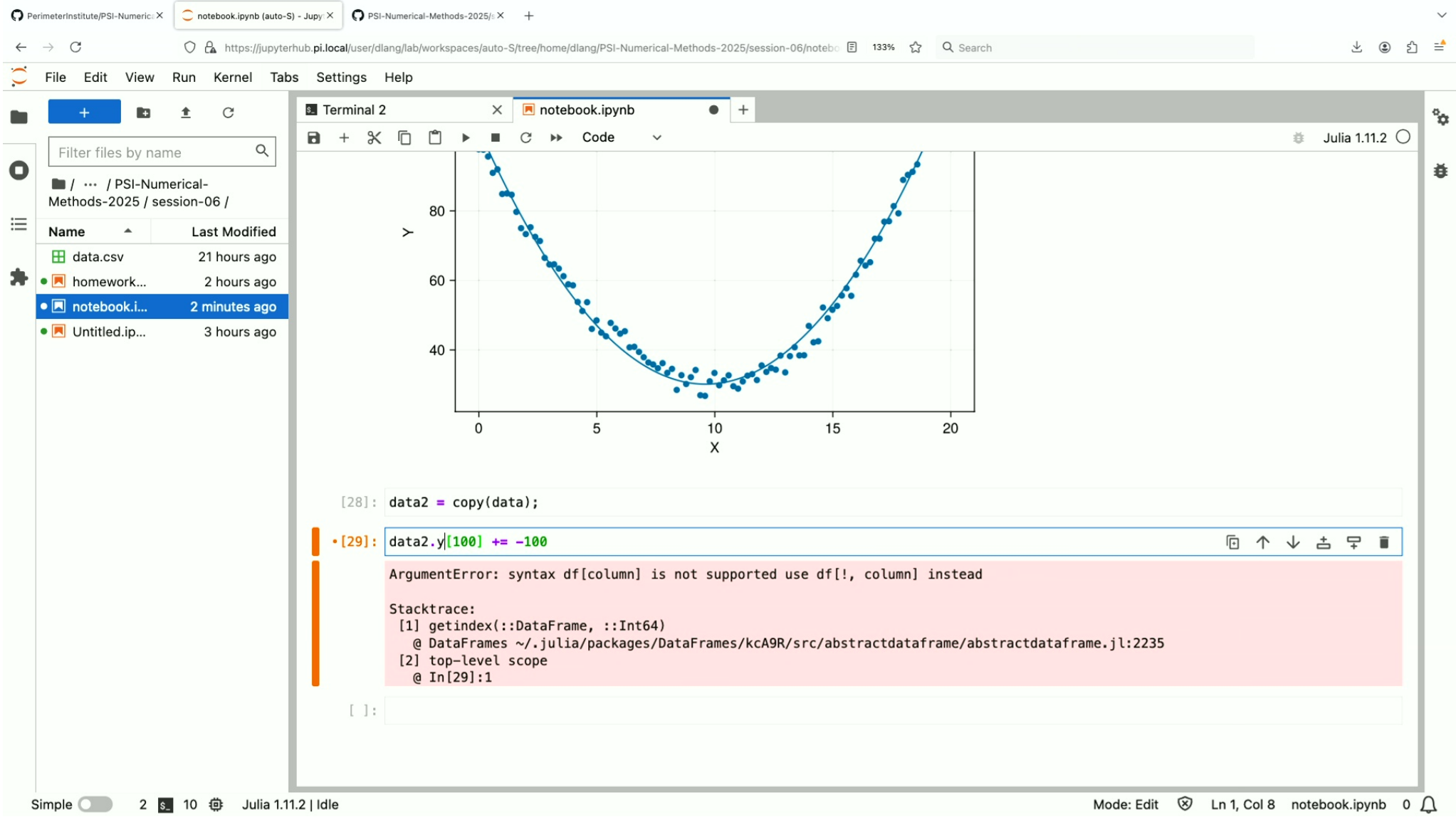
[25]:
```
yy = @. c[1] + c[2] * xx + c[3] * xx ^ 2;
```

[26]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
lines!(xx, yy)
f
```

[26]:



Simple 2 10 Julia 1.11.2 | Idle Mode: Edit Ln 3, Col 25 notebook.ipynb 0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Code
Julia 1.11.2
80
60
40
Y
0
5
10
15
20
X
[28]: data2 = copy(data);
[29]: data2.y[100] += -100
ArgumentError: syntax df[column] is not supported use df[!, column] instead
Stacktrace:
[1] getindex(::DataFrame, ::Int64)
@ DataFrames ~/.julia/packages/DataFrames/kcA9R/src/abstractdataframe/abstractdataframe.jl:2235
[2] top-level scope
@ In[29]:1
[ ]:
Simple
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Julia 1.11.2 | Idle
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Terminal 2 | notebook.ipynb

Code | Julia 1.11.2

[15]:
```
N = length(data.x)
A = zeros((N, 3))
A[:, 1] .= 1
A[:, 2] = data.x
A[:, 3] = data.x .^ 2
;
```

[17]:
```
c = A \ data.y
```

[17]:
```
3-element Vector{Float64}:
 103.83358669266383
 -15.28728222610627
   0.794631687877604
```

[23]:
```
xx = range(0, 20, 200)
yy = c[1] .+ c[2] * xx .+ c[3] * xx .^ 2;
```

[25]:
```
yy = @. c[1] + c[2] * xx + c[3] * xx ^ 2;
```

[26]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data.x, data.y)
lines!(xx, yy)
f
```

[26]:

Simple | 2 | 10 | Julia 1.11.2 | Idle | Mode: Edit | Ln 6, Col 2 | notebook.ipynb | 0

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Terminal 2 | notebook.ipynb

Code | Julia 1.11.2

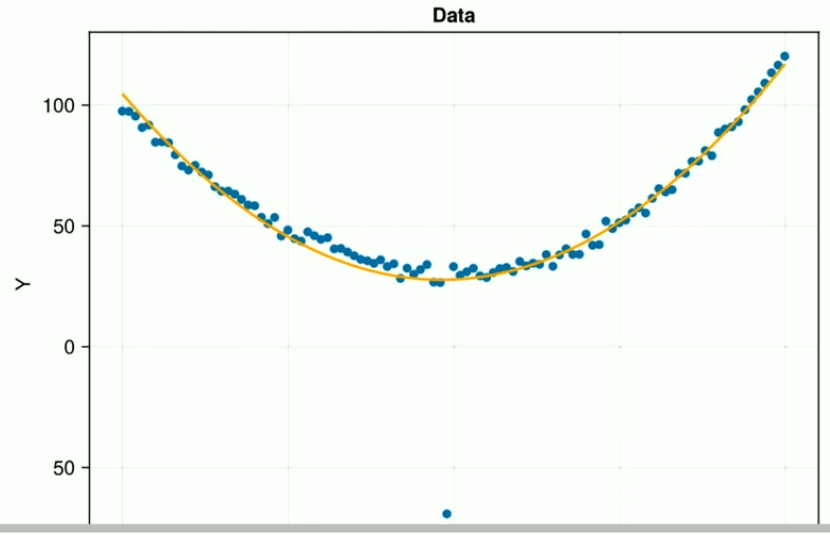
```
c2 = A \ data2.y
```

[35]:
```
3-element Vector{Float64}:
 105.18557226243723
 -16.00882953789056
   0.8310002590579658
```

[38]:
```
yy2 = @. c2[1] + c2[2] * xx + c2[3] * xx^2;
```

[40]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data2.x, data2.y)
lines!(xx, yy2, color=:orange, linewidth=2)
f
```

[40]:



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Code | Julia 1.11.2

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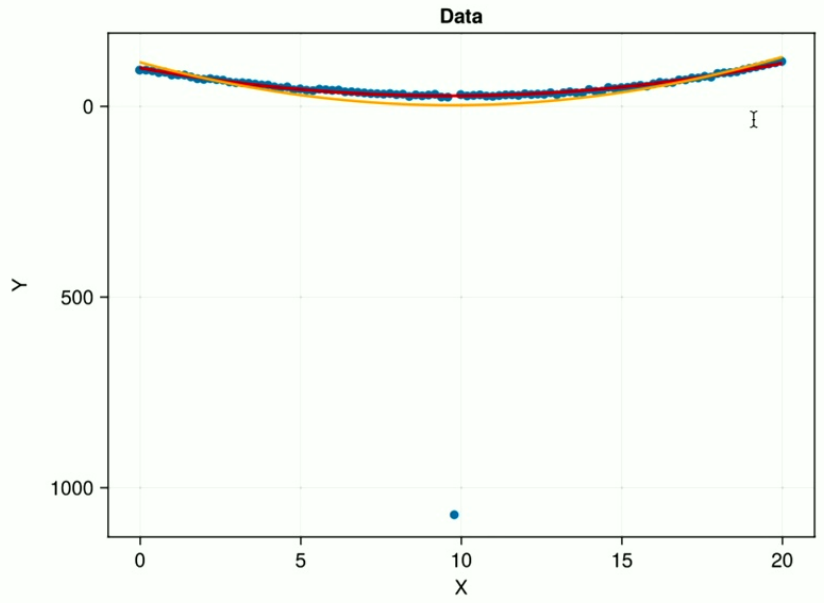
[43]:
```
data2.y[50]
```

[43]:
```
-68.8731211285464
```

[47]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y")
scatter!(data2.x, data2.y)
lines!(xx, yy, color=:red, linewidth=2)
lines!(xx, yy2, color=:orange, linewidth=2)
f
```

[47]:



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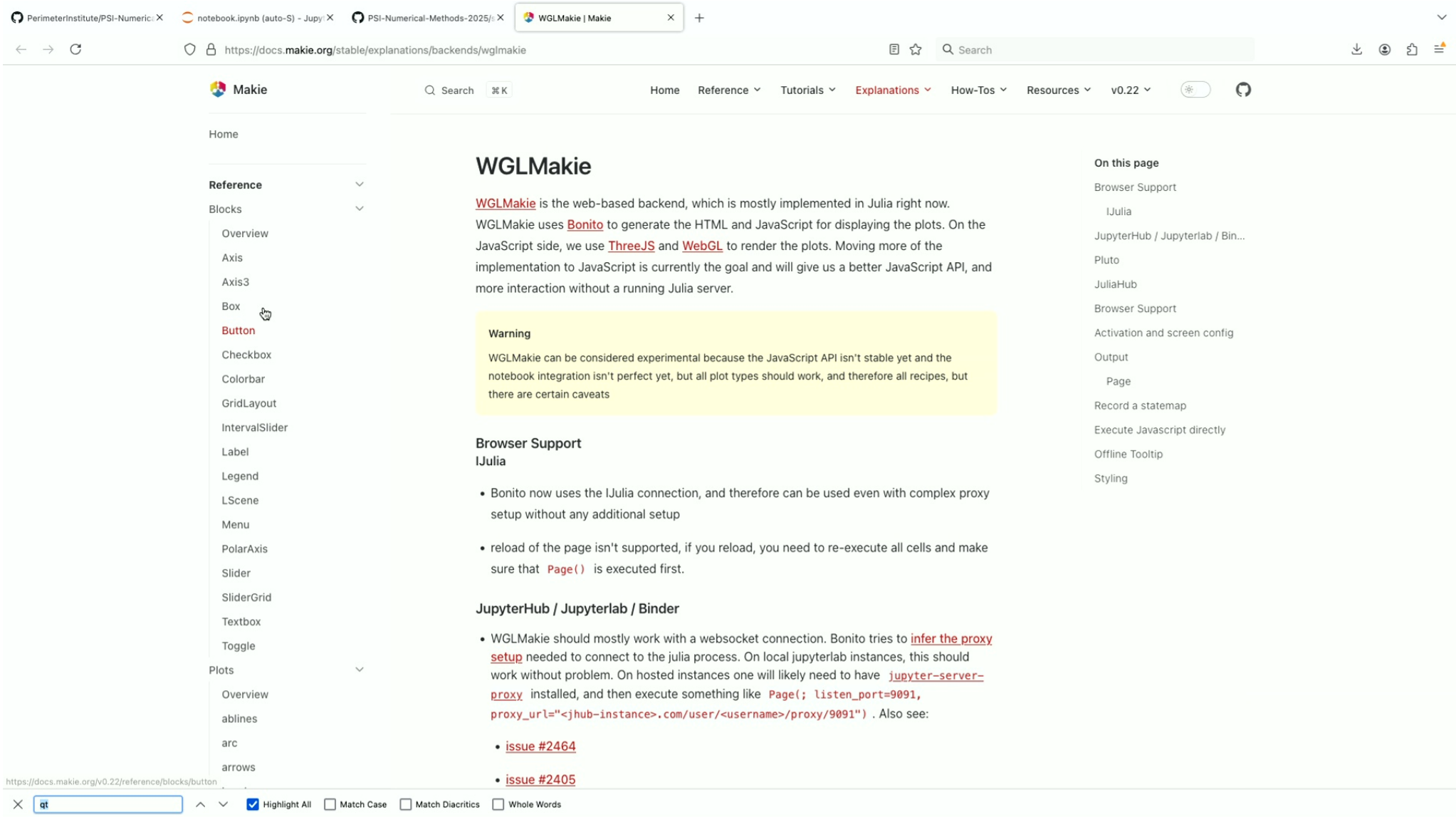
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WGLMakie | Makie
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Reference
Tutorials
Explanations
How-Tos
Resources
v0.22
Home
Reference
Blocks
Overview
Axis
Axis3
Box
Button
Checkbox
Colorbar
GridLayout
IntervalSlider
Label
Legend
LScene
Menu
PolarAxis
Slider
SliderGrid
Textbox
Toggle
Plots
Overview
ablines
arc
arrows
WGLMakie
WGLMakie is the web-based backend, which is mostly implemented in Julia right now. WGLMakie uses Bonito to generate the HTML and JavaScript for displaying the plots. On the JavaScript side, we use ThreeJS and WebGL to render the plots. Moving more of the implementation to JavaScript is currently the goal and will give us a better JavaScript API, and more interaction without a running Julia server.
Warning
WGLMakie can be considered experimental because the JavaScript API isn't stable yet and the notebook integration isn't perfect yet, but all plot types should work, and therefore all recipes, but there are certain caveats
Browser Support
IJulia
Bonito now uses the IJulia connection, and therefore can be used even with complex proxy setup without any additional setup
reload of the page isn't supported, if you reload, you need to re-execute all cells and make sure that Page() is executed first.
JupyterHub / Jupyterlab / Binder
WGLMakie should mostly work with a websocket connection. Bonito tries to infer the proxy setup needed to connect to the julia process. On local jupyterlab instances, this should work without problem. On hosted instances one will likely need to have jupyter-server-proxy installed, and then execute something like Page(; listen_port=9091, proxy_url="<jhub-instance>.com/user/<username>/proxy/9091") . Also see:
issue #2464
issue #2405
On this page
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Terminal 2 | notebook.ipynb

Code Julia 1.11.2

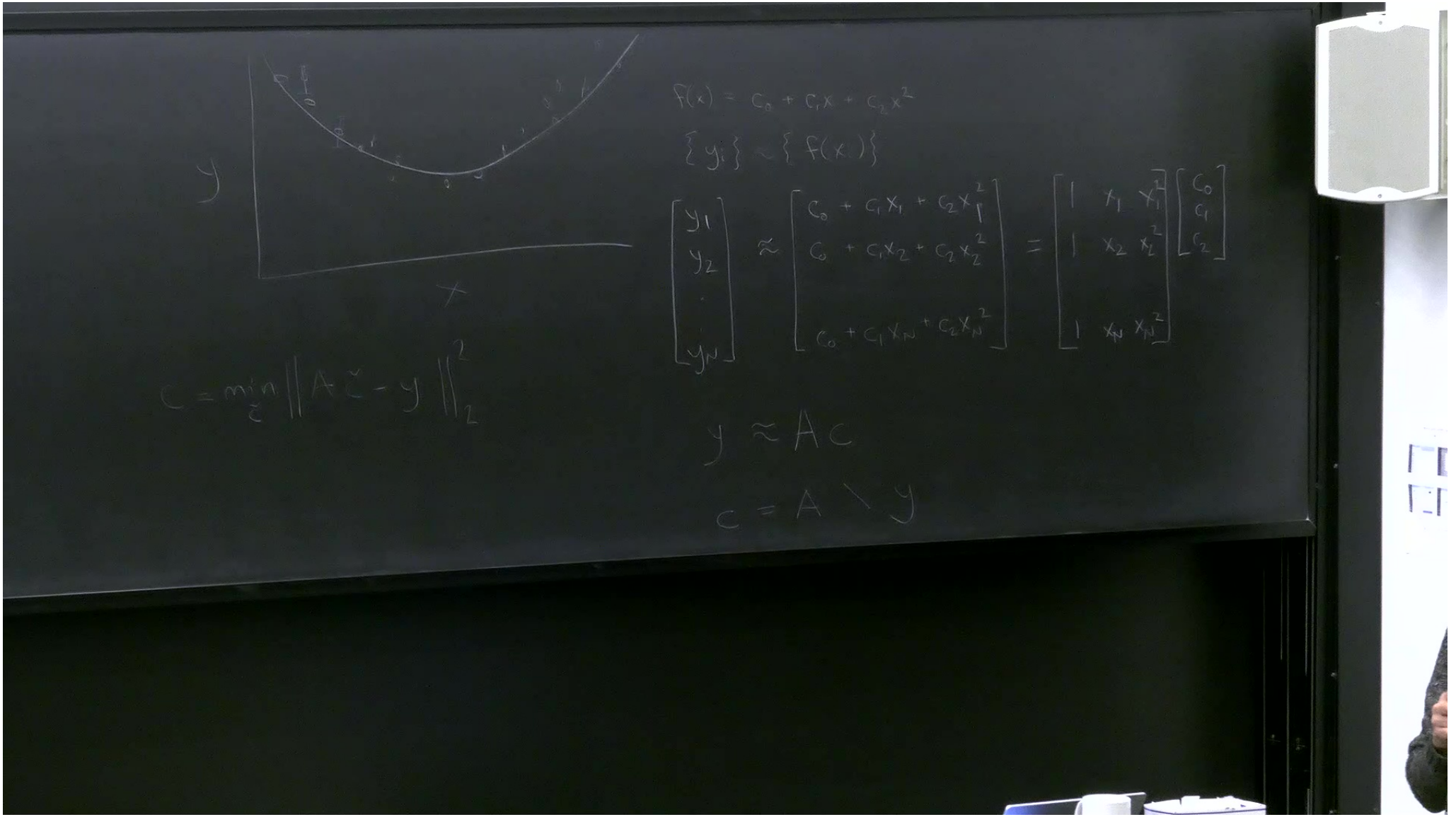
[43]:
```
data2.y[50]
```

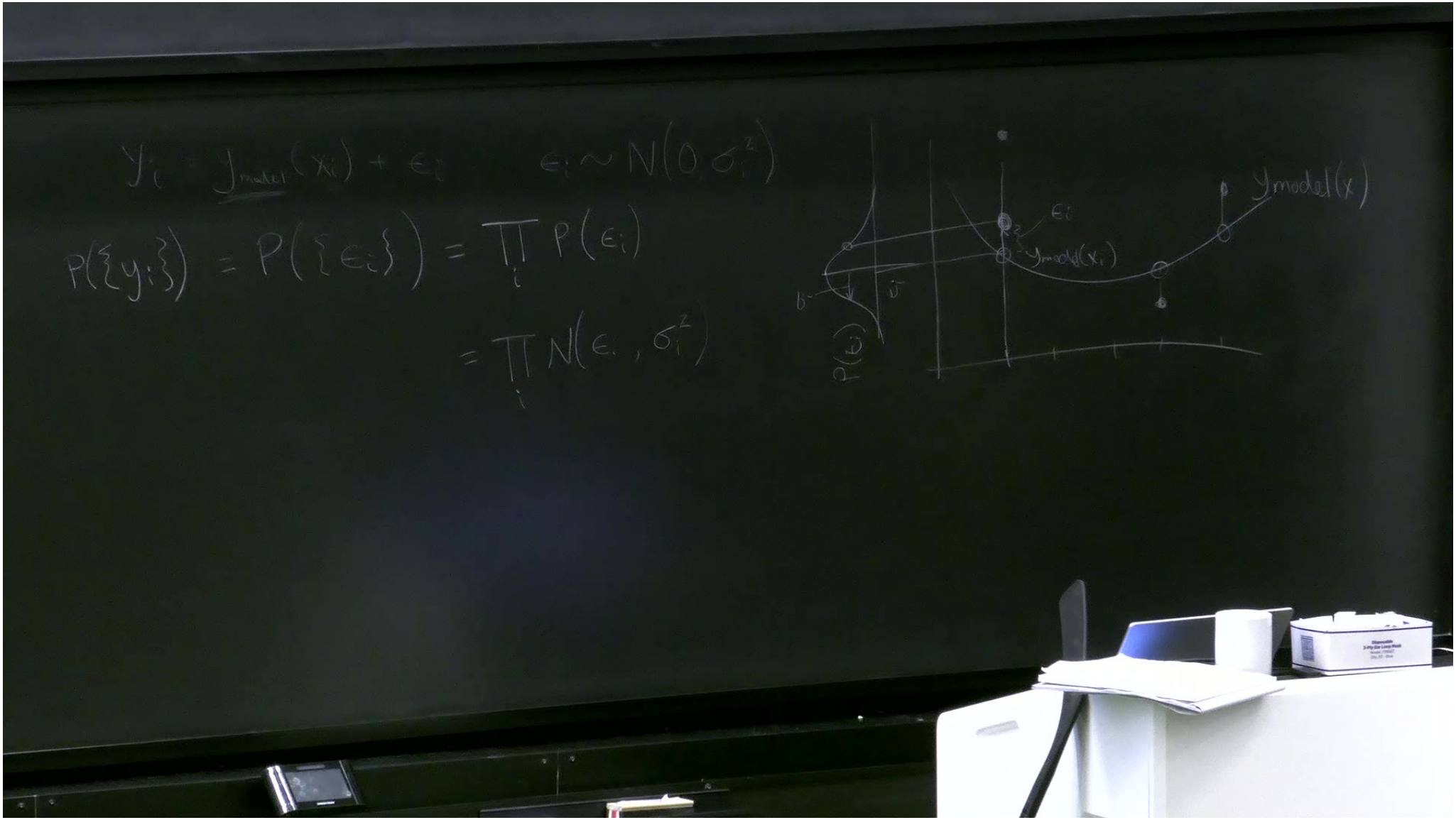
[43]:
```
-68.8731211285464
```

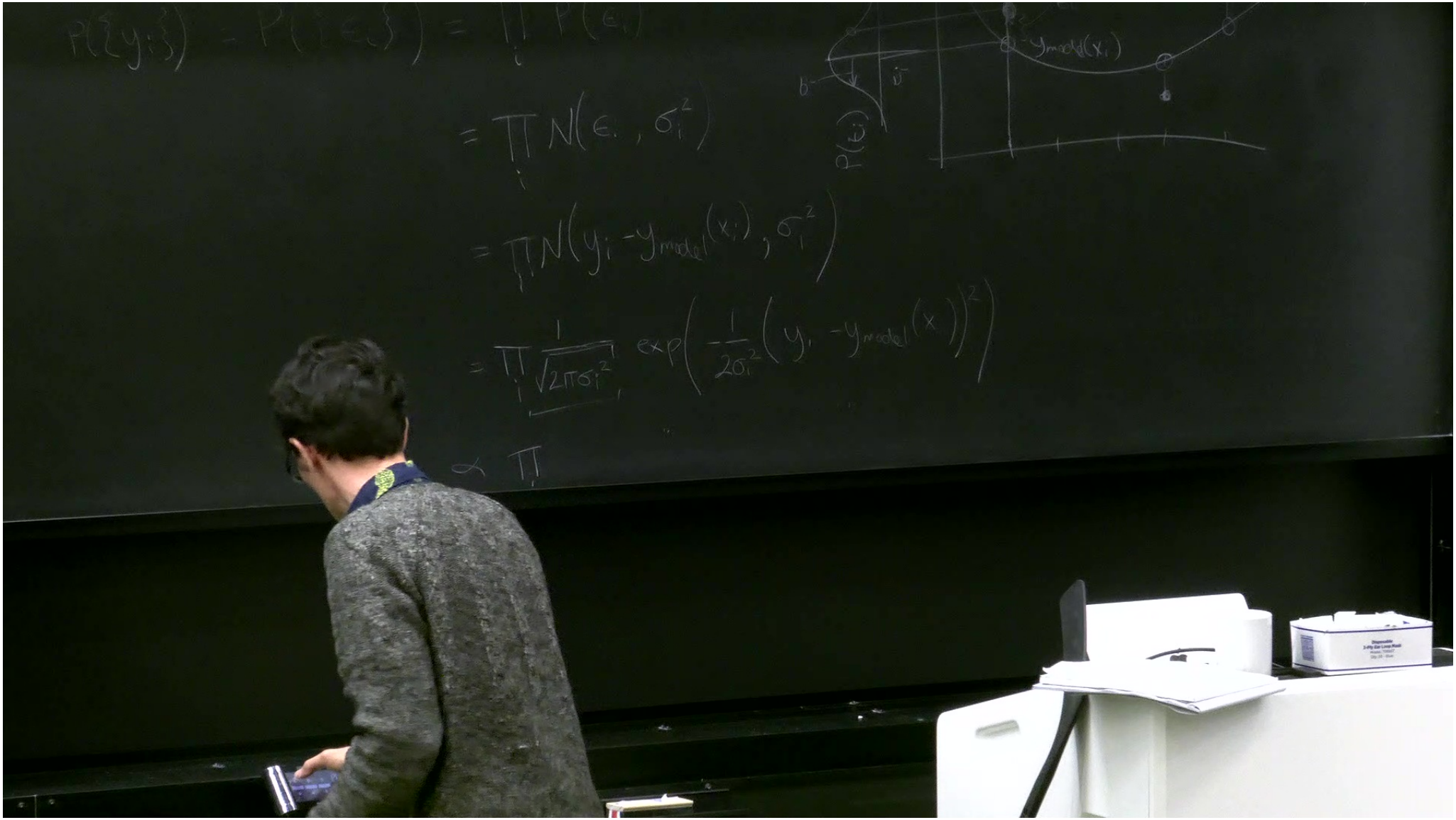
[48]:
```
f = Figure()
Axis(f[1,1], title="Data", xlabel="X", ylabel="Y", )
#scatter!(data2.x, data2.y)
lines!(xx, yy, color=:red, linewidth=2)
lines!(xx, yy2, color=:orange, linewidth=2)
f
```

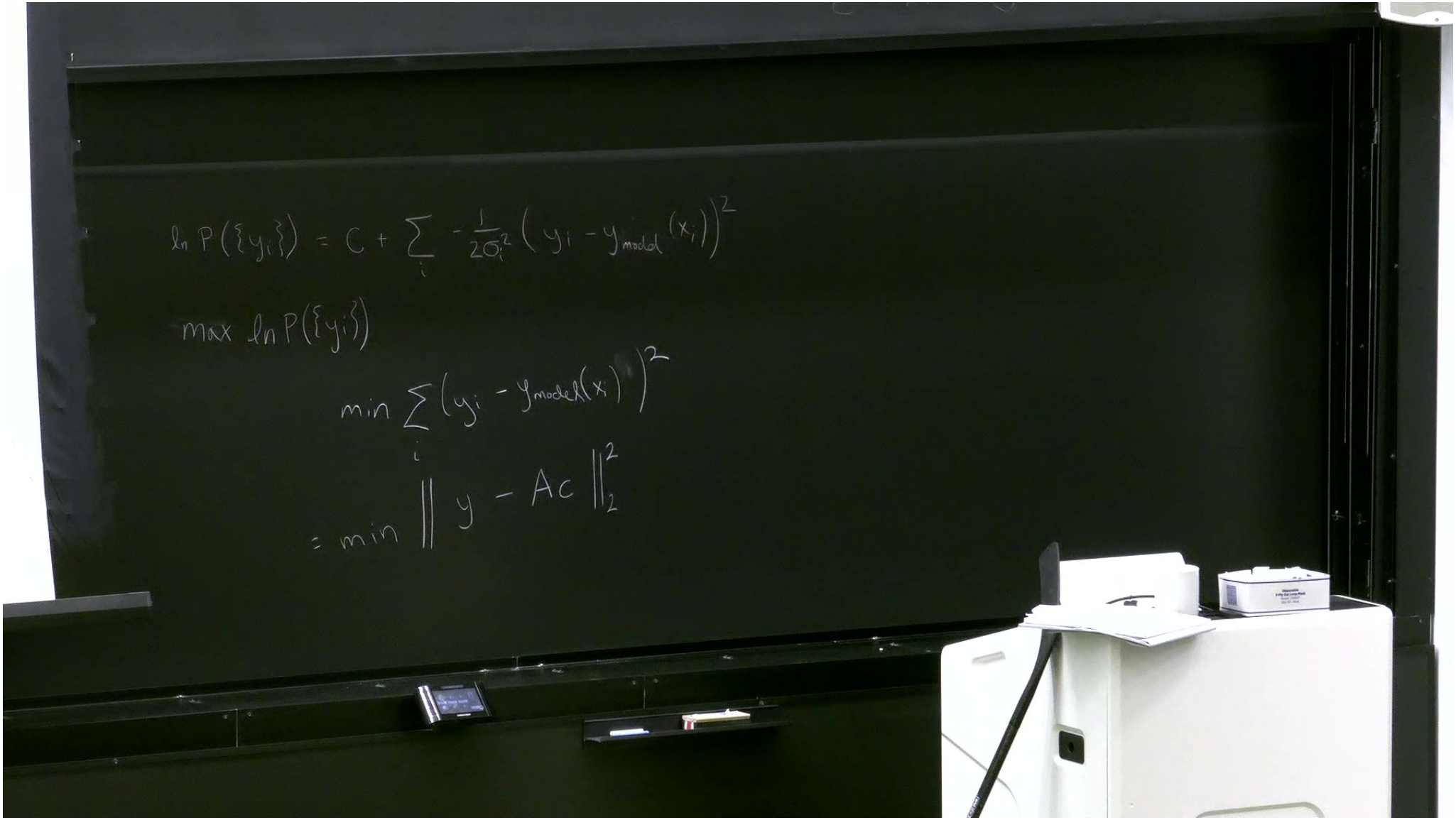
[48]:

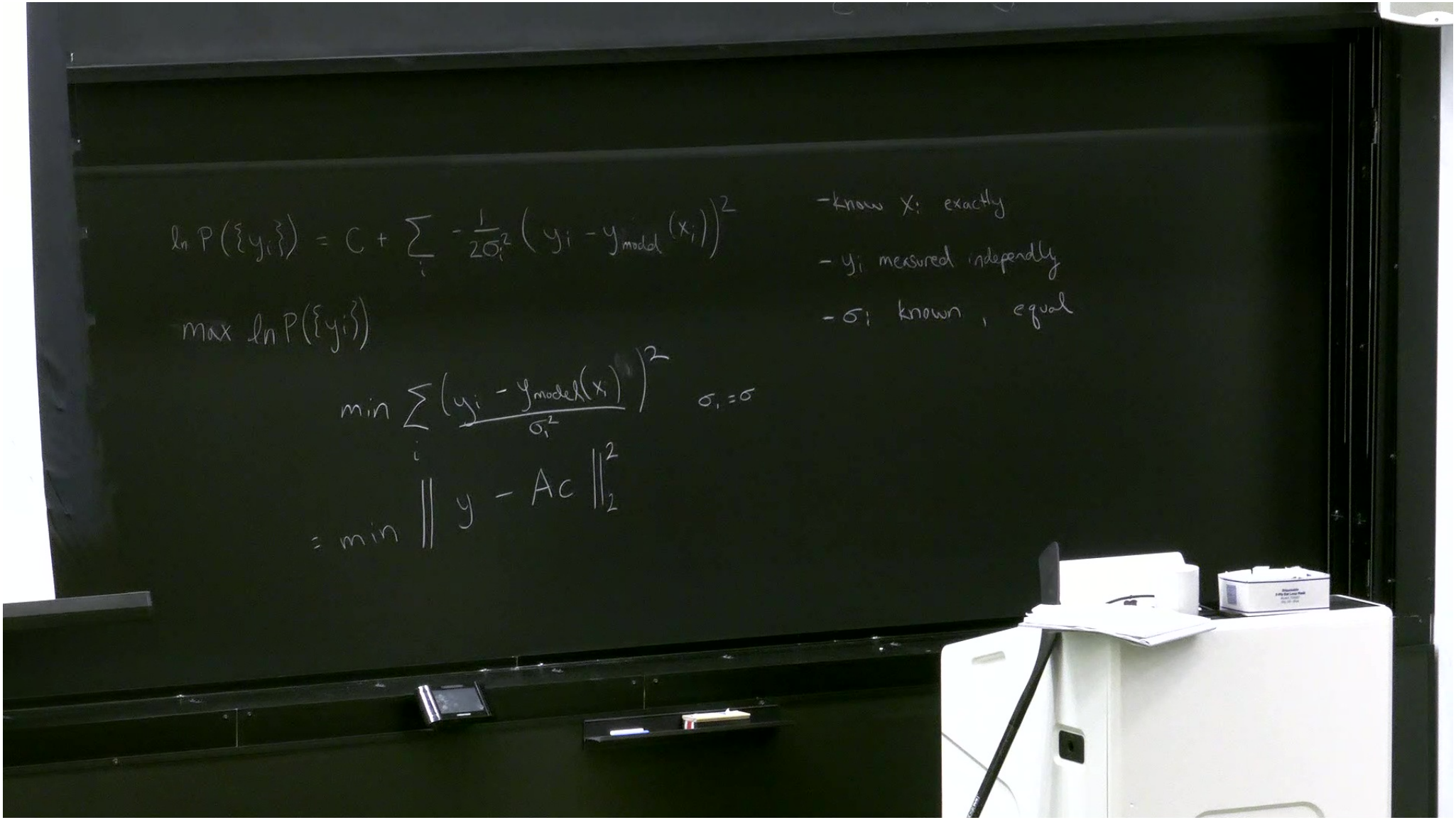
Simple 2 10 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 1 notebook.ipynb 0

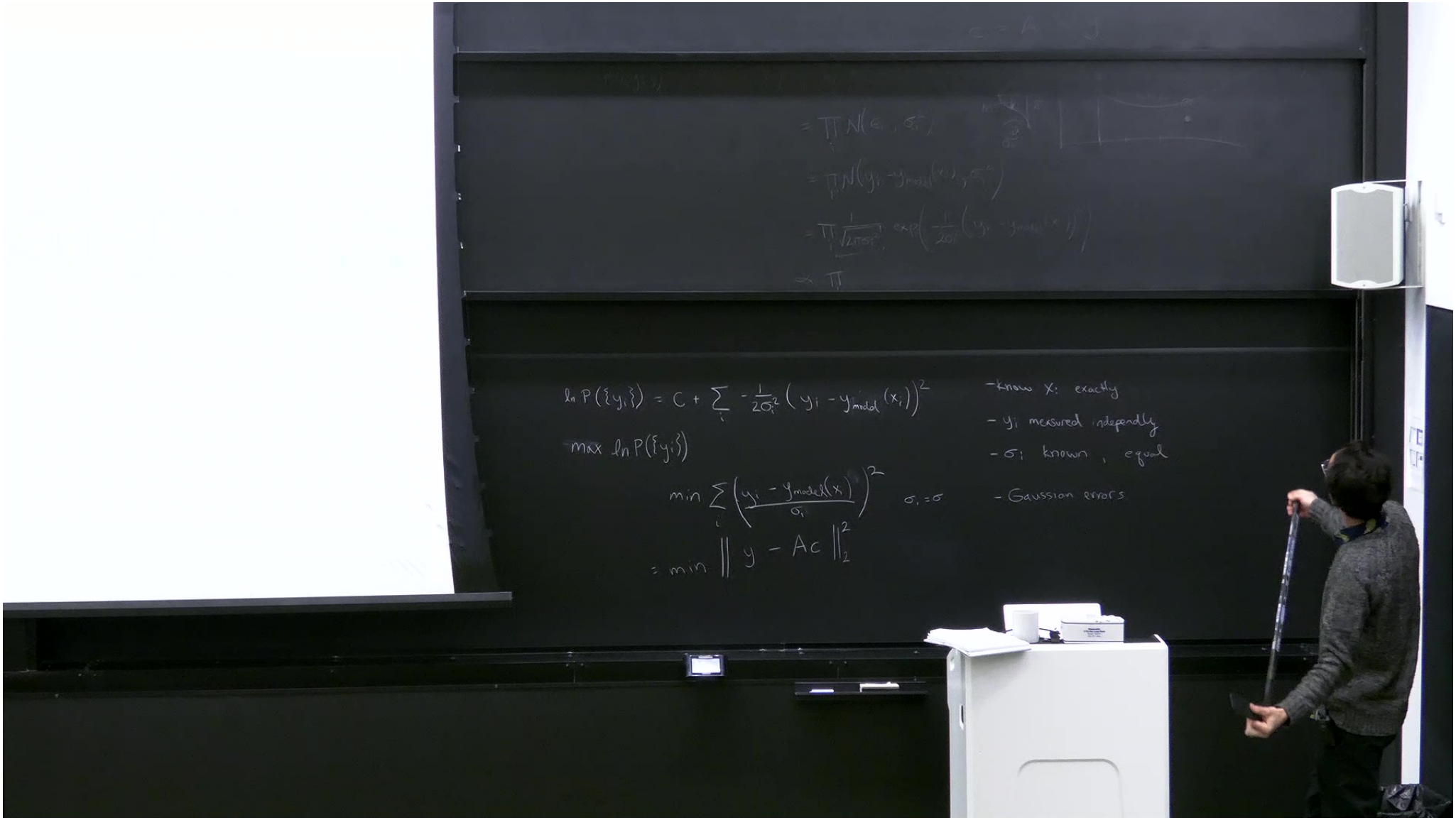

y
x
$f(x) = c_0 + c_1 x + c_2 x^2$
$\{y_i\} \approx \{f(x)\}$
$\begin{bmatrix} y_1 \\ y_2 \\ \\ y_N \end{bmatrix} \approx \begin{bmatrix} c_0 + c_1 x_1 + c_2 x_1^2 \\ c_0 + c_1 x_2 + c_2 x_2^2 \\ \\ c_0 + c_1 x_N + c_2 x_N^2 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ & & \\ 1 & x_N & x_N^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}$
$c = \min_z \|Az - y\|_2^2$
$y \approx Ac$
$c = A \backslash y$

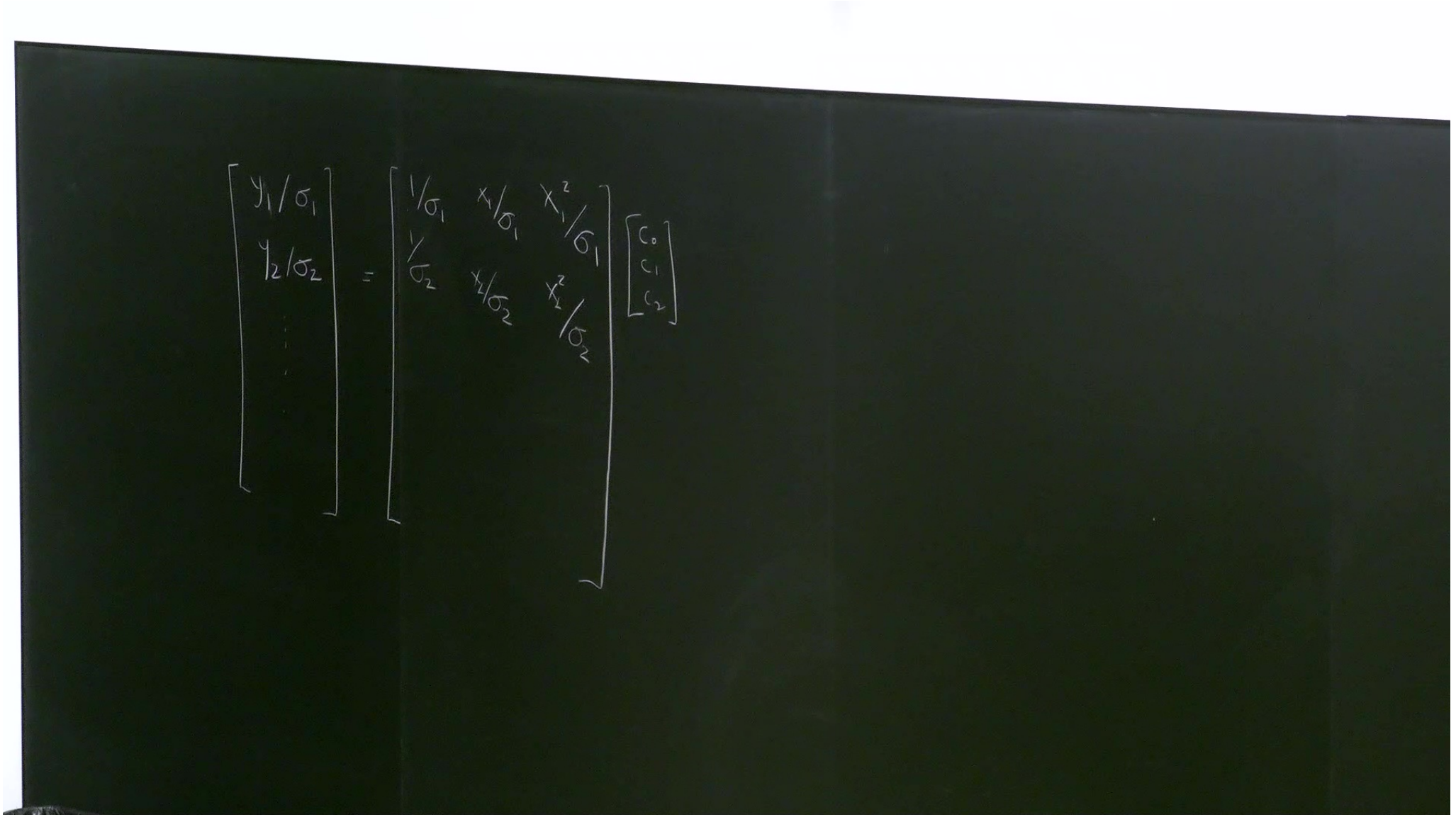

$y_i = y_{model}(x_i) + \epsilon_i \qquad \epsilon_i \sim N(0, \sigma_i^2)$
$P(\{y_i\}) = P(\{\epsilon_i\}) = \prod_i P(\epsilon_i)$
$= \prod_i N(\epsilon_i, \sigma_i^2)$
$y_{model}(x)$
ϵ_i
$y_{model}(x_i)$
$P(\epsilon_i)$


$P(\{y_i\}) = P(\{\epsilon_i\}) = \prod_i P(\epsilon_i)$
$= \prod_i N(\epsilon_i, \sigma_i^2)$
$= \prod_i N(y_i - y_{model}(x_i), \sigma_i^2)$
$= \prod_i \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{1}{2\sigma_i^2}(y_i - y_{model}(x_i))^2\right)$
$\propto \prod_i$
$y_{model}(x_i)$
$P(\epsilon_i)$


$\ln P(\{y_i\}) = C + \sum_i -\frac{1}{2\sigma_i^2}\left(y_i - y_{model}(x_i)\right)^2$
$\max \ln P(\{y_i\})$
$\min \sum_i \left(y_i - y_{model}(x_i)\right)^2$
$= \min \| y - Ac \|_2^2$


$\ln P(\{y_i\}) = C + \sum_i -\frac{1}{2\sigma_i^2}\left(y_i - y_{model}(x_i)\right)^2$
$\max \ln P(\{y_i\})$
$\min \sum_i \frac{\left(y_i - y_{model}(x_i)\right)^2}{\sigma_i^2}$
$\sigma_i = \sigma$
$= \min \| y - Ac \|_2^2$
- know x_i exactly
- y_i measured independly
- σ_i known, equal


$\ln P(\{y_i\}) = C + \sum_i -\frac{1}{2\sigma_i^2}\left(y_i - y_{model}(x_i)\right)^2$
$\max \ln P(\{y_i\})$
$\min \sum_i \left(\frac{y_i - y_{model}(x)}{\sigma_i}\right)^2$
$= \min \| y - Ac \|_2^2$
$\sigma_i = \sigma$
- know x_i exactly
- y_i measured independently
- σ_i known, equal
- Gaussian errors


$\begin{bmatrix} y_1/\sigma_1 \\ y_2/\sigma_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 1/\sigma_1 & x_1/\sigma_1 & x_1^2/\sigma_1 \\ 1/\sigma_2 & x_2/\sigma_2 & x_2^2/\sigma_2 \\ & \vdots & \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}$