

Finding Maxima and Minima of DiffEq Solutions

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0.0.1 Setup

In this tutorial we will show how to use Optim.jl to find the maxima and minima of solutions. Let's take a look at the double pendulum:

```
#Constants and setup
using OrdinaryDiffEq
initial = [0.01, 0.01, 0.01, 0.01]
tspan = (0.,100.)

#Define the problem
function double_pendulum_hamiltonian(udot,u,p,t)
    α = u[1]
    lα = u[2]
    β = u[3]
    lβ = u[4]
    udot .=
        [2(lα-(1+cos(β))lβ)/(3-cos(2β)),
         -2sin(α) - sin(α+β),
         2(-(1+cos(β))lα + (3+2cos(β))lβ)/(3-cos(2β)),
         -sin(α+β) - 2sin(β)*(((lα-lβ)lβ)/(3-cos(2β))) + 2sin(2β)*((lα^2 - 2(1+cos(β))lα*lβ
         + (3+2cos(β))lβ^2)/(3-cos(2β))^2)]
end

#Pass to solvers
poincare = ODEProblem(double_pendulum_hamiltonian, initial, tspan)

ODEProblem with uType Vector{Float64} and tType Float64. In-place: true
timespan: (0.0, 100.0)
u0: 4-element Vector{Float64}:
 0.01
 0.01
 0.01
 0.01

sol = solve(poincare, Tsit5())

retcode: Success
Interpolation: specialized 4th order "free" interpolation
t: 193-element Vector{Float64}:
 0.0
 0.08332584852065579
 0.24175300587841853
 0.4389533535703127
 0.6797301355043014
```

```

0.9647629621490508
1.3179425637594349
1.7031226016307728
2.0678503967116617
2.4717899847517866
:
95.8457309586563
96.3577910122243
96.92913461915474
97.44679415429573
97.96248479179103
98.51183391850897
99.0608253308051
99.58284388126884
100.0
u: 193-element Vector{Vector{Float64}}:
 [0.01, 0.01, 0.01, 0.01]
 [0.009170687380405334, 0.00669000455384281, 0.012420525490765841, 0.00826
6408515192909]
 [0.007673275265972504, 0.00037461737897660443, 0.016442590227730397, 0.004
636827483318277]
 [0.006125974419239289, -0.007305450189721187, 0.019967371084231897, -0.000
3364979830896869]
 [0.004966110662711131, -0.01630851653373806, 0.021440659476204722, -0.0067
05037098400474]
 [0.0047955683310194714, -0.026238103489235838, 0.01882432520883759, -0.013
913364556753736]
 [0.0060546798253553686, -0.03712455187908053, 0.010055702788069564, -0.021
038127478647375]
 [0.007900784412908646, -0.04667606960847394, -0.002673581831574513, -0.025
18303627203377]
 [0.008276510489473166, -0.05278433365633976, -0.012731546444725367, -0.025
25804037623962]
 [0.00552349681674124, -0.05525250414492613, -0.016843881882621835, -0.0218
98963191274153]
:
 [-0.014886751154788403, 0.04233275827248491, 0.0136282832580092, 0.0180290
82291419467]
 [-0.008190258536393156, 0.054422679804409874, 0.009448013826704854, 0.0177
4006800908217]
 [0.004124711787695587, 0.05674878820505975, -0.00515418739191979, 0.017596
983103942972]
 [0.013079718118471138, 0.048077043077395416, -0.01377066122508919, 0.01828
6648610391296]
 [0.015316040241448815, 0.03163095955755212, -0.008956991644884404, 0.01711
8404049844594]
 [0.011115490017375213, 0.00992901822063005, 0.007297481421219374, 0.010353
371812537674]
 [0.005713878919291721, -0.011787427051187821, 0.02050806401368854, -0.0023
10458905852316]
 [0.004211439726126673, -0.029911199361470703, 0.018750446422905413, -0.015
650712294907165]
 [0.005741239607321043, -0.04165385985159563, 0.007413270184094278, -0.0233
4897852528026]

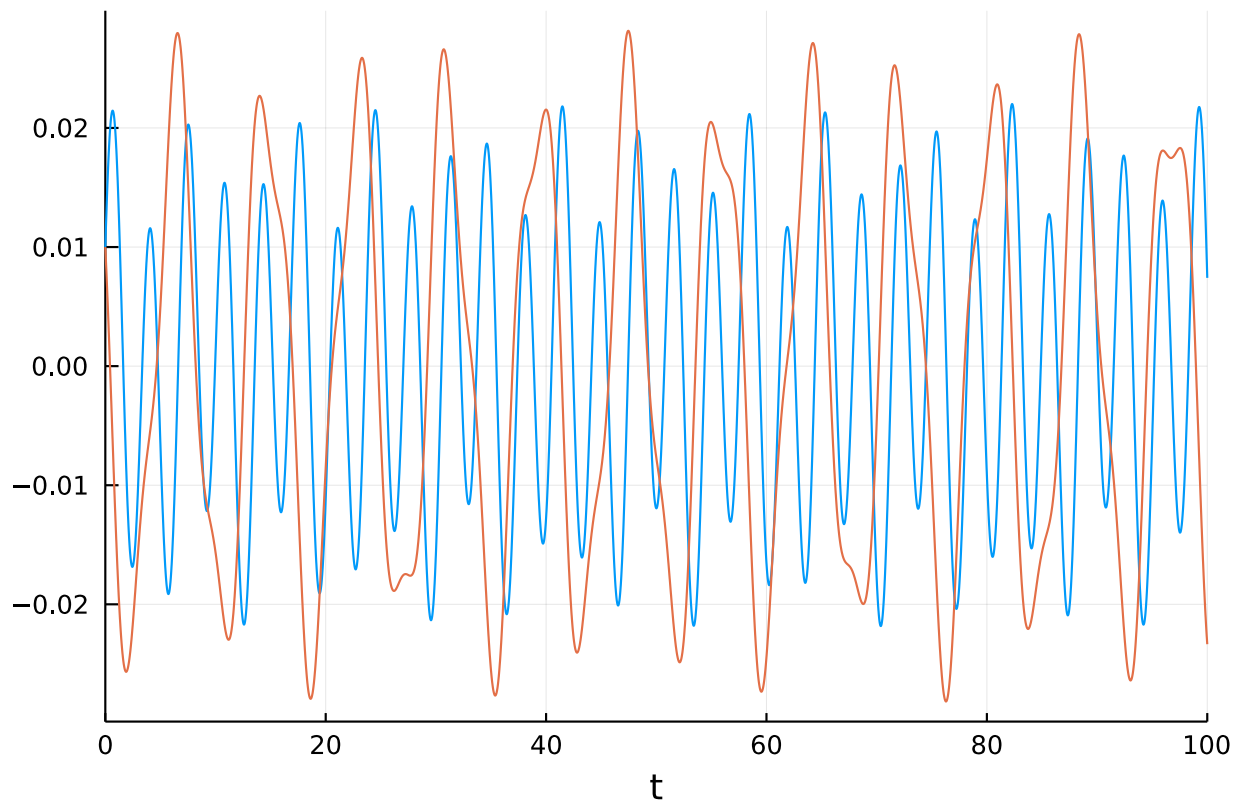
```

In time, the solution looks like:

```

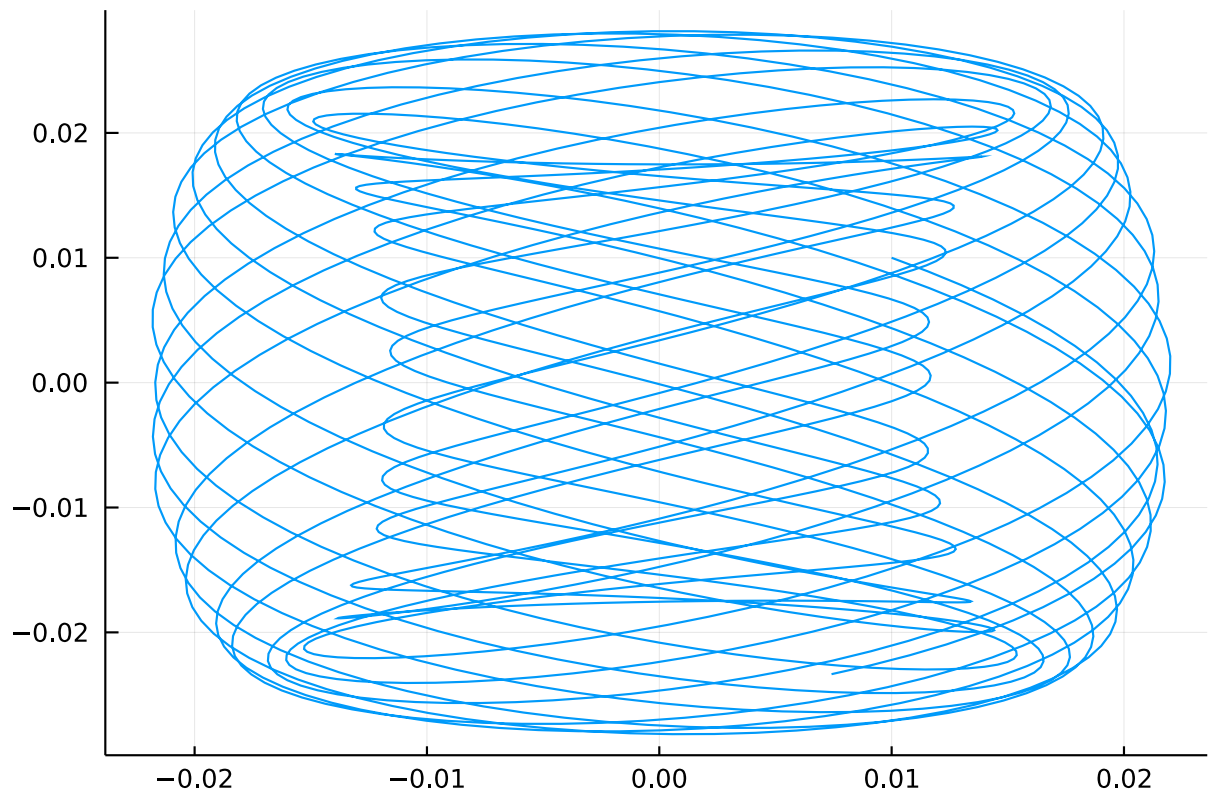
using Plots; gr()
plot(sol, vars=[(0,3),(0,4)], leg=false, plotdensity=10000)

```



while it has the well-known phase-space plot:

```
plot(sol, vars=(3,4), leg=false)
```



0.0.2 Local Optimization

Let's find out what some of the local maxima and minima are. Optim.jl can be used to minimize functions, and the solution type has a continuous interpolation which can be used. Let's look for the local optima for the 4th variable around $t=20$. Thus our optimization function is:

```
f = (t) -> sol(t,idxs=4)
```

```
#1 (generic function with 1 method)
```

`first(t)` is the same as `t[1]` which transforms the array of size 1 into a number. `idxs=4` is the same as `sol(first(t))[4]` but does the calculation without a temporary array and thus is faster. To find a local minima, we can simply call Optim on this function. Let's find a local minimum:

```
using Optim
opt = optimize(f,18.0,22.0)
```

```
Results of Optimization Algorithm
* Algorithm: Brent's Method
* Search Interval: [18.000000, 22.000000]
* Minimizer: 1.863213e+01
* Minimum: -2.793164e-02
* Iterations: 11
* Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16)
): true
* Objective Function Calls: 12
```

From this printout we see that the minimum is at $t=18.63$ and the value is $-2.79e-2$. We can get these in code-form via:

```
println(opt.minimizer)
println(opt.minimum)
```

```
18.632127451866573
-0.02793163565154488
```

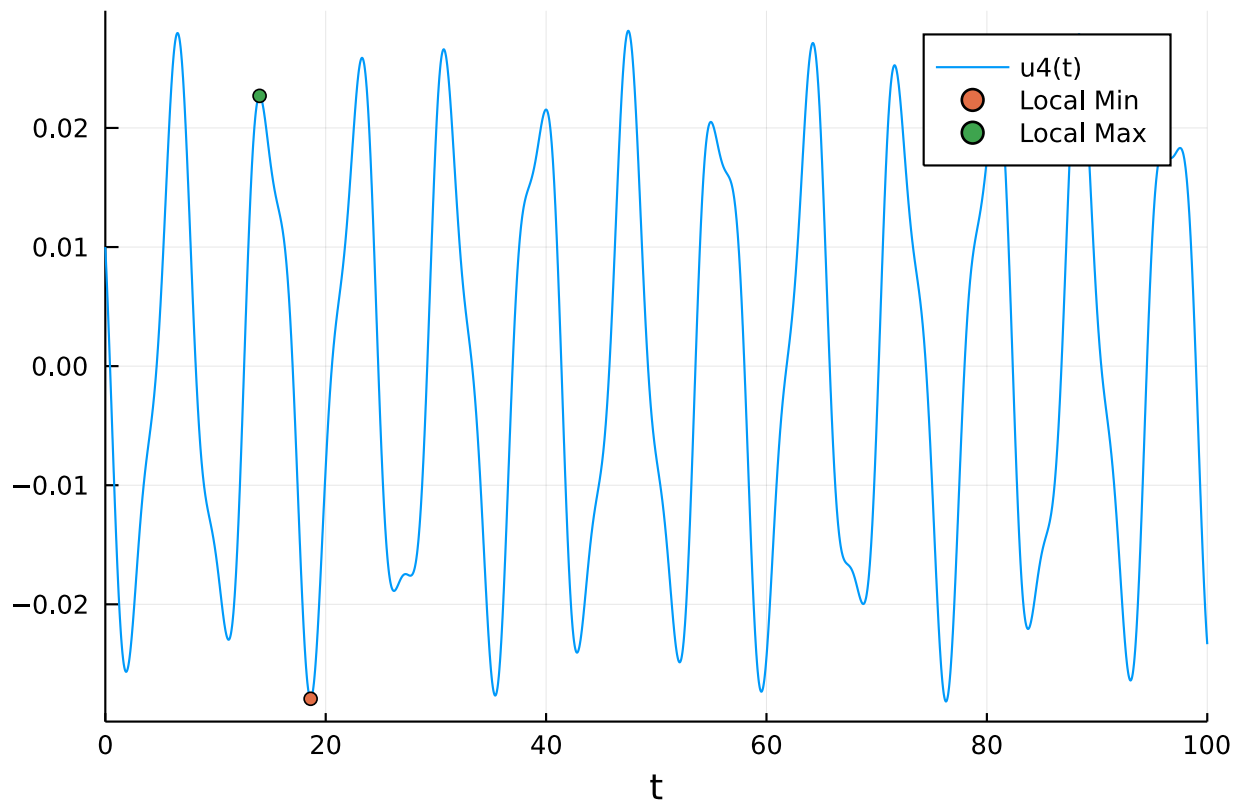
To get the maximum, we just minimize the negative of the function:

```
f = (t) -> -sol(first(t),idxs=4)
opt2 = optimize(f,0.0,22.0)
```

```
Results of Optimization Algorithm
* Algorithm: Brent's Method
* Search Interval: [0.000000, 22.000000]
* Minimizer: 1.399975e+01
* Minimum: -2.269411e-02
* Iterations: 13
* Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16)
): true
* Objective Function Calls: 14
```

Let's add the maxima and minima to the plots:

```
plot(sol, vars=(0,4), plotdensity=10000)
scatter!([opt.minimizer],[opt.minimum],label="Local Min")
scatter!([opt2.minimizer],[-opt2.minimum],label="Local Max")
```



Brent's method will locally minimize over the full interval. If we instead want a local maxima nearest to a point, we can use `BFGS()`. In this case, we need to optimize a vector `[t]`, and thus dereference it to a number using `first(t)`.

```
f = (t) -> -sol(first(t),idxs=4)
opt = optimize(f,[20.0],BFGS())
```

```
* Status: success
```

```
* Candidate solution
```

```
Final objective value:      -2.588588e-02
```

```
* Found with
```

```
Algorithm:      BFGS
```

```
* Convergence measures
```

```
|x - x'|          = 1.11e-04 < 0.0e+00
|x - x'|/|x'|     = 4.78e-06 < 0.0e+00
|f(x) - f(x')|    = 1.68e-10 < 0.0e+00
|f(x) - f(x')|/|f(x')| = 6.49e-09 < 0.0e+00
|g(x)|            = 8.44e-12 ≤ 1.0e-08
```

```
* Work counters
```

```
Seconds run:      0 (vs limit Inf)
```

```
Iterations:       4
```

```
f(x) calls:       16
```

```
∇f(x) calls:      16
```

0.0.3 Global Optimization

If we instead want to find global maxima and minima, we need to look somewhere else. For this there are many choices. A pure Julia option is BlackBoxOptim.jl, but I will use NLOpt.jl. Following the NLOpt.jl tutorial but replacing their function with our own:

```
import NLOpt, ForwardDiff

count = 0 # keep track of # function evaluations

function g(t::Vector, grad::Vector)
    if length(grad) > 0
        #use ForwardDiff for the gradients
        grad[1] = ForwardDiff.derivative((t)->sol(first(t),idxs=4),t)
    end
    sol(first(t),idxs=4)
end

opt = NLOpt.Opt(:GN_ORIG_DIRECT_L, 1)
NLOpt.lower_bounds!(opt, [0.0])
NLOpt.upper_bounds!(opt, [40.0])
NLOpt.xtol_rel!(opt, 1e-8)
NLOpt.min_objective!(opt, g)
(minf,minx,ret) = NLOpt.optimize(opt,[20.0])
println(minf, " ",minx, " ",ret)
NLOpt.max_objective!(opt, g)
(maxf,maxx,ret) = NLOpt.optimize(opt,[20.0])
println(maxf, " ",maxx, " ",ret)
```

Error: ArgumentError: Package ForwardDiff not found in current path:
- Run `import Pkg; Pkg.add("ForwardDiff")` to install the ForwardDiff package.

```
plot(sol, vars=(0,4), plotdensity=10000)
scatter!([minx],[minf],label="Global Min")
scatter!([maxx],[maxf],label="Global Max")
```

Error: UndefVarError: minx not defined

0.1 Appendix

These tutorials are a part of the SciMLTutorials.jl repository, found at: <https://github.com/SciML/SciMLTutorials.jl>. For more information on high-performance scientific machine learning, check out the SciML Open Source Software Organization <https://sciml.ai>.

To locally run this tutorial, do the following commands:

```
using SciMLTutorials
SciMLTutorials.weave_file("tutorials/ode_extras","03-ode_minmax.jmd")
```

Computer Information:

```
Julia Version 1.6.2
Commit 1b93d53fc4 (2021-07-14 15:36 UTC)
Platform Info:
```

OS: Linux (x86_64-pc-linux-gnu)
CPU: AMD EPYC 7502 32-Core Processor
WORD_SIZE: 64
LIBM: libopenlibm
LLVM: libLLVM-11.0.1 (ORCJIT, znver2)

Environment:

JULIA_DEPOT_PATH = /root/.cache/julia-buildkite-plugin/depots/a6029d3a-f78b-41ea-bc9
JULIA_NUM_THREADS = 16

Package Information:

```
Status `~/var/lib/buildkite-agent/builds/5-amdci4-julia-csail-mit-edu/julia-lang/s
[f3b72e0c] DiffEqDevTools v2.27.2
[0c46a032] DifferentialEquations v6.17.1
[961ee093] ModelingToolkit v5.17.3
[76087f3c] NLopt v0.6.2
[2774e3e8] NLSolve v4.5.1
[429524aa] Optim v1.3.0
[1dea7af3] OrdinaryDiffEq v5.56.0
[91a5bcdd] Plots v1.15.2
[30cb0354] SciMLTutorials v0.9.0
[37e2e46d] LinearAlgebra
[2f01184e] SparseArrays
```

And the full manifest:

```
Status `~/var/lib/buildkite-agent/builds/5-amdci4-julia-csail-mit-edu/julia-lang/s
[c3fe647b] AbstractAlgebra v0.16.0
[1520ce14] AbstractTrees v0.3.4
[79e6a3ab] Adapt v3.3.0
[ec485272] ArnoldiMethod v0.1.0
[4fba245c] ArrayInterface v3.1.15
[4c555306] ArrayLayouts v0.7.0
[aae01518] BandedMatrices v0.16.9
[6e4b80f9] BenchmarkTools v1.0.0
[764a87c0] BoundaryValueDiffEq v2.7.1
[fa961155] CEnum v0.4.1
[00ebfdb7] CSTParser v2.5.0
[d360d2e6] ChainRulesCore v0.9.44
[b630d9fa] CheapThreads v0.2.5
[523fee87] CodecBzip2 v0.7.2
[944b1d66] CodecZlib v0.7.0
[35d6a980] ColorSchemes v3.12.1
[3da002f7] ColorTypes v0.11.0
[5ae59095] Colors v0.12.8
[861a8166] Combinatorics v1.0.2
[a80b9123] CommonMark v0.8.1
```

[38540f10] CommonSolve v0.2.0
[bbf7d656] CommonSubexpressions v0.3.0
[34da2185] Compat v3.30.0
[8f4d0f93] Conda v1.5.2
[187b0558] ConstructionBase v1.2.1
[d38c429a] Contour v0.5.7
[a8cc5b0e] Crayons v4.0.4
[9a962f9c] DataAPI v1.6.0
[864edb3b] DataStructures v0.18.9
[e2d170a0] DataValueInterfaces v1.0.0
[bcd4f6db] DelayDiffEq v5.31.0
[2b5f629d] DiffEqBase v6.62.2
[459566f4] DiffEqCallbacks v2.16.1
[f3b72e0c] DiffEqDevTools v2.27.2
[5a0ffddc] DiffEqFinancial v2.4.0
[c894b116] DiffEqJump v6.14.2
[77a26b50] DiffEqNoiseProcess v5.7.3
[055956cb] DiffEqPhysics v3.9.0
[163ba53b] DiffResults v1.0.3
[b552c78f] DiffRules v1.0.2
[0c46a032] DifferentialEquations v6.17.1
[c619ae07] DimensionalPlotRecipes v1.2.0
[b4f34e82] Distances v0.10.3
[31c24e10] Distributions v0.24.18
[ffbed154] DocStringExtensions v0.8.4
[e30172f5] Documenter v0.26.3
[d4d017d3] ExponentialUtilities v1.8.4
[e2ba6199] ExprTools v0.1.3
[c87230d0] FFMPEG v0.4.0
[7034ab61] FastBroadcast v0.1.8
[9aa1b823] FastClosures v0.3.2
[1a297f60] FillArrays v0.11.7
[6a86dc24] FiniteDiff v2.8.0
[53c48c17] FixedPointNumbers v0.8.4
[59287772] Formatting v0.4.2
[f6369f11] ForwardDiff v0.10.18
[069b7b12] FunctionWrappers v1.1.2
[28b8d3ca] GR v0.57.4
[5c1252a2] GeometryBasics v0.3.12
[42e2da0e] Grisu v1.0.2
[cd3eb016] HTTP v0.9.9
[eafb193a] Highlights v0.4.5
[0e44f5e4] Hwloc v2.0.0
[7073ff75] IJulia v1.23.2
[b5f81e59] IOCapture v0.1.1
[615f187c] IfElse v0.1.0
[d25df0c9] Inflate v0.1.2
[83e8ac13] IniFile v0.5.0
[c8e1da08] IterTools v1.3.0

[42fd0dbc] IterativeSolvers v0.9.1
 [82899510] IteratorInterfaceExtensions v1.0.0
 [692b3bcd] JLLWrappers v1.3.0
 [682c06a0] JSON v0.21.1
 [7d188eb4] JSONSchema v0.3.3
 [98e50ef6] JuliaFormatter v0.13.7
 [b964fa9f] LaTeXStrings v1.2.1
 [2ee39098] LabelledArrays v1.6.1
 [23fbe1c1] Latexify v0.15.5
 [093fc24a] LightGraphs v1.3.5
 [d3d80556] LineSearches v7.1.1
 [2ab3a3ac] LogExpFunctions v0.2.4
 [bdcacae8] LoopVectorization v0.12.23
 [1914dd2f] MacroTools v0.5.6
 [b8f27783] MathOptInterface v0.9.22
 [fdb3010] MathProgBase v0.7.8
 [739be429] MbedTLS v1.0.3
 [442fcdcd] Measures v0.3.1
 [e1d29d7a] Missings v1.0.0
 [961ee093] ModelingToolkit v5.17.3
 [46d2c3a1] MuladdMacro v0.2.2
 [f9640e96] MultiScaleArrays v1.8.1
 [ffc61752] Mustache v1.0.10
 [d8a4904e] MutableArithmetics v0.2.19
 [d41bc354] NLSolversBase v7.8.0
 [76087f3c] NLOpt v0.6.2
 [2774e3e8] NLSolve v4.5.1
 [77ba4419] NaNMath v0.3.5
 [8913a72c] NonlinearSolve v0.3.8
 [6fe1bfb0] OffsetArrays v1.9.0
 [429524aa] Optim v1.3.0
 [bac558e1] OrderedCollections v1.4.1
 [1dea7af3] OrdinaryDiffEq v5.56.0
 [90014a1f] PDMats v0.11.0
 [65888b18] ParameterizedFunctions v5.10.0
 [d96e819e] Parameters v0.12.2
 [69de0a69] Parsers v1.1.0
 [ccf2f8ad] PlotThemes v2.0.1
 [995b91a9] PlotUtils v1.0.10
 [91a5bcdd] Plots v1.15.2
 [e409e4f3] PoissonRandom v0.4.0
 [f517fe37] Polyester v0.3.1
 [85a6dd25] PositiveFactorizations v0.2.4
 [21216c6a] Preferences v1.2.2
 [1fd47b50] QuadGK v2.4.1
 [74087812] Random123 v1.3.1
 [fb686558] RandomExtensions v0.4.3
 [e6cf234a] RandomNumbers v1.4.0
 [3cdcf5f2] RecipesBase v1.1.1

[01d81517] RecipesPipeline v0.3.2
[731186ca] RecursiveArrayTools v2.11.4
[f2c3362d] RecursiveFactorization v0.1.12
[189a3867] Reexport v1.0.0
[ae029012] Requires v1.1.3
[ae5879a3] ResettableStacks v1.1.0
[79098fc4] Rmath v0.7.0
[47965b36] RootedTrees v1.0.0
[7e49a35a] RuntimeGeneratedFunctions v0.5.2
[476501e8] SLEEF Pirates v0.6.20
[1bc83da4] SafeTestsets v0.0.1
[0bca4576] SciMLBase v1.13.4
[30cb0354] SciMLTutorials v0.9.0
[6c6a2e73] Scratch v1.0.3
[efcf1570] Setfield v0.7.0
[992d4aef] Showoff v1.0.3
[699a6c99] SimpleTraits v0.9.3
[b85f4697] SoftGlobalScope v1.1.0
[a2af1166] SortingAlgorithms v1.0.0
[47a9eef4] SparseDiffTools v1.13.2
[276daf66] SpecialFunctions v1.4.1
[aedffcd0] Static v0.2.4
[90137ffa] StaticArrays v1.2.0
[82ae8749] StatsAPI v1.0.0
[2913bbd2] StatsBase v0.33.8
[4c63d2b9] StatsFuns v0.9.8
[9672c7b4] SteadyStateDiffEq v1.6.2
[789caeaf] StochasticDiffEq v6.34.1
[7792a7ef] StrideArraysCore v0.1.11
[09ab397b] StructArrays v0.5.1
[c3572dad] Sundials v4.4.3
[d1185830] SymbolicUtils v0.11.2
[0c5d862f] Symbolics v0.1.25
[3783bdb8] TableTraits v1.0.1
[bd369af6] Tables v1.4.2
[8290d209] ThreadingUtilities v0.4.4
[a759f4b9] TimerOutputs v0.5.9
[0796e94c] Tokenize v0.5.16
[3bb67fe8] TranscodingStreams v0.9.5
[a2a6695c] TreeViews v0.3.0
[5c2747f8] URIs v1.3.0
[3a884ed6] UnPack v1.0.2
[1986cc42] Unitful v1.7.0
[3d5dd08c] VectorizationBase v0.20.11
[81def892] VersionParsing v1.2.0
[19fa3120] VertexSafeGraphs v0.1.2
[44d3d7a6] Weave v0.10.8
[ddb6d928] YAML v0.4.6
[c2297ded] ZMQ v1.2.1

[a5390f91] ZipFile v0.9.3
[700de1a5] ZygoteRules v0.2.1
[6e34b625] Bzip2_jll v1.0.6+5
[83423d85] Cairo_jll v1.16.0+6
[5ae413db] EarCut_jll v2.1.5+1
[2e619515] Expat_jll v2.2.10+0
[b22a6f82] FFMPEG_jll v4.3.1+4
[a3f928ae] Fontconfig_jll v2.13.1+14
[d7e528f0] FreeType2_jll v2.10.1+5
[559328eb] FriBidi_jll v1.0.5+6
[0656b61e] GLFW_jll v3.3.4+0
[d2c73de3] GR_jll v0.57.2+0
[78b55507] Gettext_jll v0.21.0+0
[7746bdde] Glib_jll v2.68.1+0
[e33a78d0] Hwloc_jll v2.4.1+0
[aacddb02] JpegTurbo_jll v2.0.1+3
[c1c5ebd0] LAME_jll v3.100.0+3
[dd4b983a] LZ0_jll v2.10.1+0
[dd192d2f] LibVPX_jll v1.9.0+1
[e9f186c6] Libffi_jll v3.2.2+0
[d4300ac3] Libgcrypt_jll v1.8.7+0
[7e76a0d4] Libglvnd_jll v1.3.0+3
[7add5ba3] Libgpg_error_jll v1.42.0+0
[94ce4f54] Libiconv_jll v1.16.1+0
[4b2f31a3] Libmount_jll v2.35.0+0
[89763e89] Libtiff_jll v4.1.0+2
[38a345b3] Libuuid_jll v2.36.0+0
[079eb43e] NLOpt_jll v2.7.0+0
[e7412a2a] Ogg_jll v1.3.4+2
[458c3c95] OpenSSL_jll v1.1.1+6
[efe28fd5] OpenSpecFun_jll v0.5.4+0
[91d4177d] Opus_jll v1.3.1+3
[2f80f16e] PCRE_jll v8.44.0+0
[30392449] Pixman_jll v0.40.1+0
[ea2cea3b] Qt5Base_jll v5.15.2+0
[f50d1b31] Rmath_jll v0.3.0+0
[fb77eaff] Sundials_jll v5.2.0+1
[a2964d1f] Wayland_jll v1.17.0+4
[2381bf8a] Wayland_protocols_jll v1.18.0+4
[02c8fc9c] XML2_jll v2.9.12+0
[aed1982a] XSLT_jll v1.1.34+0
[4f6342f7] Xorg_libX11_jll v1.6.9+4
[0c0b7dd1] Xorg_libXau_jll v1.0.9+4
[935fb764] Xorg_libXcursor_jll v1.2.0+4
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[d091e8ba] Xorg_libXfixes_jll v5.0.3+4
[a51aa0fd] Xorg_libXi_jll v1.7.10+4
[d1454406] Xorg_libXinerama_jll v1.1.4+4

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 [ea2f1a96] Xorg_libXrender_jll v0.9.10+4
 [14d82f49] Xorg_libpthread_stubs_jll v0.1.0+3
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 [c5fb5394] Xorg_xtrans_jll v1.4.0+3
 [8f1865be] ZeroMQ_jll v4.3.2+6
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 [b53b4c65] libpng_jll v1.6.38+0
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 [f27f6e37] libvorbis_jll v1.3.6+6
 [1270edf5] x264_jll v2020.7.14+2
 [dfaa095f] x265_jll v3.0.0+3
 [d8fb68d0] xkbcommon_jll v0.9.1+5
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 [6462fe0b] Sockets

[2f01184e] SparseArrays
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[c8ffd9c3] MbedTLS_jll
[14a3606d] MozillaCACerts_jll
[4536629a] OpenBLAS_jll
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