Title: Numerical Methods Lecture

Speakers: Dustin Lang

Collection: Numerical Methods 2023/24

Date: January 25, 2024 - 10:15 AM

URL: https://pirsa.org/24010024

emcee: An Affine-Invariant Sampler

Dustin Lang
Perimeter Institute for Theoretical Physics

PSI Numerical Methods, 2024-01-25

Borrowing heavily from Dan Foreman-Mackey's slides
https://speakerdeck.com/dfm/data-analysis-with-mcmc1
These slides are available at

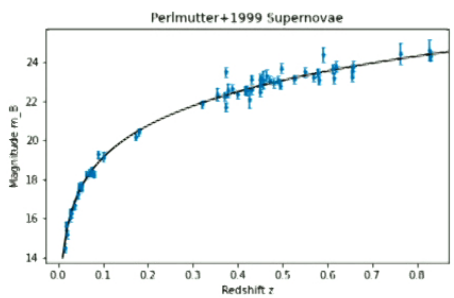
https://github.com/dstndstn/MCMC-talk/emcee-slides

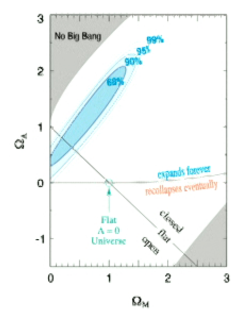
1

Recap from last lecture (1)

- Markov Chain Monte Carlo (MCMC) *draws samples from a probability distribution* when you can *numerically evaluate* the probability function (up to a constant)
- Used extensively in data analysis: *inferring* parameters of models, given observed data
- *Usually* in a Bayesian context; the probability function we run MCMC on is the *posterior* probability:

$$\text{posterior}(\text{params}|\text{data}) \propto \text{prior}(\text{params}) \times \text{likelihood}(\text{data}|\text{params})$$

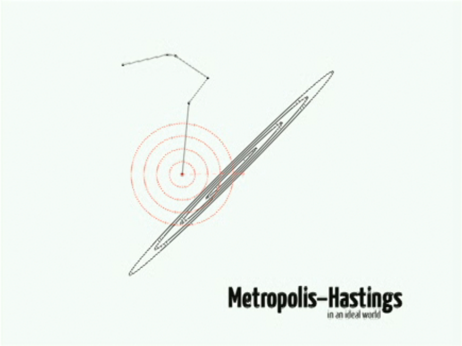




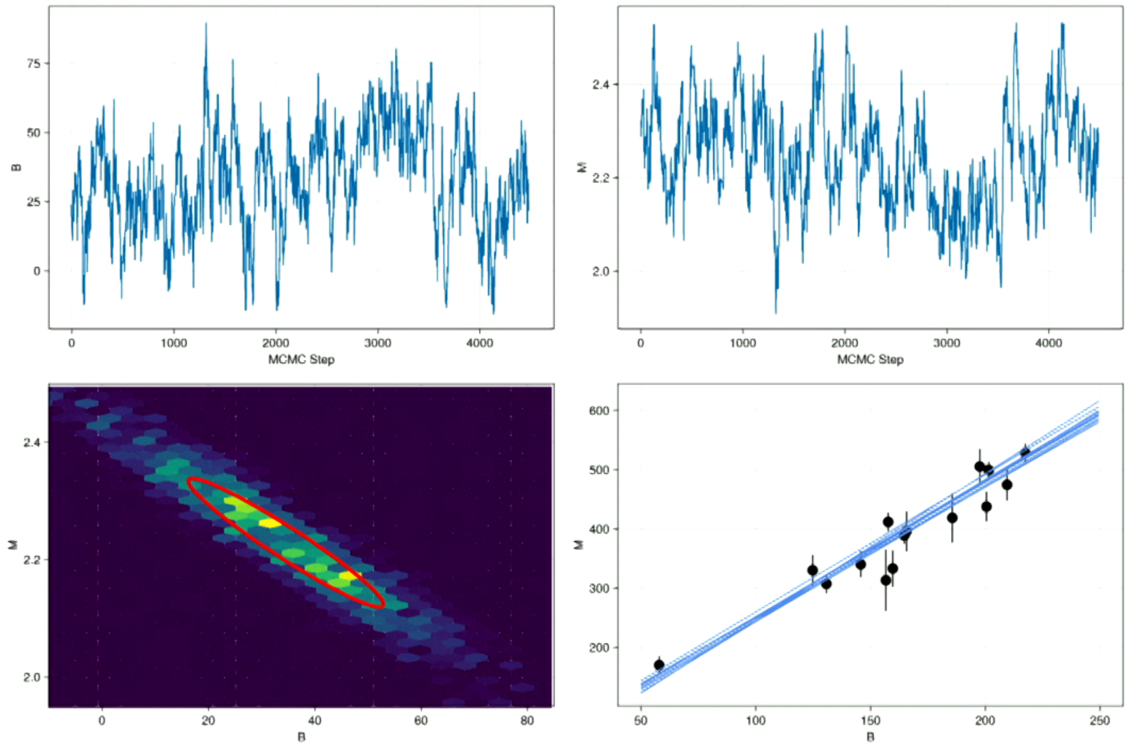
2

Recap from last lecture (2)

- The "classic" Markov Chain Monte Carlo algorithm is *Metropolis–Hastings*, which moves a *walker* or *particle* around the *state space* (*model parameter space*)
- A randomly-drawn *proposed* jump gets *evaluated* (by calling the probability function), and then *accepted*, or not
- A big difficulty is to *customize* the *proposal distribution* to get the algorithm to work efficiently



MCMC for model parameter inference



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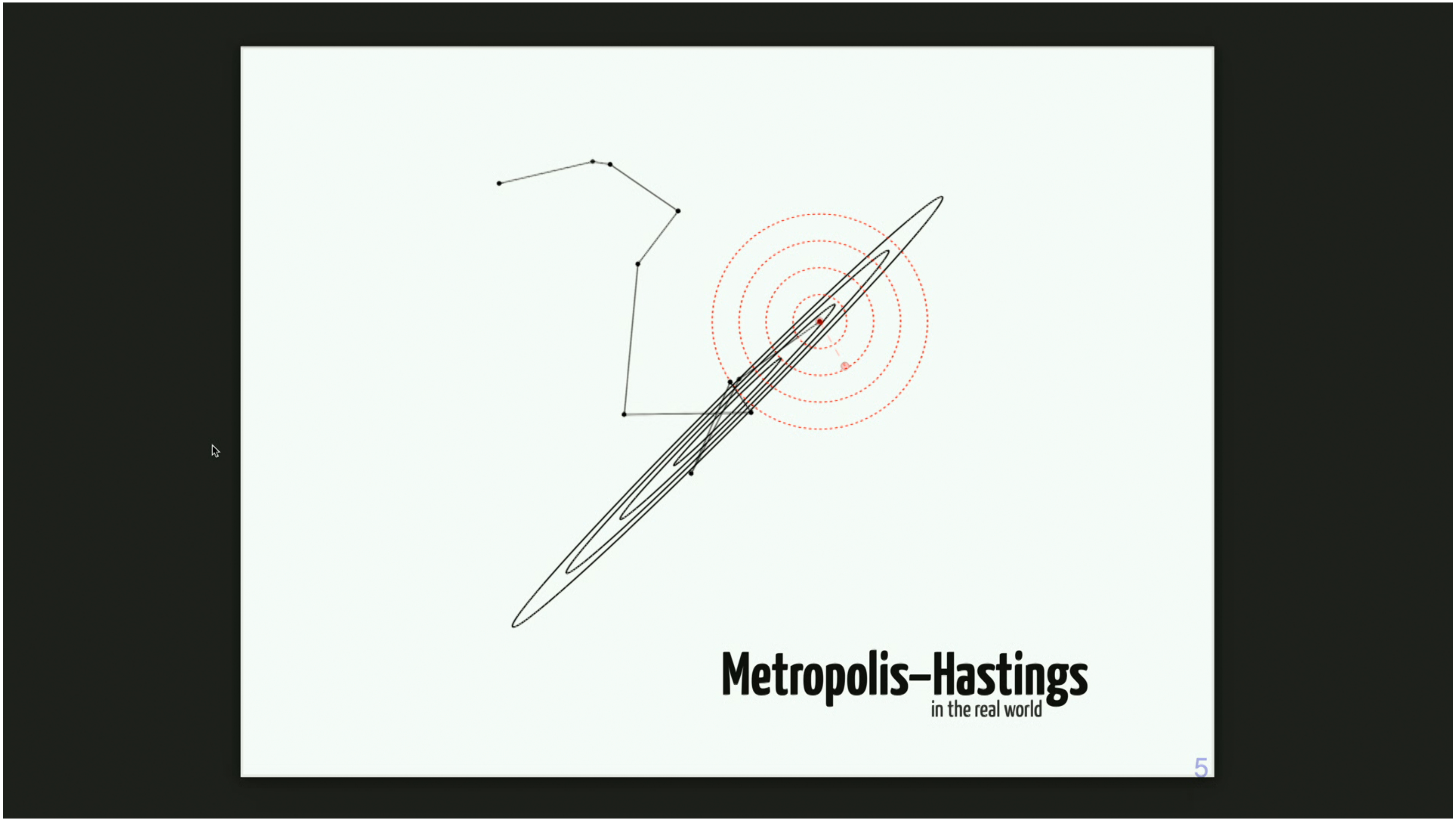

Metropolis–Hastings
in the real world
5

Jonathan Goodman

Jonathan Weare

"Ensemble samplers with affine invariance"

(dfm.io/mcmc-gw10)

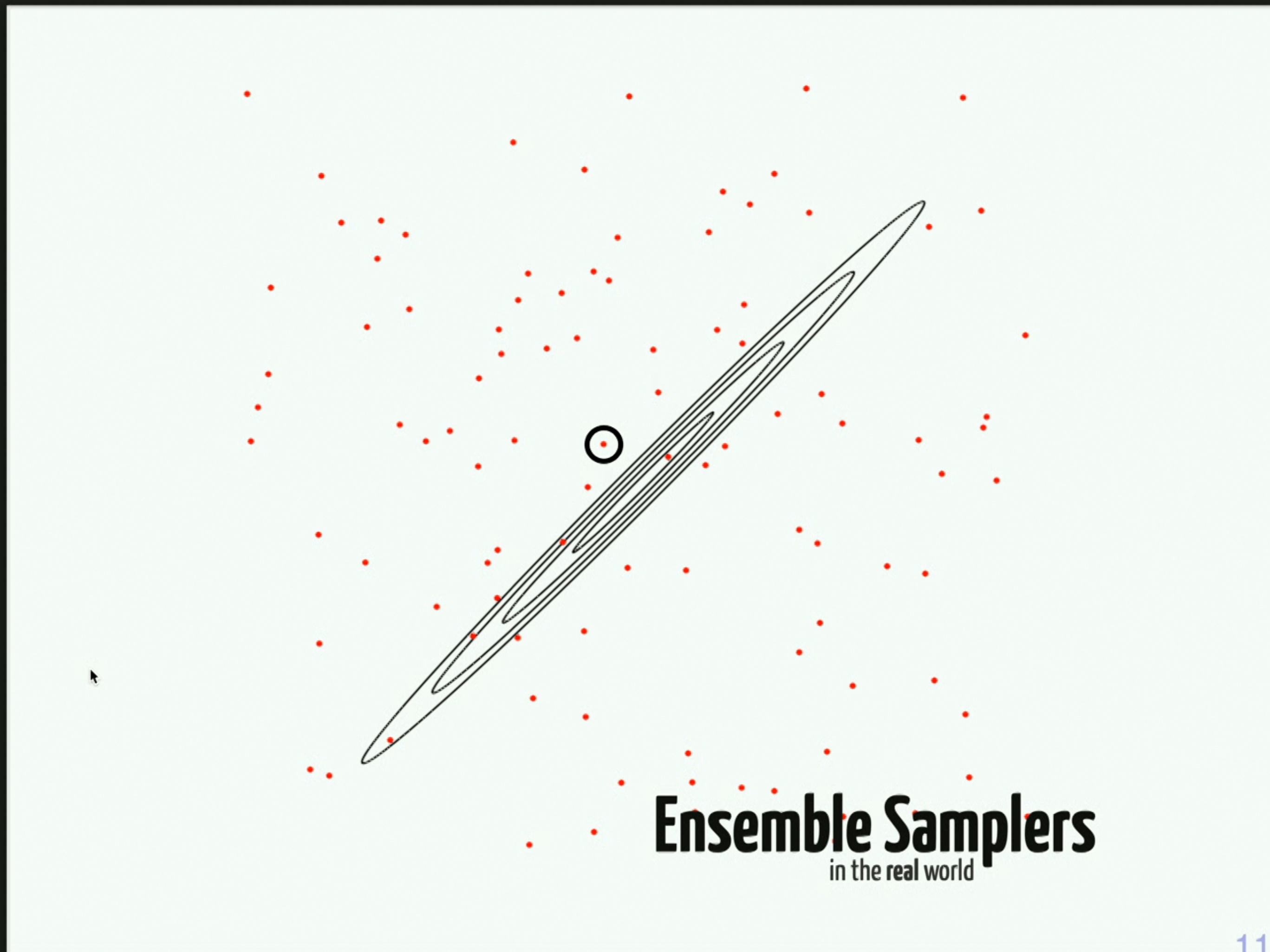
8

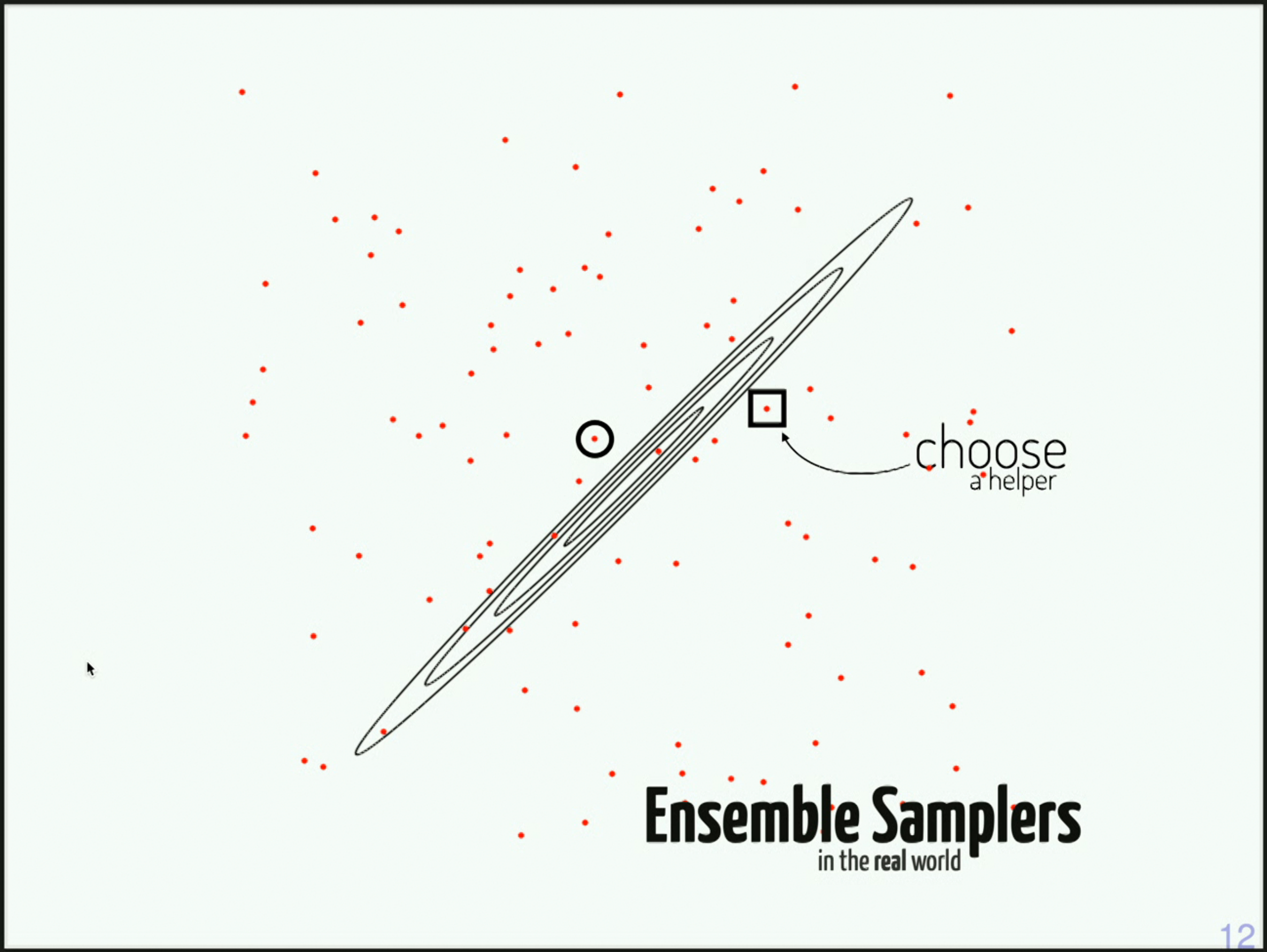
introducing **emcee** the MCMC Hammer

arxiv.org/abs/1202.3665

dan.iel.fm/emcee


Ensemble Samplers
in the real world
10


Ensemble Samplers
in the real world
11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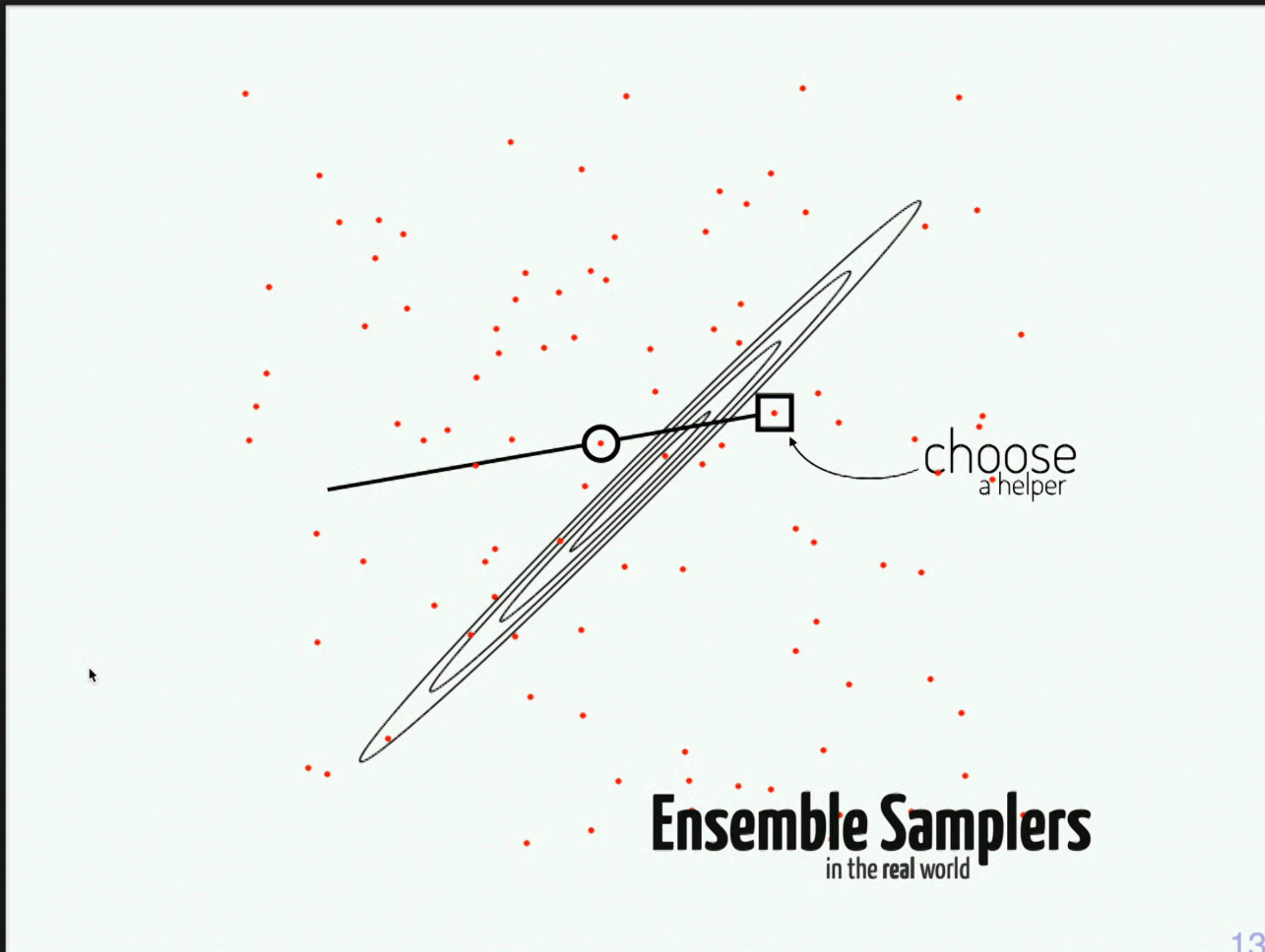
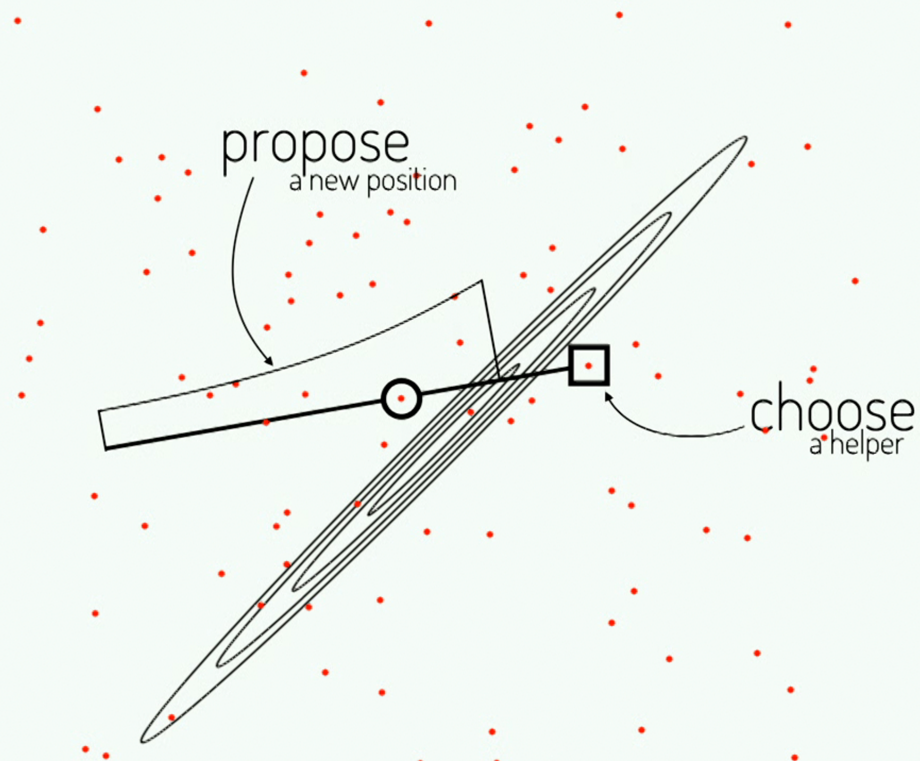
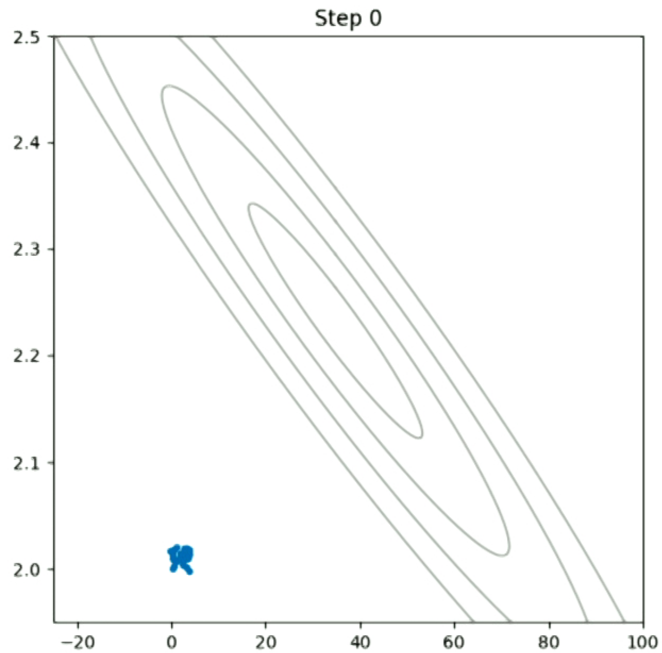
Ensemble Samplers
in the real world
12


choose
a helper
Ensemble Samplers
in the real world
13



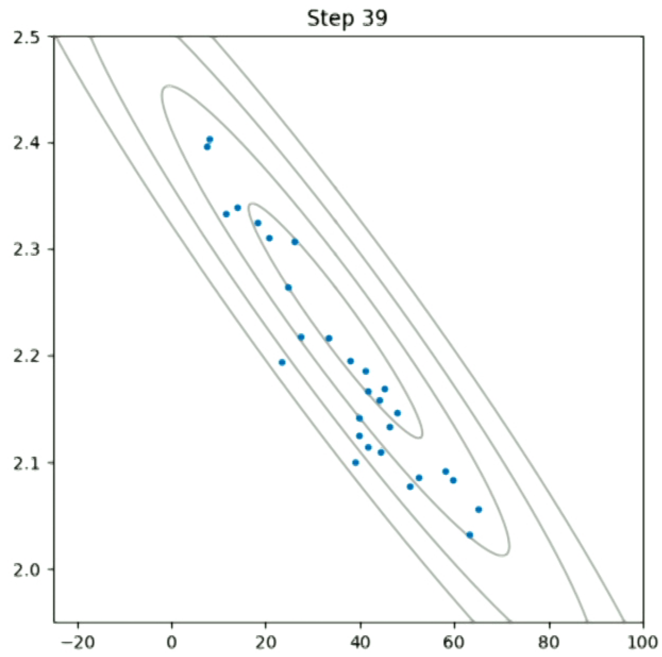
Ensemble Samplers
in the **real** world

Emcee demo



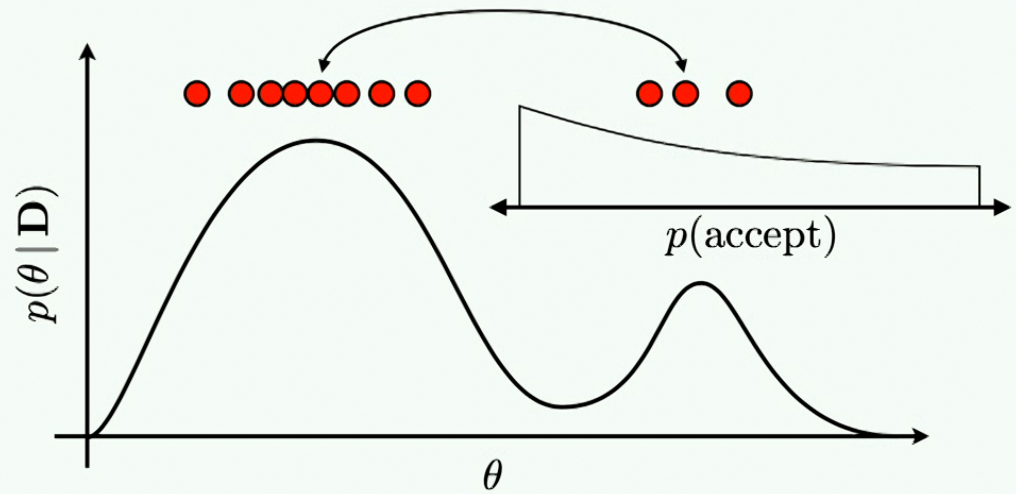
15

Emcee demo



54

what about multimodal densities?



Differential Evolution move

- emcee allows us to use different *move* types (different *proposal* functions)
- The Differential Evolution (DE) move can improve the sampling for multi-modal distributions
- DE move: randomly select *two* “helpers”
- Propose moving by their vector difference
- (If they are from different modes, this proposes *jumping between modes*)
- Mixing in a fraction of DE moves with the regular “Stretch” move works well!

Summary

- Traditional Metropolis–Hastings MCMC suffers from a *lack of affine invariance* – requires *tuning parameters* that change for each specific probability function
- *Ensemble samplers* like emcee use the *distribution of the walkers* to achieve *affine invariance*
- $\rightarrow$ much easier to use, and faster sampling
- (Huge side effect: parallelizable!)
- Multi-modal distributions still hard, but *DE Move* can help

https://symmetry.pi.local/user/dlang/lab/workspaces/auto-w/tree/home/dlang/MCMC-talk/notebooks-julia/MCMC-homework

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Launcher | MCMC-homework-hints.ipy

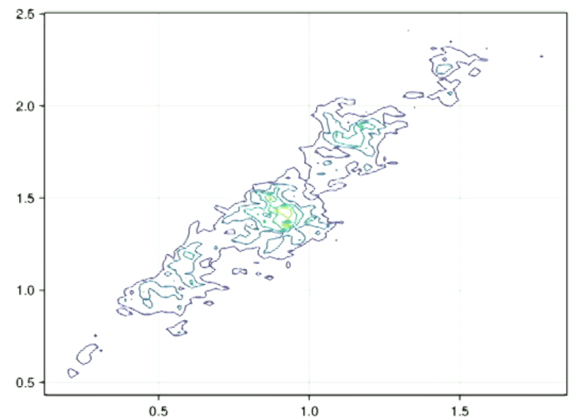
Code | Julia 1.9.3

0.08 1.86

[19]:
```
counts = bincounts(h);
xc,yc = bincenters(h);
```

[20]:
```
contour(xc, yc, counts) #, levels=[10,50,100])
```

[20]:



[21]:
```
import Pkg; Pkg.add("AffineInvariantMCMC")
```

```
   Resolving package versions...
   Installed RobustPmap ────────── v1.0.2
   Installed JLD2 ──────────────── v0.4.45
   Installed AffineInvariantMCMC ─ v1.2.2
    Updating `~/.julia/environments/v1.9/Project.toml`
  [a0f608ac] + AffineInvariantMCMC v1.2.2
    Updating `~/.julia/environments/v1.9/Manifest.toml`
  [a0f608ac] + AffineInvariantMCMC v1.2.2
  [033835bb] + JLD2 v0.4.45
  [27aeedcb] + RobustPmap v1.0.2
Precompiling project...
  ✓ JLD2
  ✓ RobustPmap
  ✓ AffineInvariantMCMC
  3 dependencies successfully precompiled in 26 seconds. 297 already precompiled. 1 skipped during auto due to previous errors.
```

[25]:
```
using AffineInvariantMCMC
```

[101]:
```
numdims = 3
```

Simple 0 3 Julia 1.9.3 | Idle Mode: Command Ln 1, Col 20 MCMC-homework-hints.ipynb

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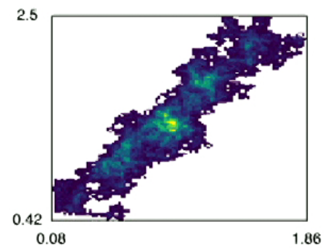
Code — Julia 1.9.3

[17]:
```
using FHist
```

[18]:
```
h = FHist.Hist2D((chain[:,2], chain[:,3]); nbins=(100,100))
```

[18]:

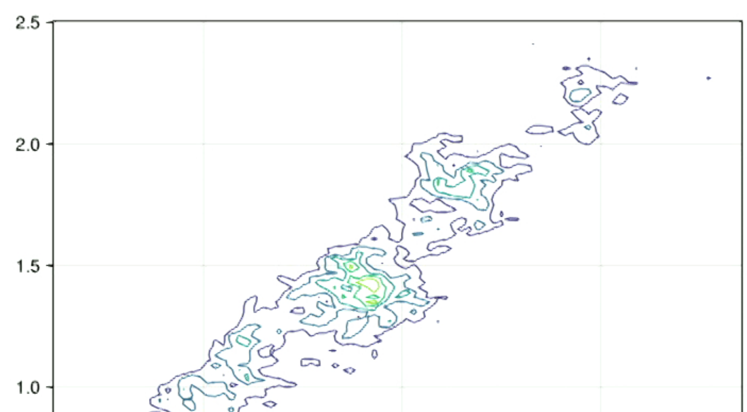


- edges: (0.08:0.02:1.86, 0.42:0.02:2.5)
- bin counts: [0 0 … 0 0; 0 0 … 0 0; … ; 0 0 … 0 0; 0 0 … 0 0]
- maximum count: 135
- total count: 50000

[19]:
```
counts = bincounts(h);
xc,yc = bincenters(h);
```

[20]:
```
contour(xc, yc, counts) #, levels=[10,50,100])
```

[20]:



Simple 0 3 Julia 1.9.3 | Idle Mode: Edit Ln 1, Col 60 MCMC-homework-hints.ipynb

I haven't actually tried fine-tuning the step sizes myself, nor in fact have I tried making the histogram and contour plot!

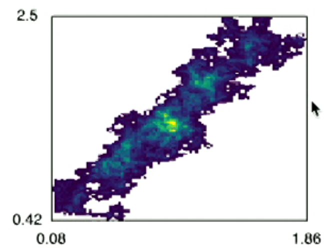
[16]:
```julia
using Pkg
Pkg.add("FHist")
```

```
  Resolving package versions...
 No Changes to `~/.julia/environments/v1.9/Project.toml`
 No Changes to `~/.julia/environments/v1.9/Manifest.toml`
```

[17]:
```julia
using FHist
```

[18]:
```julia
h = FHist.Hist2D((chain[:,2], chain[:,3]); nbins=(100,100))
```

[18]:



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- bin counts: [0 0 ... 0 0; 0 0 ... 0 0; ... ; 0 0 ... 0 0; 0 0 ... 0 0]
- maximum count: 135
- total count: 50000

[19]:
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xc,yc = bincenters(h);
```

[20]:
```julia
contour(xc, yc, counts) #, levels=[10,50,100])
```

[20]:

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Julia 1.9.3

[21]:
```
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```

```
   Resolving package versions...
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Precompiling project...
  ✓ JLD2
  ✓ RobustPmap
  ✓ AffineInvariantMCMC
  3 dependencies successfully precompiled in 26 seconds. 297 already precompiled. 1 skipped during auto due to previous errors.
```

[25]:
```
using AffineInvariantMCMC
```

[101]:
```
numdims = 3
numwalkers = 50
thinning = 10
numsamples_perwalker = 10000
burnin = 100

logprob_func = p -> begin
    (M,Om,Ode) = p
    if Om < 0 || Ode < 0
        return -Inf
    end
    try
        return supernova_log_likelihood(data.z, data.mag, data.sigma_mag, p[1], p[2], p[3])
    catch e
        return -Inf
    end
end
initial = [abs_mag, 0.5, 0.5] .+ randn(numdims, numwalkers)*0.01

chain, ll = AffineInvariantMCMC.sample(logprob_func, numwalkers, initial, burnin, 1)
```

Simple 0 3 Julia 1.9.3 | Idle   Mode: Edit Ln 2, Col 23 MCMC-homework-hints.ipynb

[25]:
```
using AffineInvariantMCMC
```

[104]:
```
numdims = 3
numwalkers = 50
thinning = 10
numsamples_perwalker = 10000
burnin = 100

logprob_func = p -> begin
    (M,Om,Ode) = p
    if Om < 0 || Ode < 0
        return -Inf
    end
    try
        return supernova_log_likelihood(data.z, data.mag, data.sigma_mag, p[1], p[2], p[3])
    catch e
        return -Inf
    end
end
initial = [abs_mag, 0.5, 0.5] .+ randn(numdims, numwalkers)*0.01

chain, ll = AffineInvariantMCMC.sample(logprob_func, numwalkers, initial, burnin, 1)
chain, ll = AffineInvariantMCMC.sample(logprob_func, numwalkers, chain[:,:,end], numsamples_perwalker, thinning)
flatchain, flatllhoodvals = AffineInvariantMCMC.flattenmcmcarray(chain, ll)
;
```

```
Progress: 100%|████████████████████████████████| Time: 0:00:08
```

[105]:
```
size(chain)
```

[105]:
```
(3, 50, 1000)
```

[106]:
```
size(flatchain)
```

[106]:
```
(3, 50000)
```

[103]:
```
S = 10
scatter(flatchain[2,1:S:end], flatchain[3,1:S:end])
```

[103]:

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```
        return supernova_log_likelihood(data.z, data.mag, data.sigma_mag, p[1], p[2], p[3])
    catch e
        return -Inf
    end
end
initial = [abs_mag, 0.5, 0.5] .+ randn(numdims, numwalkers)*0.01

chain, ll = AffineInvariantMCMC.sample(logprob_func, numwalkers, initial, burnin, 1)
chain, ll = AffineInvariantMCMC.sample(logprob_func, numwalkers, chain[:,:,end], numsamples_perwalker, thinning)
flatchain, flatllhoodvals = AffineInvariantMCMC.flattenmcmcarray(chain, ll)
;
```

Progress: 100%| | Time: 0:00:08

[105]: `size(chain)`

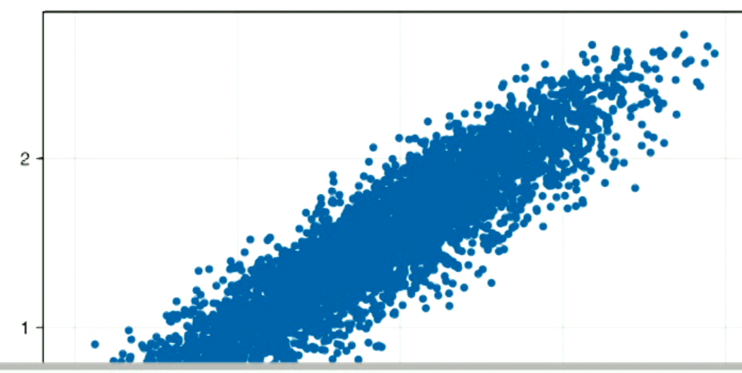
[105]: (3, 50, 1000)

[106]: `size(flatchain)`

[106]: (3, 50000)

[103]:
```
S = 10
scatter(flatchain[2,1:S:end], flatchain[3,1:S:end])
```

[103]:



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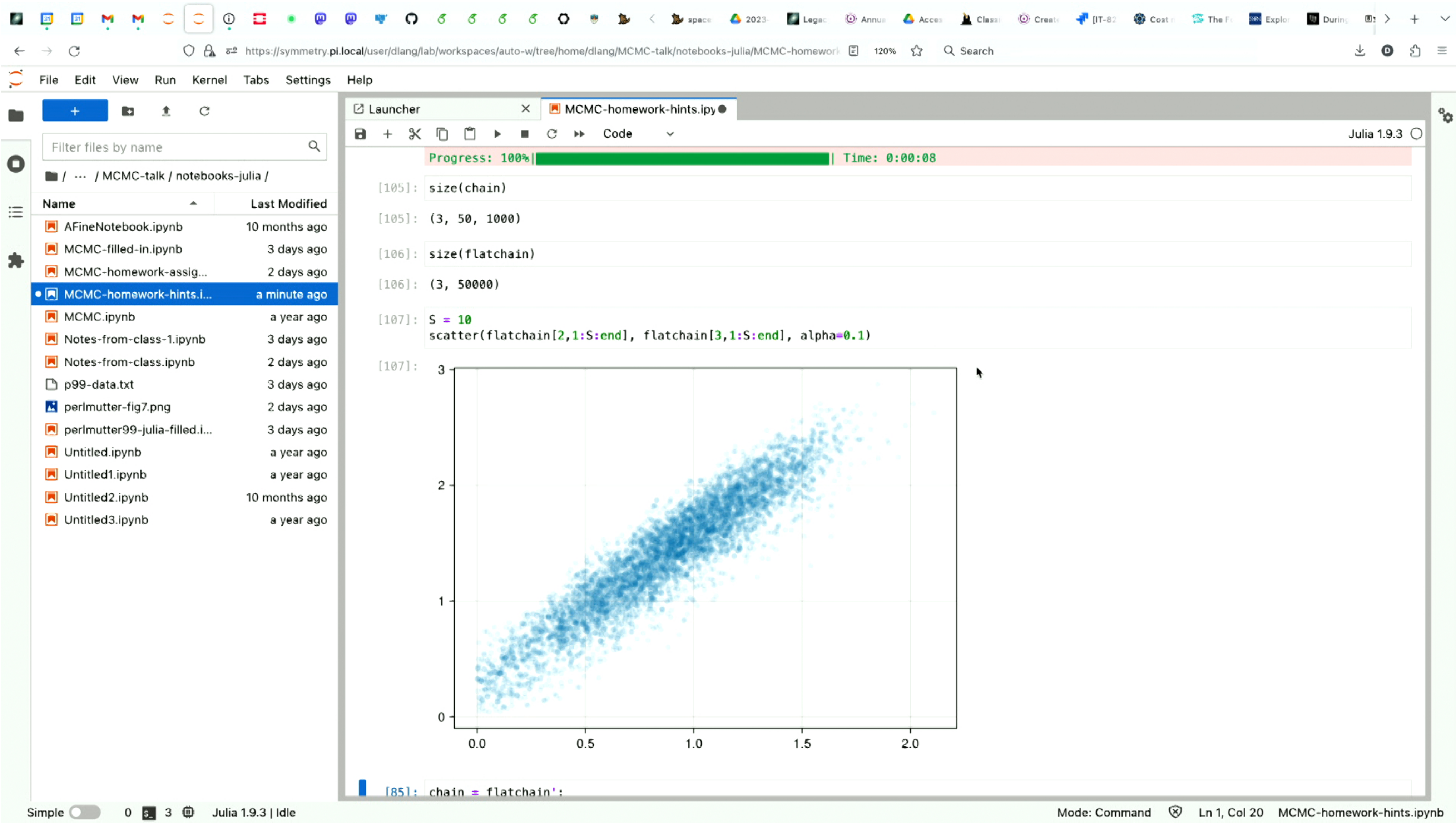
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Launcher
MCMC-homework-hints.ipy
Code
Julia 1.9.3
Progress: 100%| | Time: 0:00:08
[105]: size(chain)
[105]: (3, 50, 1000)
[106]: size(flatchain)
[106]: (3, 50000)
[107]: S = 10
scatter(flatchain[2,1:S:end], flatchain[3,1:S:end], alpha=0.1)
[107]:
[85]: chain = flatchain';
Simple 0 3 Julia 1.9.3 | Idle
Mode: Command Ln 1, Col 20 MCMC-homework-hints.ipynb

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Untitled3.ipynb	a year ago

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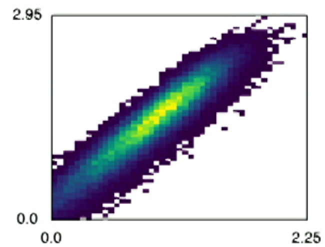
Julia 1.9.3

[108]:
```
chain = flatchain';
```

[109]:
```
h = FHist.Hist2D((chain[:,2], chain[:,3]); nbins=(100,100))
```

[109]:

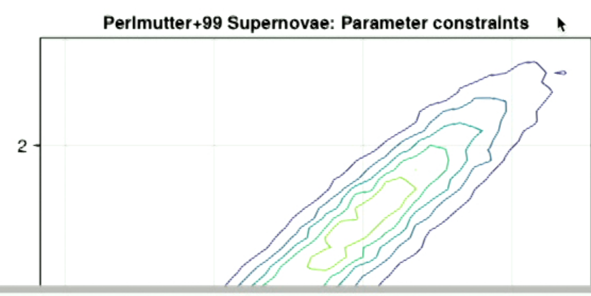


- edges: (0.0:0.05:2.25, 0.0:0.05:2.95)
- bin counts: [17 27 … 0 0; 16 22 … 0 0; … ; 0 0 … 0 0; 0 0 … 0 0]
- maximum count: 262
- total count: 50000

[98]:
```
counts = bincounts(h);
xc,yc = bincenters(h);

f = Figure(size=(500,500))
Axis(f[1,1], title="Perlmutter+99 Supernovae: Parameter constraints", xlabel=L"\Omega_M", ylabel=L"\Omega_{\Lambda}")
contour!(xc, yc, counts) #, levels=[10,50,100])
lines!([0,1], [1,0])
f
```

[98]:



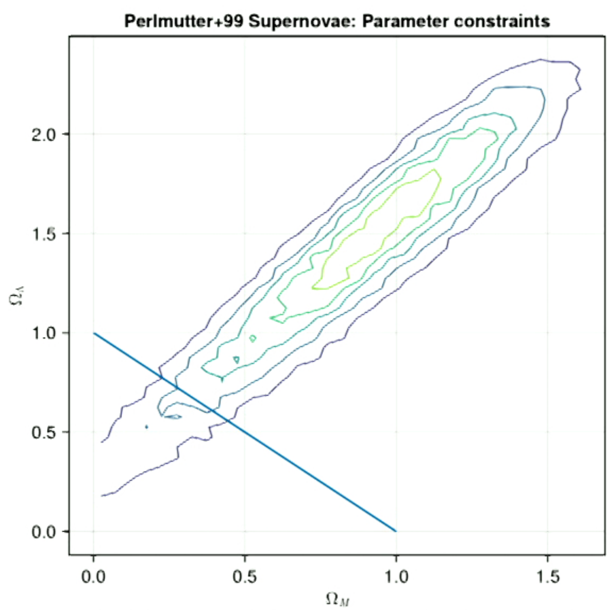
Simple 0 3 Julia 1.9.3 | Idle Mode: Command Ln 4, Col 23 MCMC-homework-hints.ipynb

[110]:

```
counts = bincounts(h);
xc,yc = bincenters(h);

f = Figure(size=(500,500))
Axis(f[1,1], title="Perlmutter+99 Supernovae: Parameter constraints", xlabel=L"\Omega_M", ylabel=L"\Omega_{\Lambda}")
contour!(xc, yc, counts) #, levels=[10,50,100])
lines!([0,1], [1,0])
f
```

[110]:



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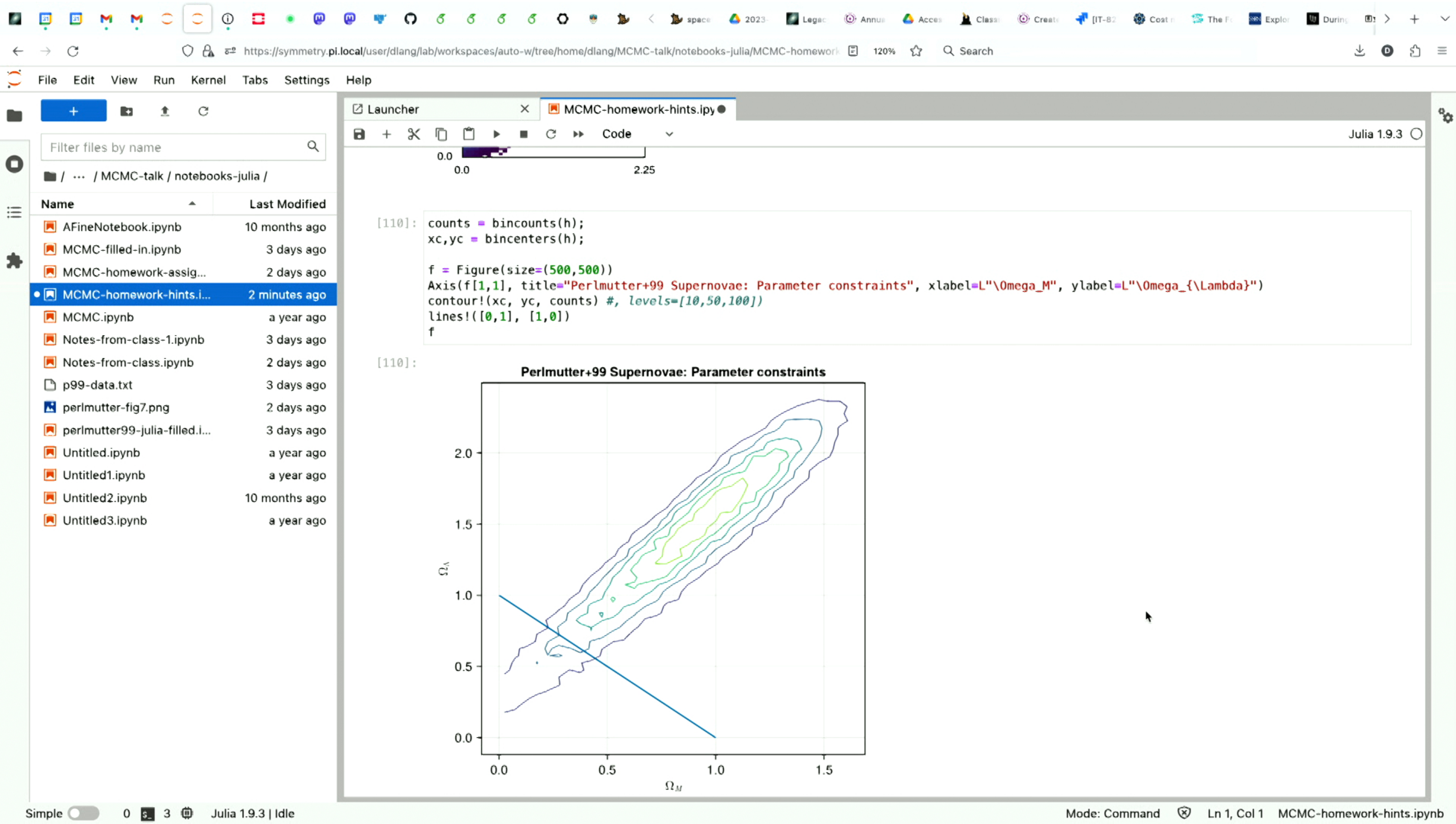
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Untitled1.ipynb a year ago
Untitled2.ipynb 10 months ago
Untitled3.ipynb a year ago
Launcher
MCMC-homework-hints.ipy
Code
Julia 1.9.3
[110]:
counts = bincounts(h);
xc,yc = bincenters(h);
f = Figure(size=(500,500))
Axis(f[1,1], title="Perlmutter+99 Supernovae: Parameter constraints", xlabel=L"\Omega_M", ylabel=L"\Omega_{\Lambda}")
contour!(xc, yc, counts) #, levels=[10,50,100])
lines!([0,1], [1,0])
f
[110]:
Perlmutter+99 Supernovae: Parameter constraints
Simple 0 3 Julia 1.9.3 | Idle
Mode: Command Ln 1, Col 1 MCMC-homework-hints.ipynb

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/ ··· / MCMC-talk / notebooks-julia /

Name	Last Modified
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MCMC-homework-hints.i...	13 minutes ago
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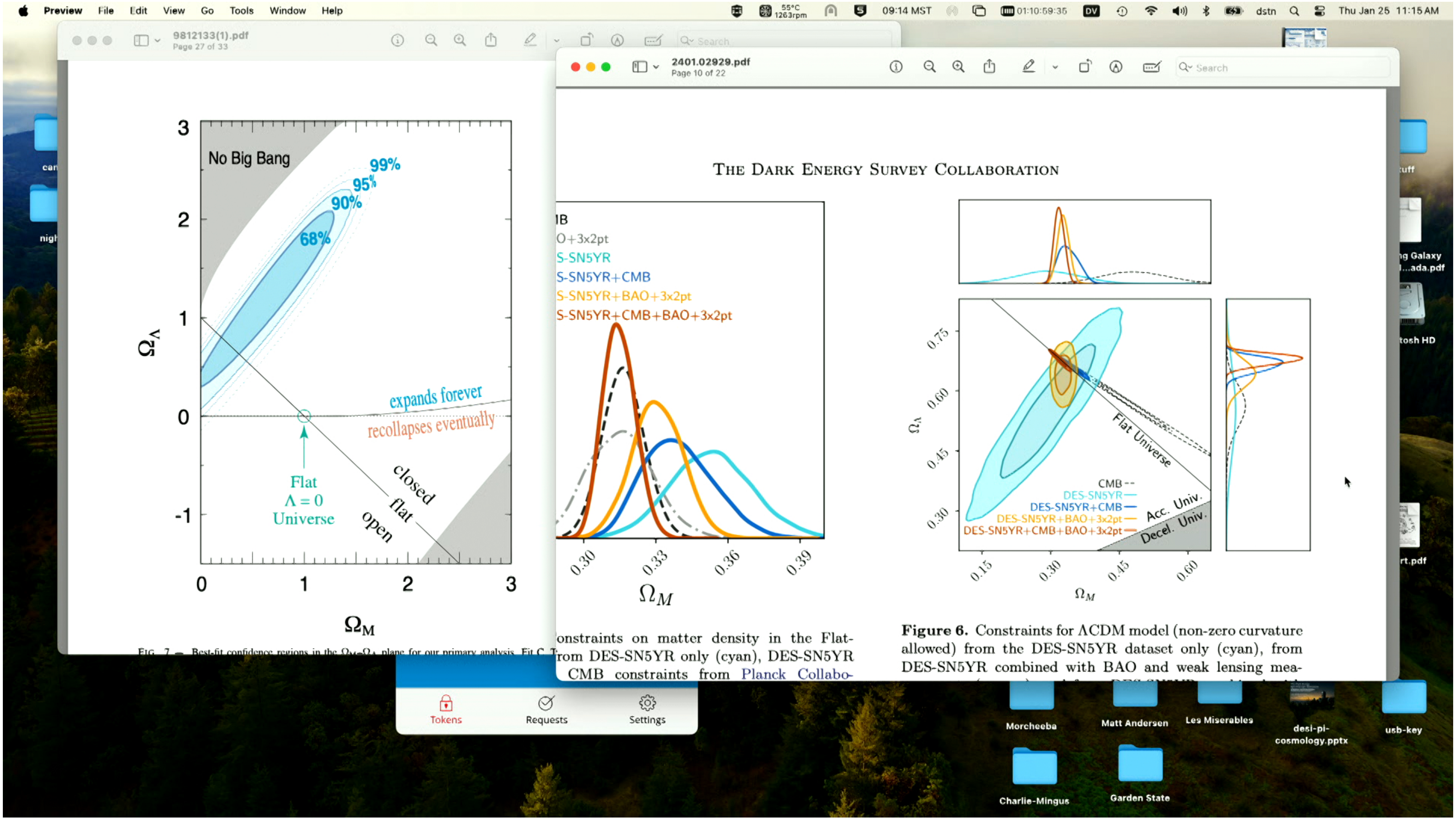
p99-data.txt	3 days ago
perlmutter-fig7.png	2 days ago
perlmutter99-julia-filled.i...	3 days ago
Untitled.ipynb	a year ago
Untitled1.ipynb	a year ago
Untitled2.ipynb	10 months ago
Untitled3.ipynb	a year ago

[111]:

```julia
Om_lo,Om_hi = 0.0, 2.0
Ode_lo,Ode_hi = 0.0, 2.0
MM = range(Om_lo, stop=Om_hi, length=100)
DD = range(Ode_lo, stop=Ode_hi, length=100)
LL = zeros((length(MM), length(DD)))
for i in 1:length(MM)
    for j in 1:length(DD)
        #try
            LL[i, j] = supernova_log_likelihood(data.z, data.mag, data.sigma_mag, abs_mag, MM[i], DD[j])
        #catch e
        #    LL[i, j] = -Inf
        #end
    end
end

maxlogprob = maximum(LL)

f = Figure()
Axis(f[1,1], title="Supernova constraints", xlabel="Omega matter", ylabel="Omega darkenergy")
hm = heatmap!(MM, DD, LL, colorrange=[maxlogprob-20, maxlogprob])
Colorbar(f[:, end+1], hm)
f
```

```
DomainError with -0.0006210338577678176:
sqrt will only return a complex result if called with a complex argument. Try sqrt(Complex(x)).

Stacktrace:
  [1] throw_complex_domainerror(f::Symbol, x::Float64)
    @ Base.Math ./math.jl:33
  [2] sqrt
    @ ./math.jl:677 [inlined]
  [3] a2E
    @ ~/.julia/packages/Cosmology/eZT7X/src/Cosmology.jl:65 [inlined]
  [4] #3
    @ ~/.julia/packages/Cosmology/eZT7X/src/Cosmology.jl:181 [inlined]
  [5] evalrule(f::Cosmology.var"#3#4"{Cosmology.ClosedLCDM{Float64}}, a::Float64, b::Float64, x::Vector{Float64}, w::Vector{Float64}, g
w::Vector{Float64}, nrm::typeof(LinearAlgebra.norm))
    @ QuadGK ~/.julia/packages/QuadGK/OtnWt/src/evalrule.jl:30
  [6] #6
    @ ~/.julia/packages/QuadGK/OtnWt/src/adapt.jl:15 [inlined]
  [7] ntuple
    @ ./ntuple.jl:48 [inlined]
```

Simple 0 3 Julia 1.9.3 | Idle   Mode: Edit   Ln 17, Col 1   MCMC-homework-hints.ipynb



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Thu Jan 25 11:15 AM
9812133(1).pdf
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No Big Bang
99%
95%
90%
68%
expands forever
recollapses eventually
Flat
Λ = 0
Universe
closed
flat
open
Ω_Λ
Ω_M
2401.02929.pdf
Page 10 of 22
The Dark Energy Survey Collaboration
S-SN5YR
S-SN5YR+CMB
S-SN5YR+BAO+3x2pt
S-SN5YR+CMB+BAO+3x2pt
Flat Universe
CMB
DES-SN5YR
DES-SN5YR+CMB
DES-SN5YR+BAO+3x2pt
DES-SN5YR+CMB+BAO+3x2pt
Acc. Univ.
Decel. Univ.
Figure 6. Constraints for ΛCDM model (non-zero curvature allowed) from the DES-SN5YR dataset only (cyan), from DES-SN5YR combined with BAO and weak lensing mea-
onstraints on matter density in the Flat-
rom DES-SN5YR only (cyan), DES-SN5YR
CMB constraints from Planck Collabo-
Tokens
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