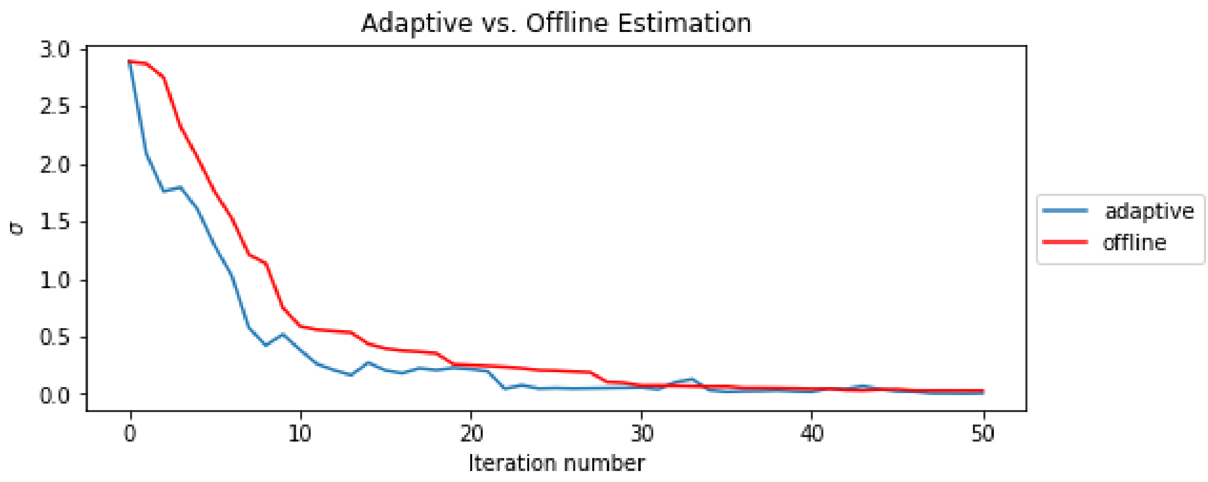
SMC with HMC resampling for some threshold ESS

1-d squared cosine (precession)

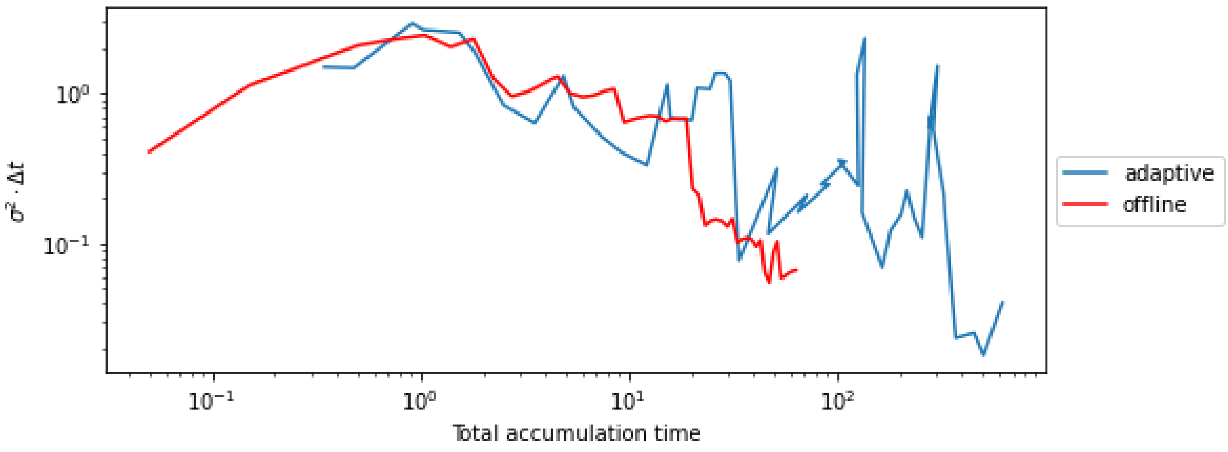
Sample run for 1000 particles, 30 steps:
Adaptive:
- Variance: 0.0001
- MSE: 0.0000 (actual error 0.00)
- Final precision: 0.03

Offline:
- Variance: 0.0121
- MSE: 0.0041 (actual error 0.06)
- Final precision: 0.28

(n=1000; N=30; f_max=10; threshold=n/2; runs=1; 1d, SHMC)



Adaptive estimation: k=1.00; 1 guess(es) per step
8 resampler calls, at steps: 2, 6, 9, 13, 16, 21, 22, 29
Offline estimation: increment=0.08
4 resampler calls, at steps: 5, 11, 22, 28



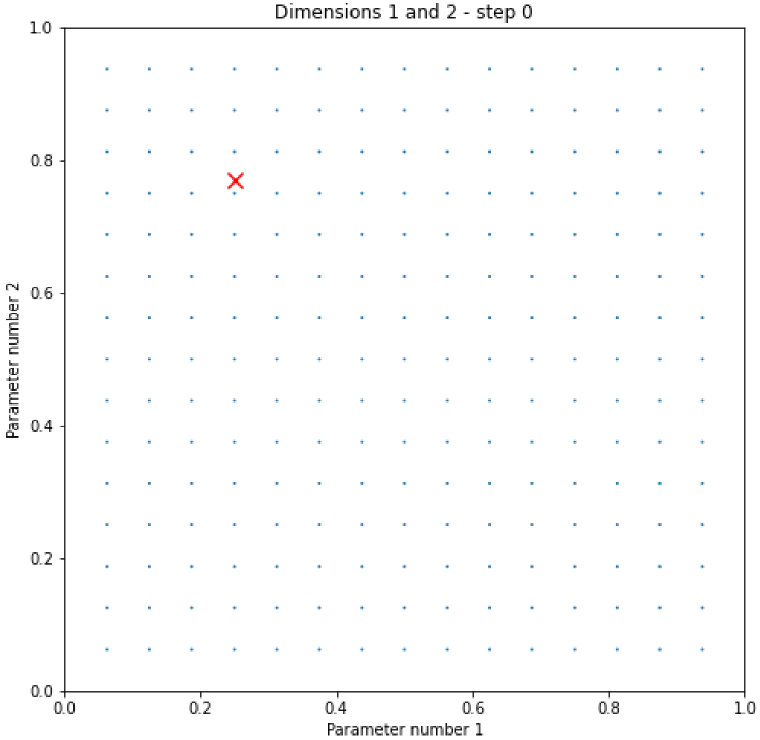
HMC: m=cov^-1, L=20, eta=0.0001
MH: s=cov, factor=1
* Percentage of HMC steps: 79.8%.
* Hamiltonian Monte Carlo: 98% mean particle acceptance rate.
* Metropolis-Hastings: 90% mean particle acceptance rate.

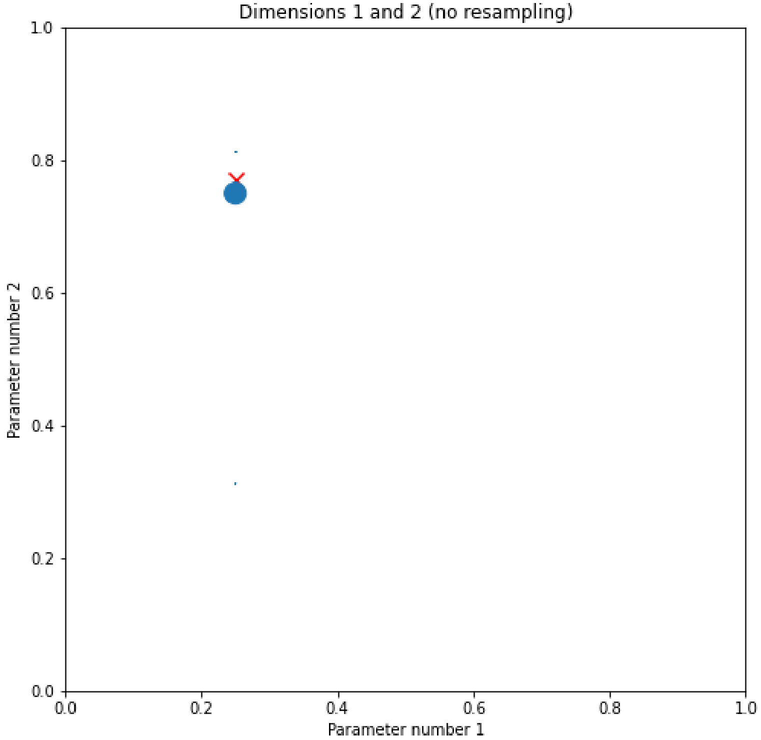
Multi-parameter case: multivariate squared cosine

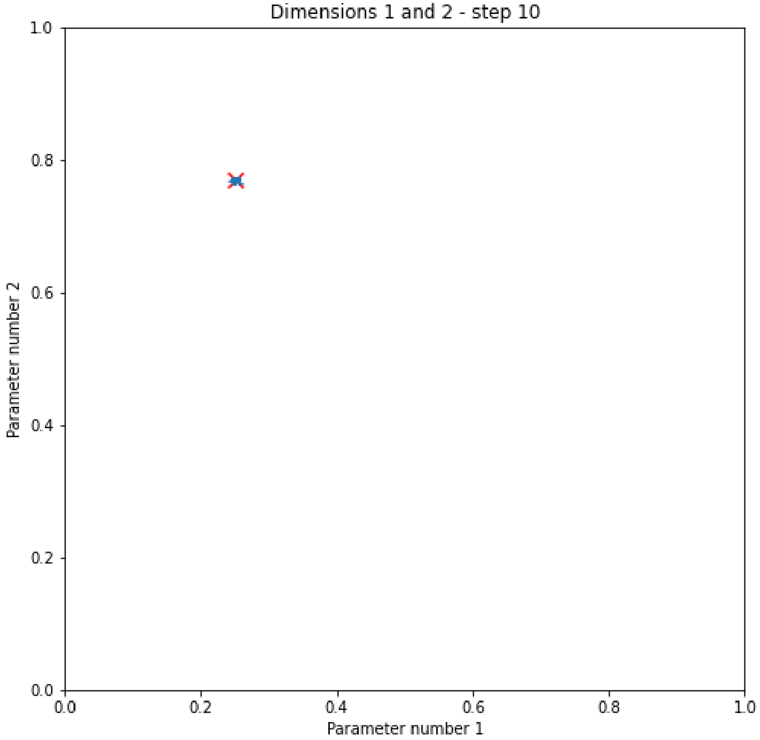
starting point

no resampling (for reference)

Final distribution:





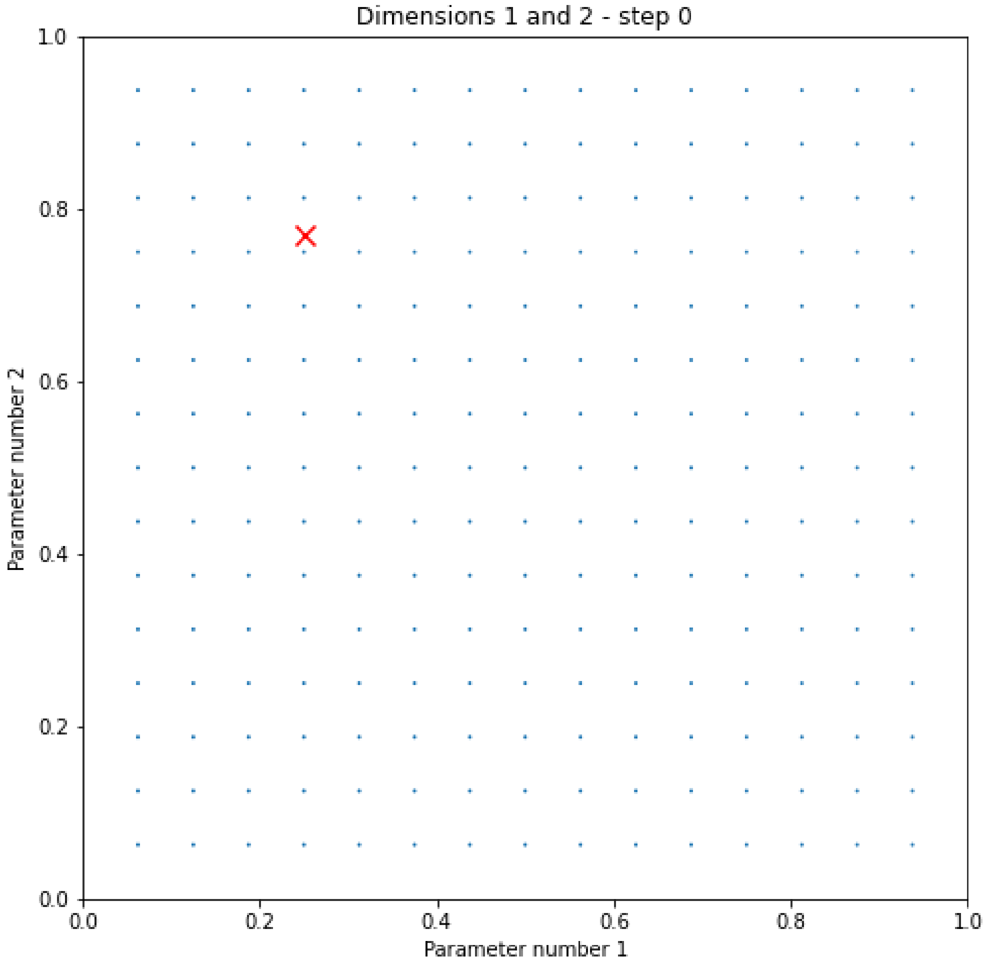


- Offline estimation: random times <= 50
- Uniform prior distribution (square lattice)
- 1 group of particles
- Data chunksize = 10 (10 experiments added per SMC step)
- HMC: Cov^-1, L=10, eta=0.005
- n=15^2; N=100; resampling threshold = 100; 2d

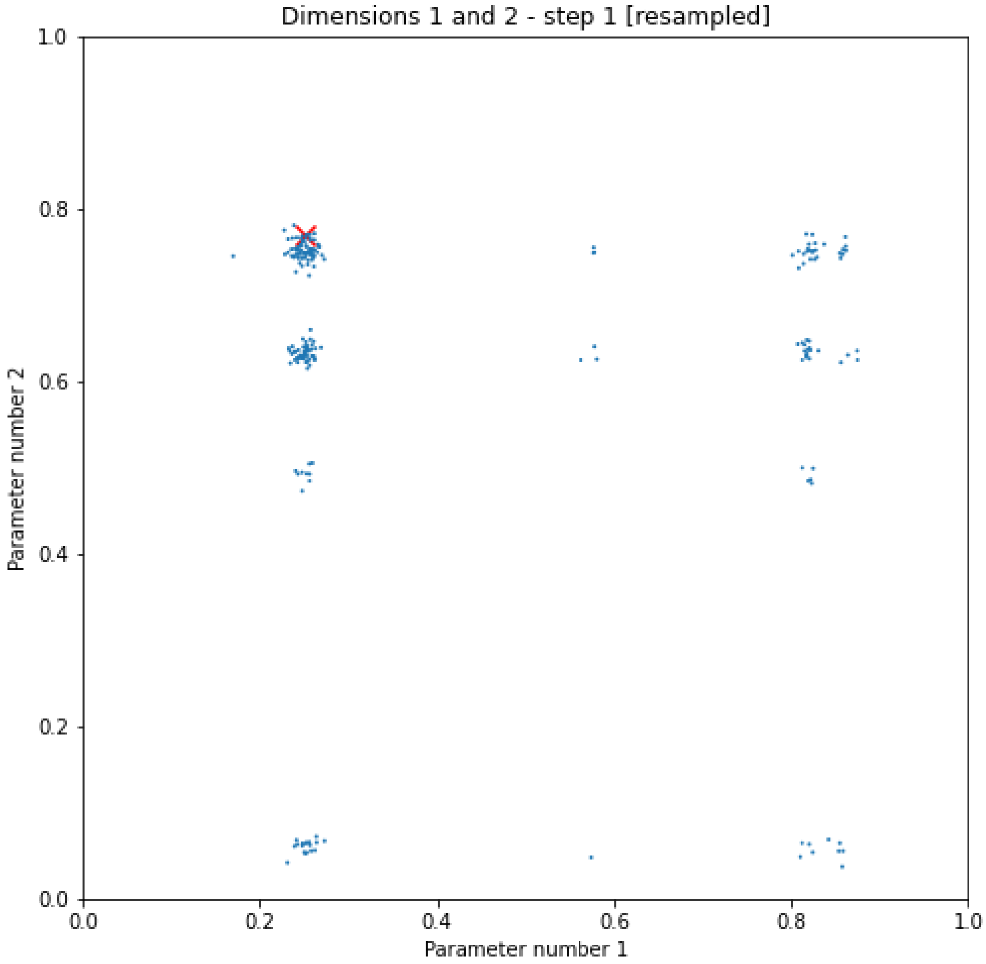
* Total resampler calls: 5.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 100% mean particle acceptance rate.

Bivariate squared cosine – step by step run of the algorithm

(100 experiments with chunksize 10 → 10 steps)

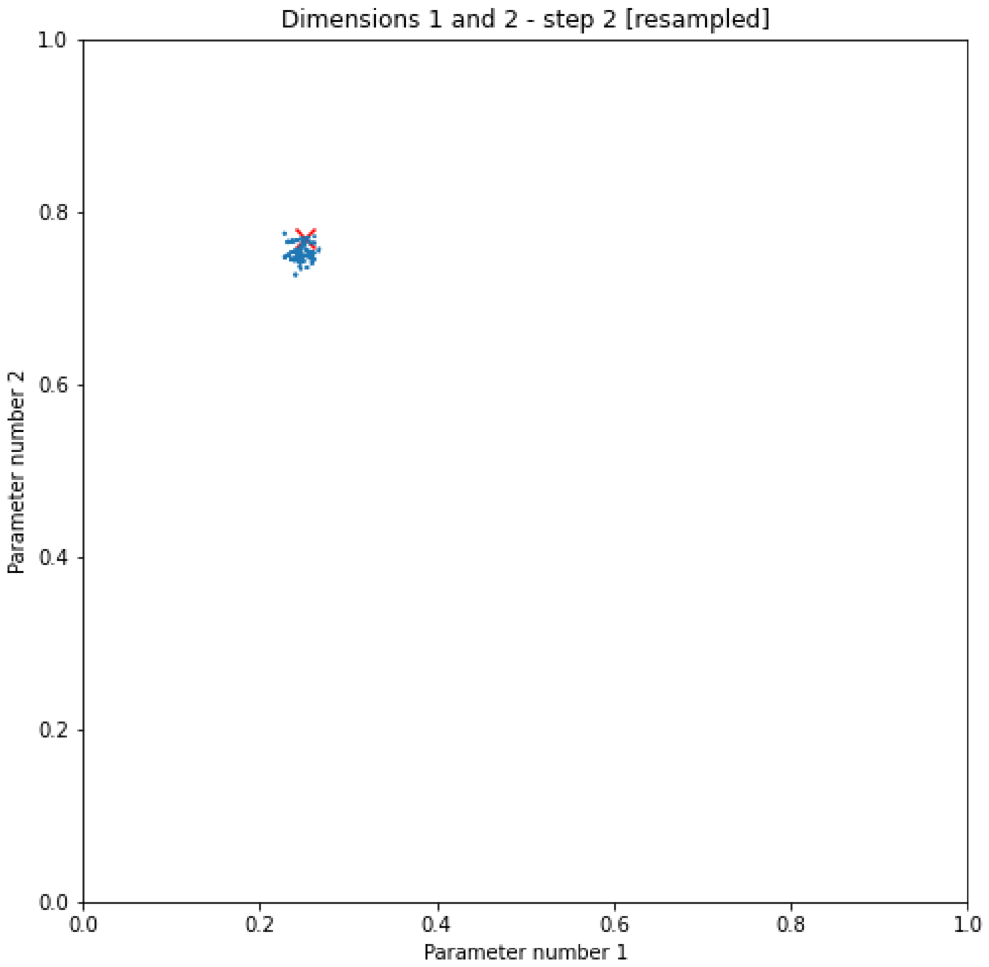


Bivariate squared cosine – step by step run of the algorithm

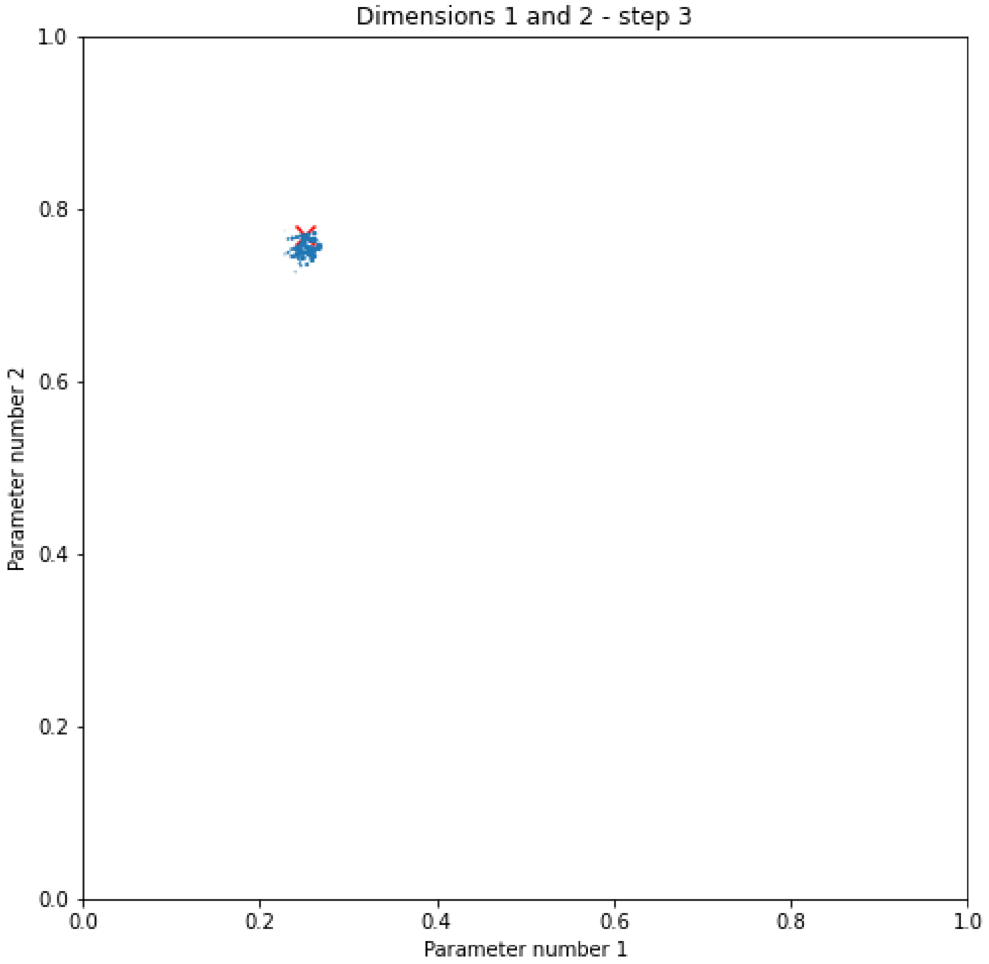


Bivariate squared cosine – step by step run of the algorithm

(100 experiments with chunksize 10 → 10 steps)

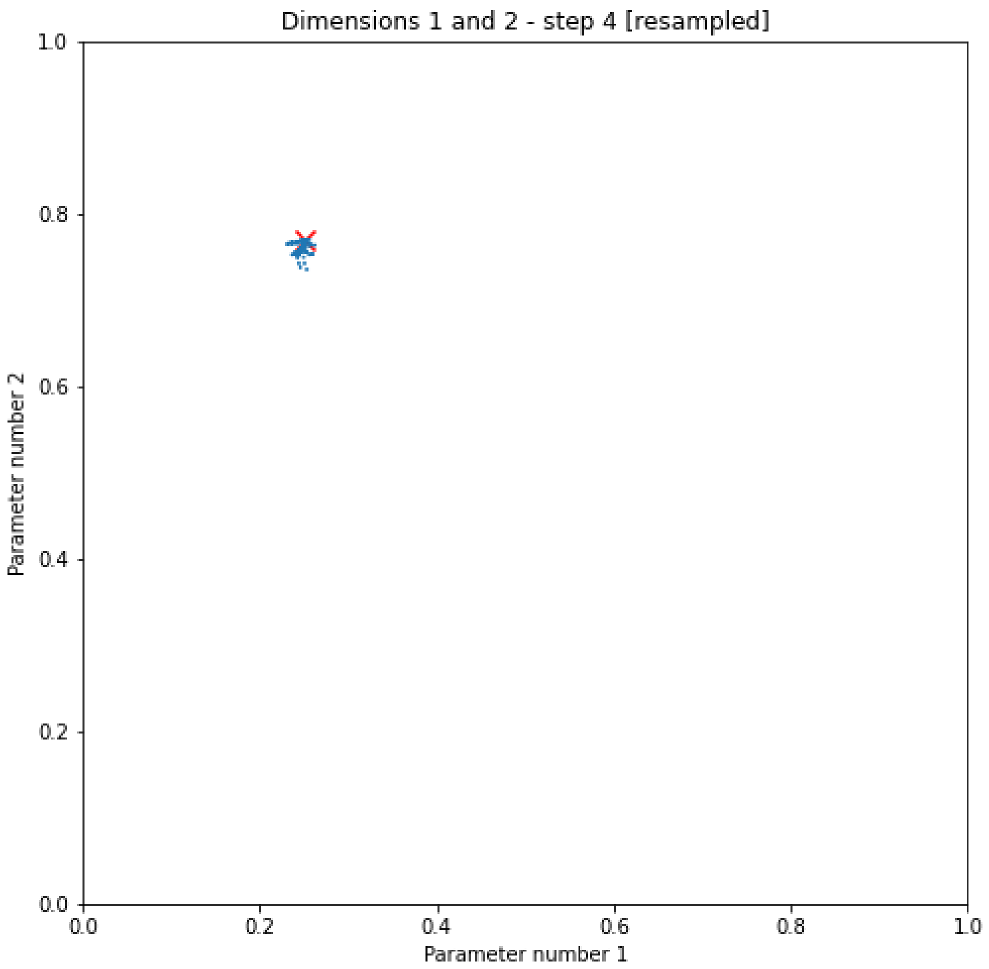


Bivariate squared cosine – step by step run of the algorithm

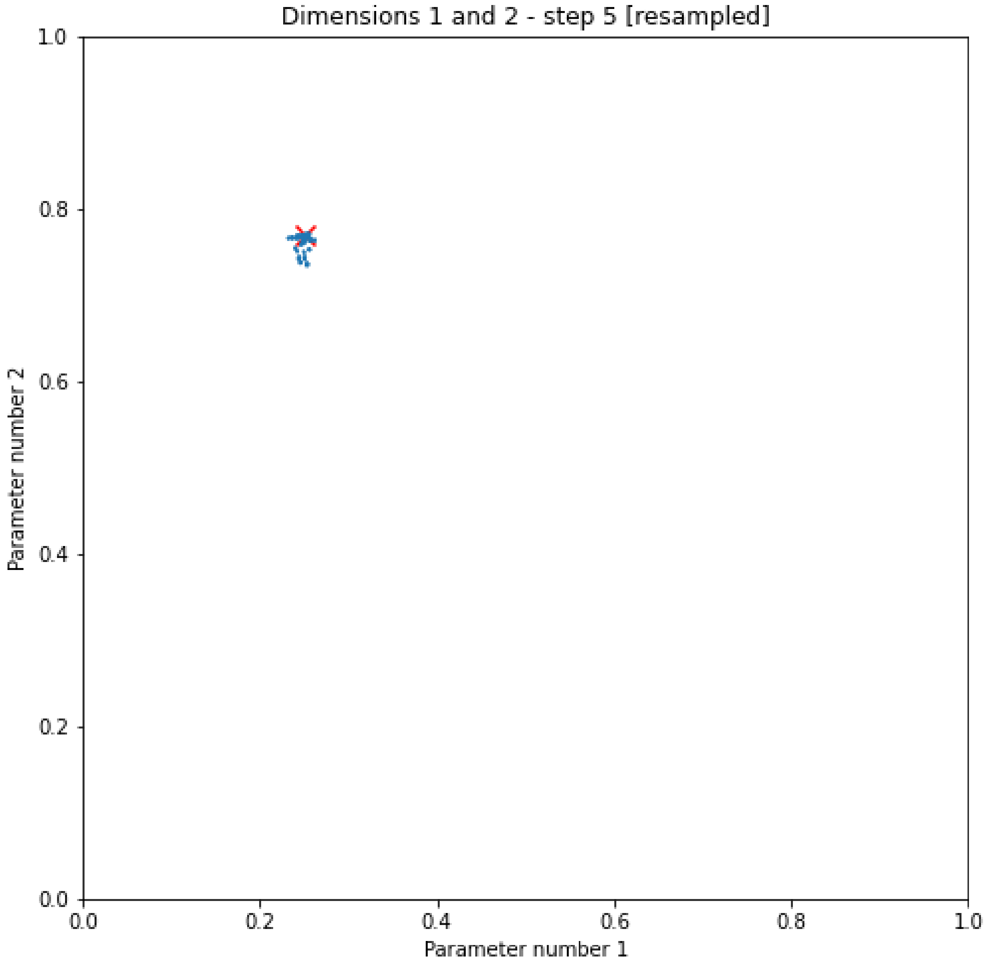


Bivariate squared cosine – step by step run of the algorithm

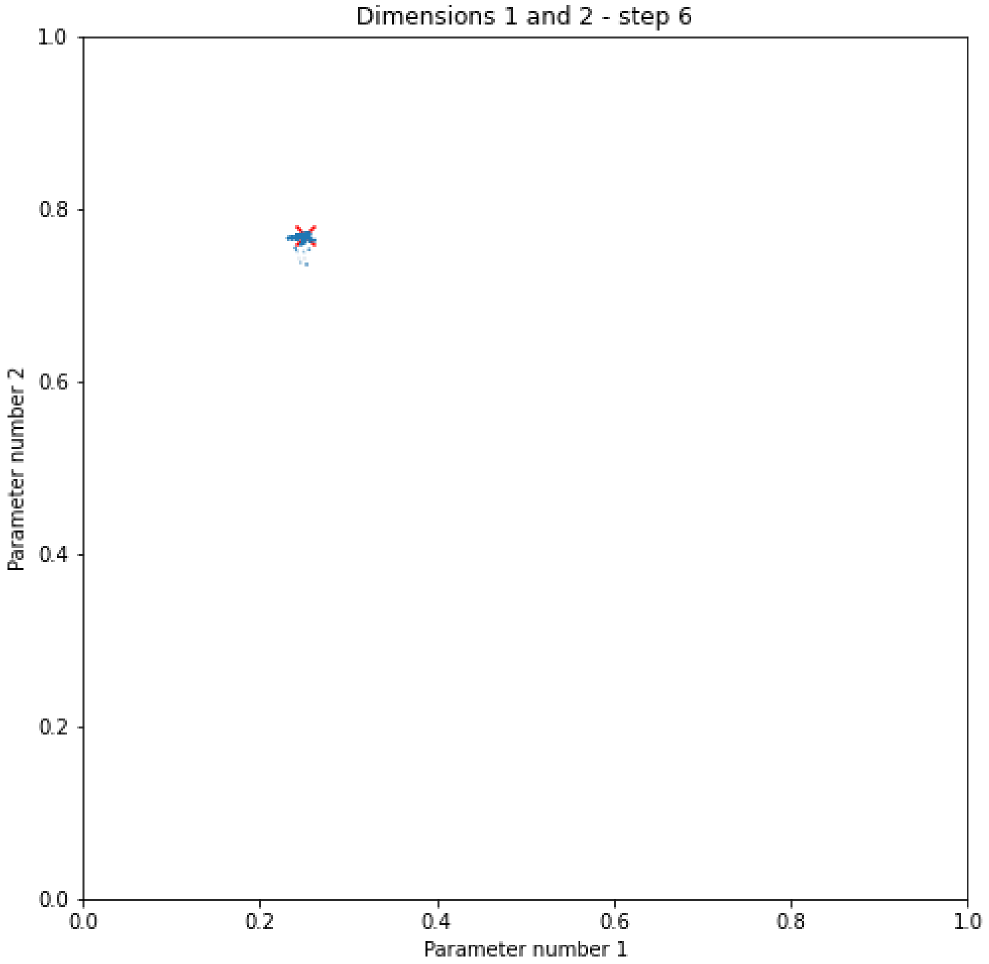
(100 experiments with hunksize 10 → 10 steps)



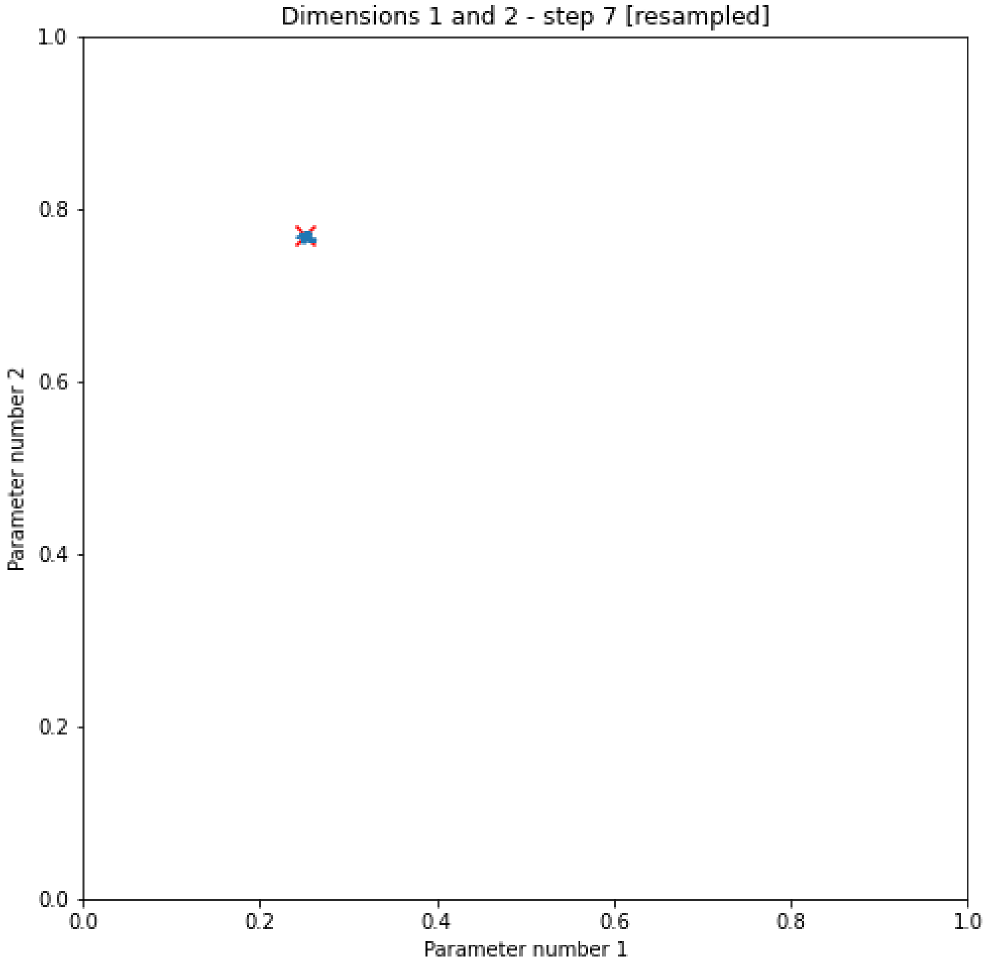
Bivariate squared cosine – step by step run of the algorithm



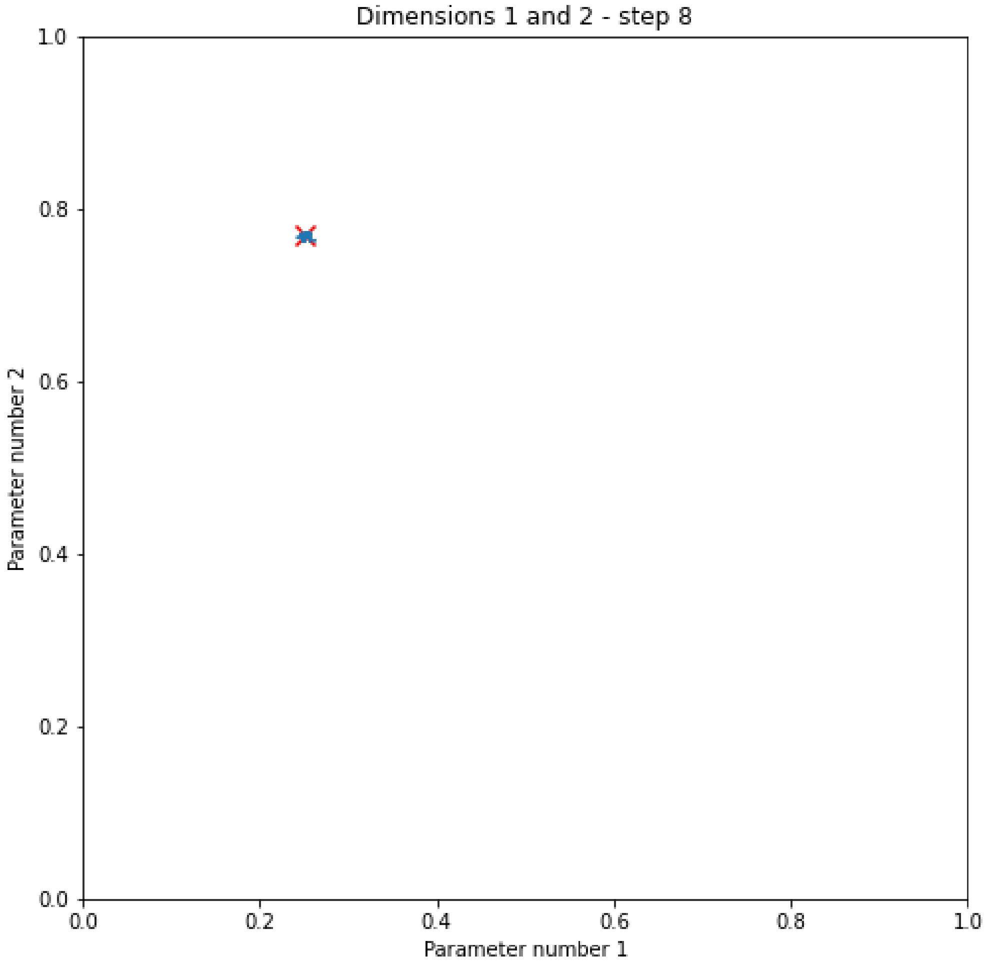
Bivariate squared cosine – step by step run of the algorithm



Bivariate squared cosine – step by step run of the algorithm



Bivariate squared cosine – step by step run of the algorithm



Multi-parameter, multi-modal case: squared cosine sum (univariate)

$$\frac{1}{dim}\sum_{d=1}^{dim}\cos^2(\boldsymbol{\theta_d}\frac{t}{2})$$

$$\vec{\boldsymbol{\theta}} = ?$$

(redundancy → all permutations)

- Measurement times chosen in advance and at random, $t_k \in [0,100]$
- Data chunksize of 1 used for all graphs here (i.e. umulative data up to datum *k* used at k^{th} step)
- Flat prior over region $\boldsymbol{\theta_d} \in [0,1]$ for each of theta's dimensions *d* (cubic lattice - as oposed to uniform sampling - for easier analysis of the particle variability induced by resampling when compared to original grid, and also to ensure all space is covered for lower particle numbers)
- HMC mass chosen as the inverse of the (diagonal) covariance matrix
- Metropolis-Hastings with multivariate normal proposals, variance matrix proportional to the covariance matrix (for some factor of choice)
- HMC mutations performed by default when resampling, M-H used when HMC acceptance probability falls below some threshold
- Other parameters (leapfrog integration parameters ε and L, number of particles *n*, number of experiments *N*, M-H proportionality factor, resampling and HMC/M-H thresholds) chosen for each run and dimension
- Single group of particles used for all graphs here (vs. splitting particles into several groups, running the algorithm independently for every one, and taking the sum distribution)
- One Markov move per particle/step

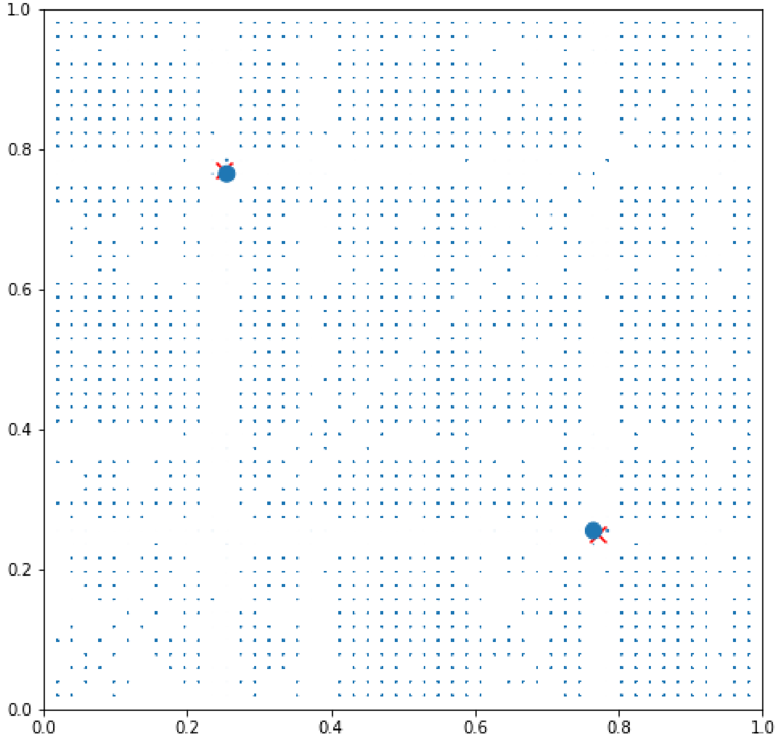
2-d squared cosine - I

Denser grid for fixed lattice (left); particle density changed only through re-weighting. For enough particles and data the particles closest to the modes tend to outgrow others, but naturally fall off-center relative to the true values (worst case scenario they don't mark them at all)

HMC resampling (right): all particles are displaced towards modes. High likelihood regions are better covered

No resampling (for reference)

50^2 particles

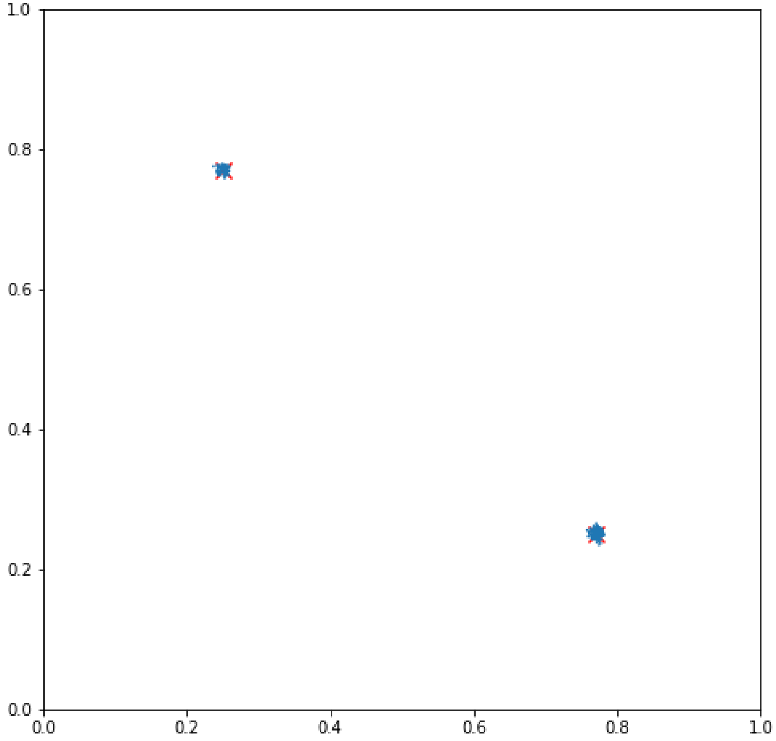


Offline estimation; random times <= 100

HMC: M=Cov^-1, L=10, eta=0.01

n=50^2/15^2; N=100; resampling threshold=100

15^2 particles

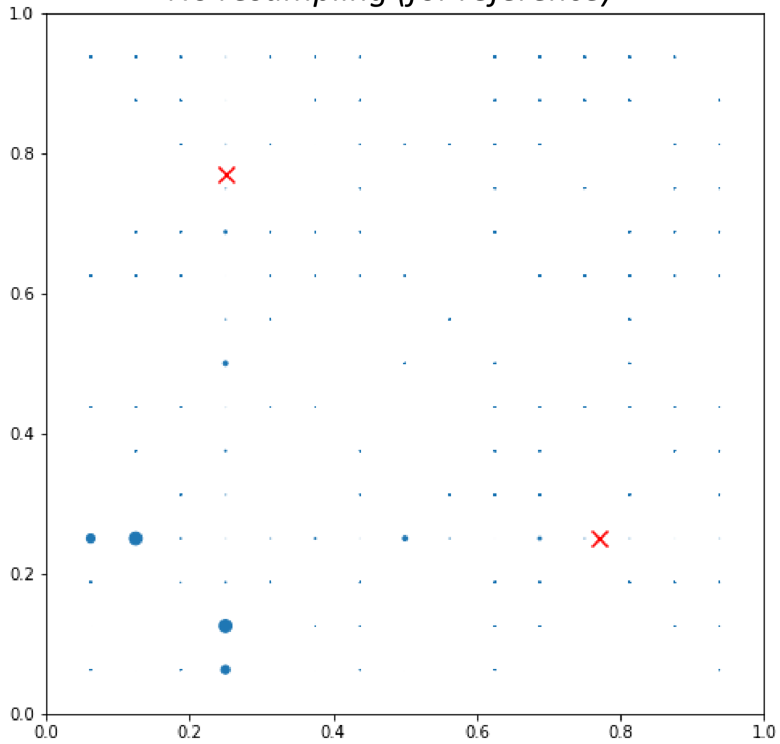


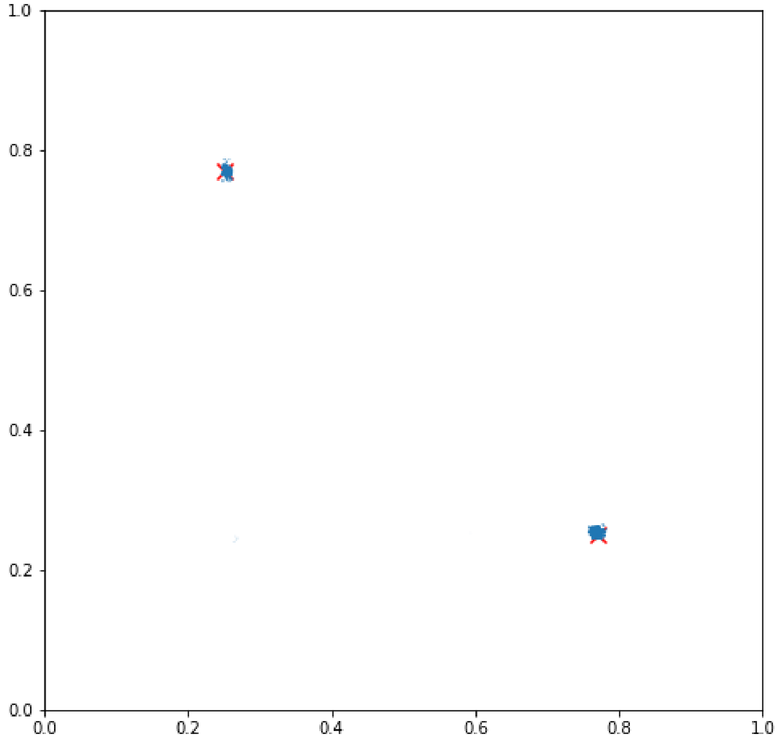
* Total resampler calls: 8.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 90% mean particle acceptance rate.

2-d squared cosine - II

Here for the same (15^2) number of particles; fixed lattice struggles more to find the modes in the parameter space as dimensionality increases (as expected)

No resampling (for reference)





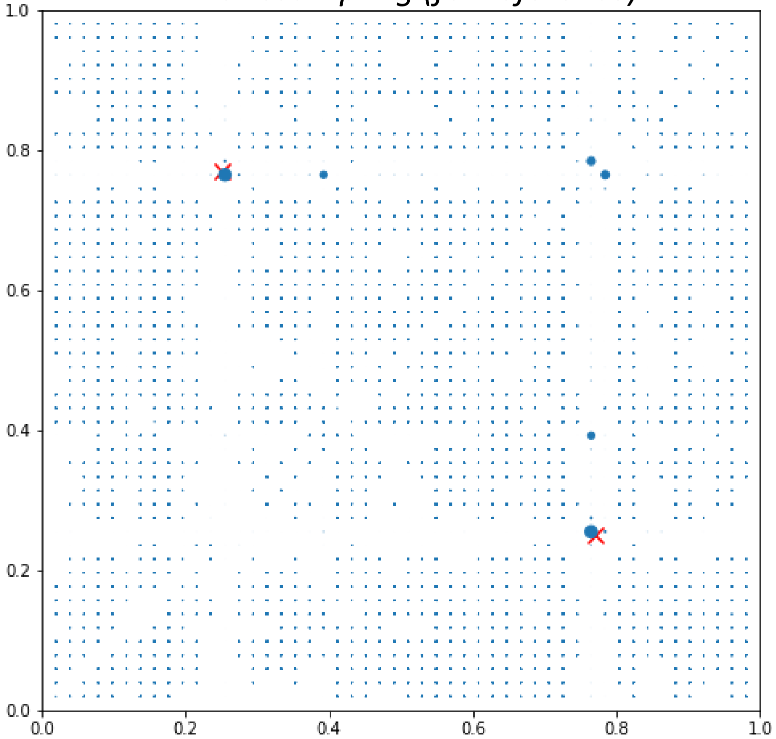
Offline estimation; random times <= 100
HMC: M=Cov^-1, L=10, eta=0.01
MH: S=Cov, factor=0.1
n=15^2; N=100; resampling threshold=100

* Total resampler calls: 8.
* Percentage of HMC steps: 99.9%.
* Hamiltonian Monte Carlo: 89% mean particle acceptance rate.
* Metropolis-Hastings: 50% mean particle acceptance rate.

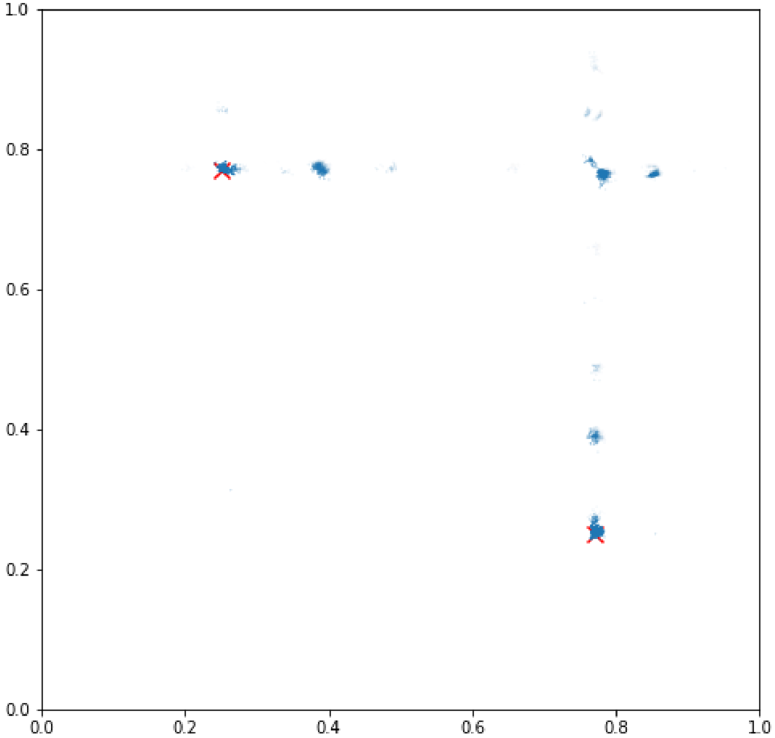
2-d squared cosine - III

Occasionally (for worse sets of measurement data) there is ambiguity in the probability density that doesn't seem to be justified by overly coarse discretization (as suggested by its affecting both cases equally, even with quite dense fixed lattice – left – or HMC mutations – right)

No resampling (for reference)



50^2 particles

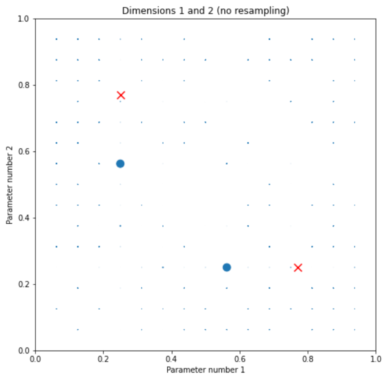


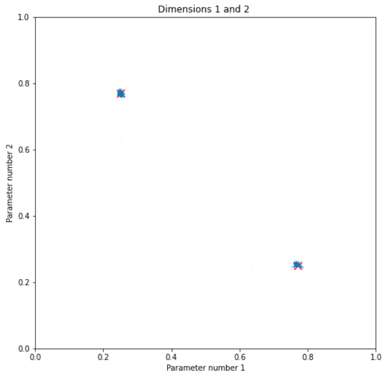
15^2 particles

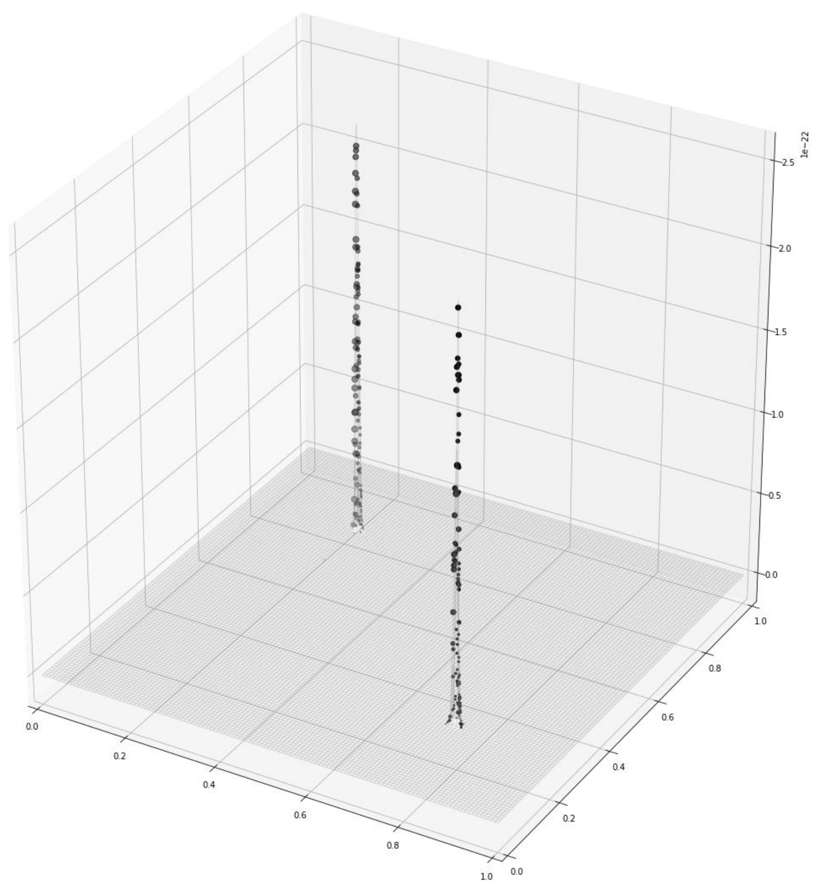
Offline estimation; random times <= 100
HMC: M=Cov^-1, L=10, eta=0.01
MH: S=Cov, factor=0.1
n=15^2; N=100; resampling threshold=100

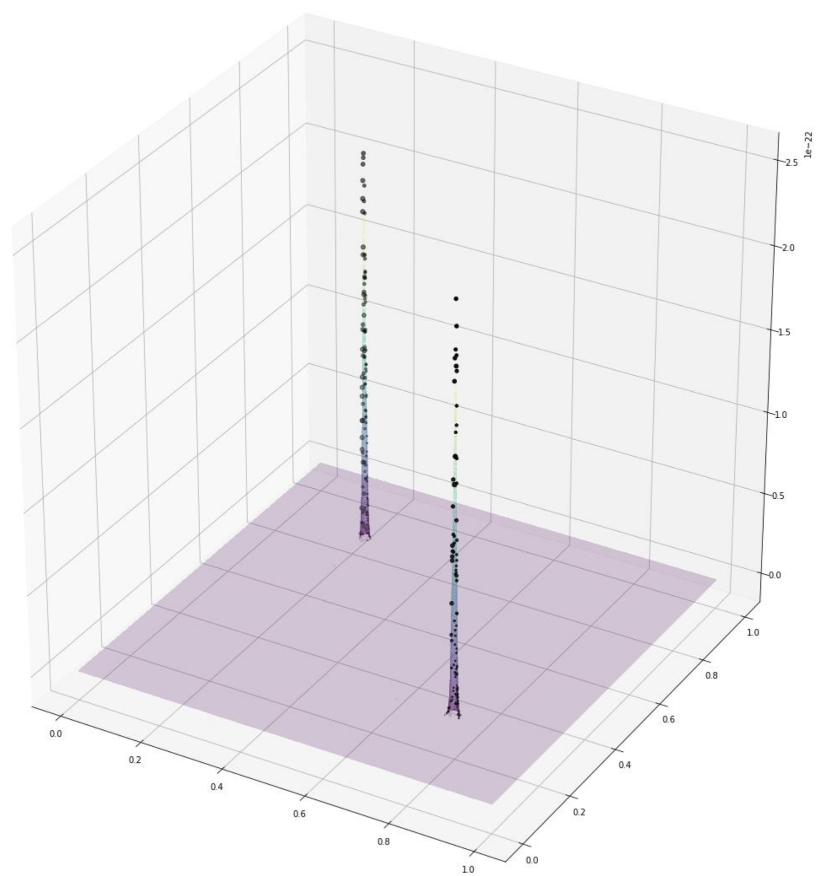
* Total resampler calls: 3.
* Percentage of HMC steps: 99.9%.
* Hamiltonian Monte Carlo: 87% mean particle acceptance rate.
* Metropolis-Hastings: 67% mean particle acceptance rate.

Likelihood vs. distribution plots









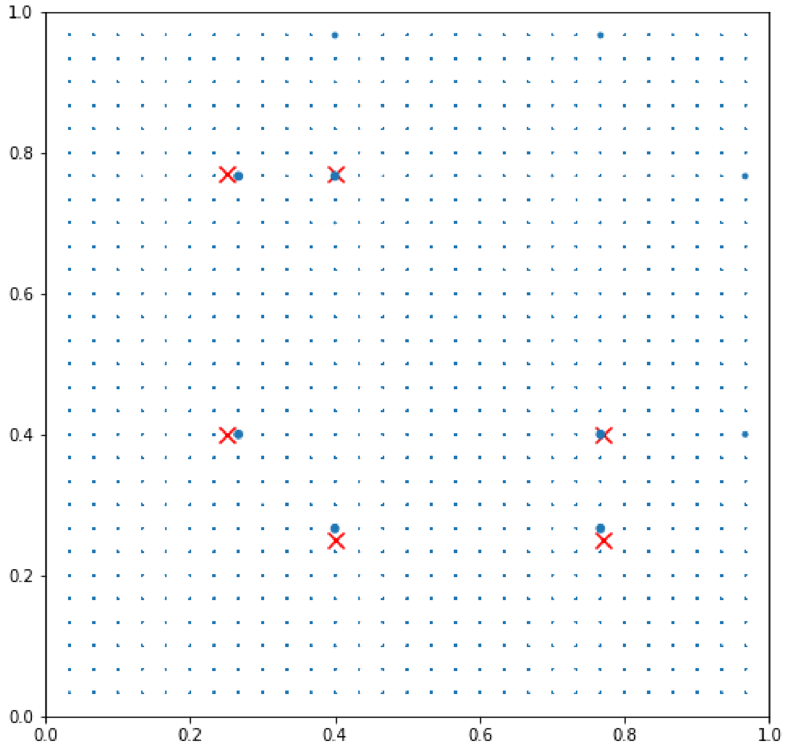
Offline estimation: random times <= 100
Uniform prior distribution, data chunksize = 20
1 particle group
HMC: Cov^-1, L=10, eta=0.0100000000
> n=15.00^2; N=100; 2d sum of squared cosines

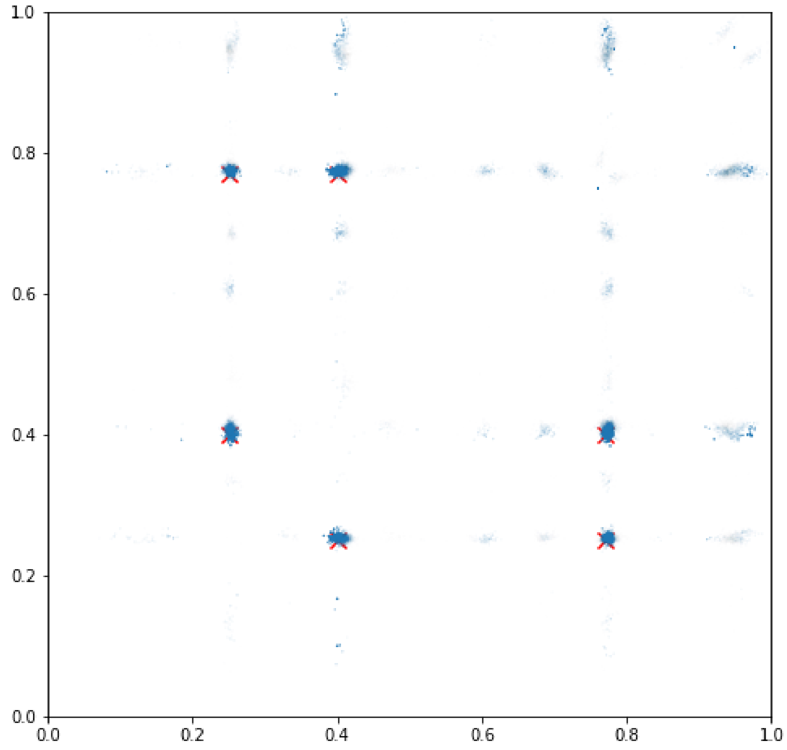
* Total resampler calls: 3.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 84% mean particle acceptance rate.

3-d squared cosine - I

(projections onto plane, third dimension omitted but similar)

No resampling (for reference)





Offline estimation; random times <= 100
HMC: M=Cov^-1, L=10, eta=0.005
n=29^3; N=200; resampling threshold=50

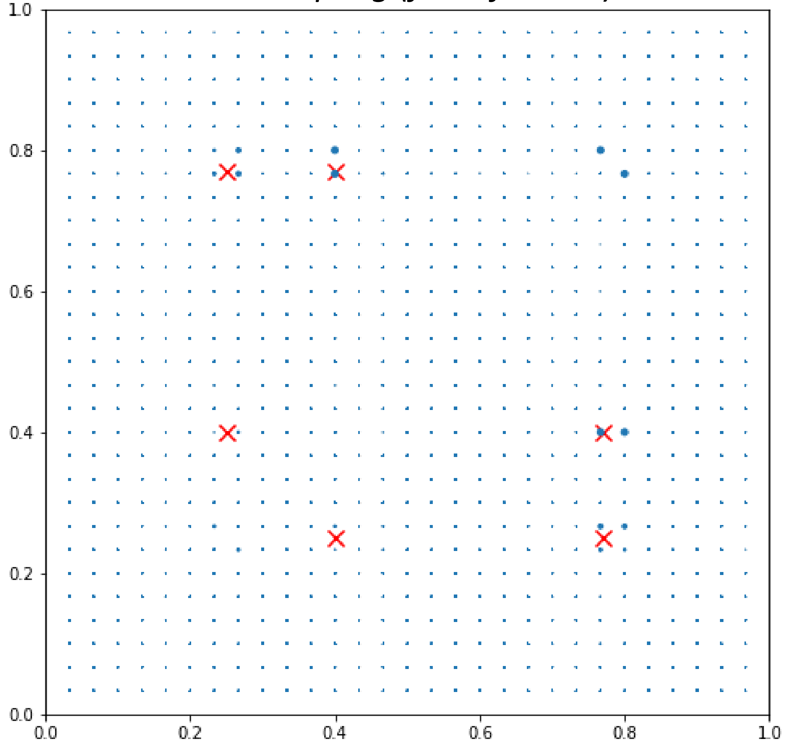
* Total resampler calls: 1.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 93% mean particle acceptance rate.

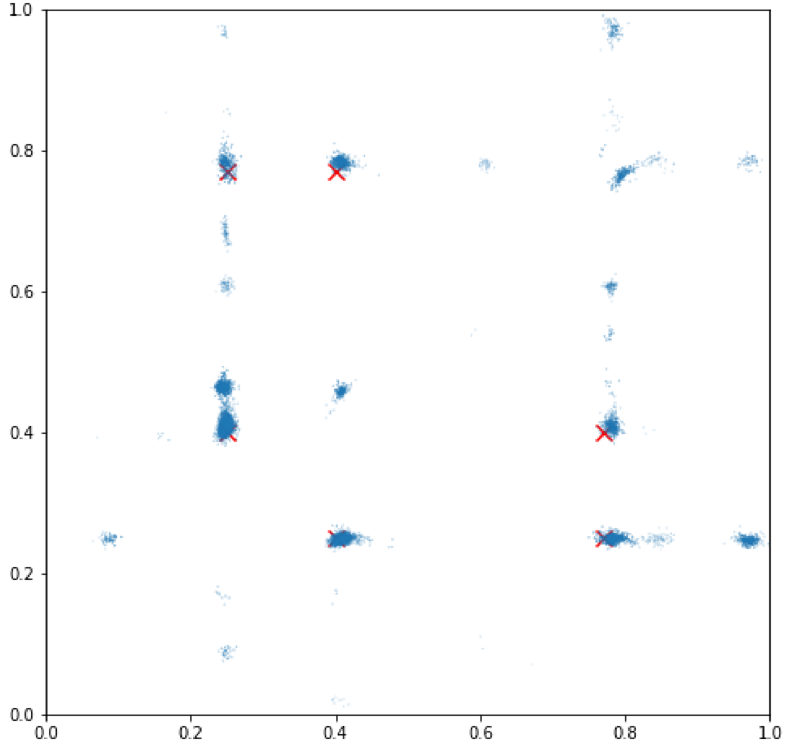
3-d squared cosine - II

(projections onto plane)

Seemingly more ambiguous set of measurement data, as in 2-d

No resampling (for reference)



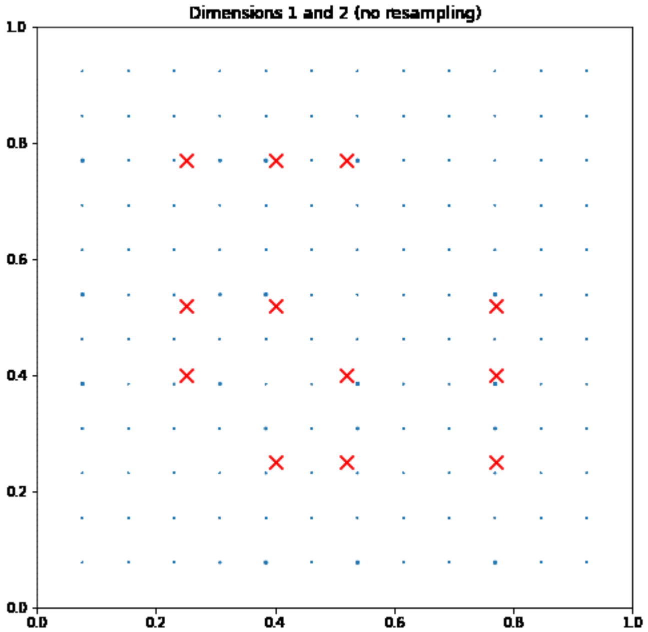


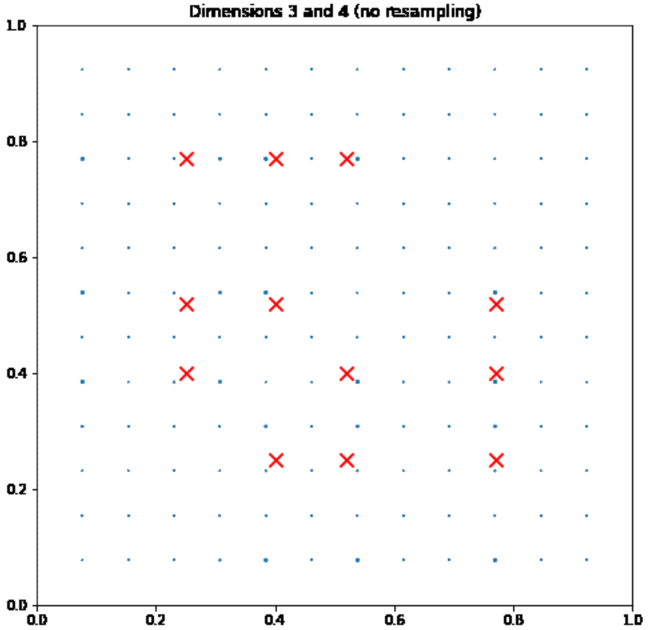
Offline estimation; random times <= 100
HMC: M=Cov^-1, L=10, eta=0.01
MH: S=Cov, factor=0.1000
n=29^3; N=200; resampling threshold=n/2

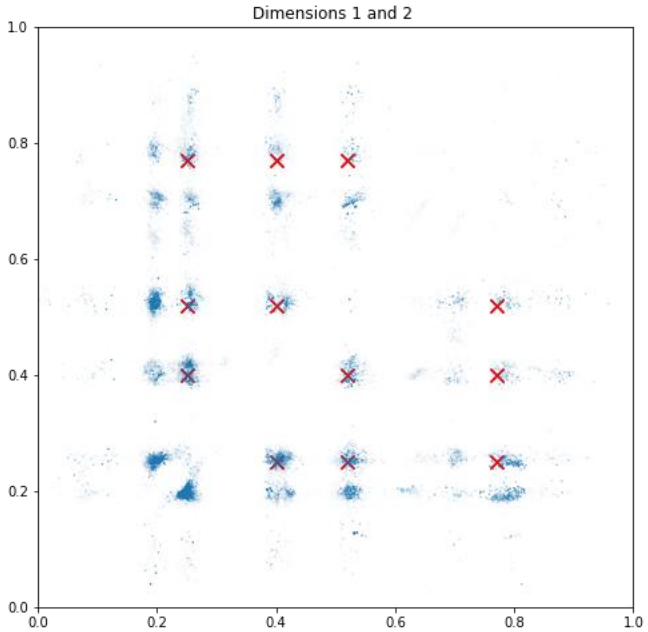
* Total resampler calls: 20.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 85% mean particle acceptance rate.
* Metropolis-Hastings: 67% mean particle acceptance rate.

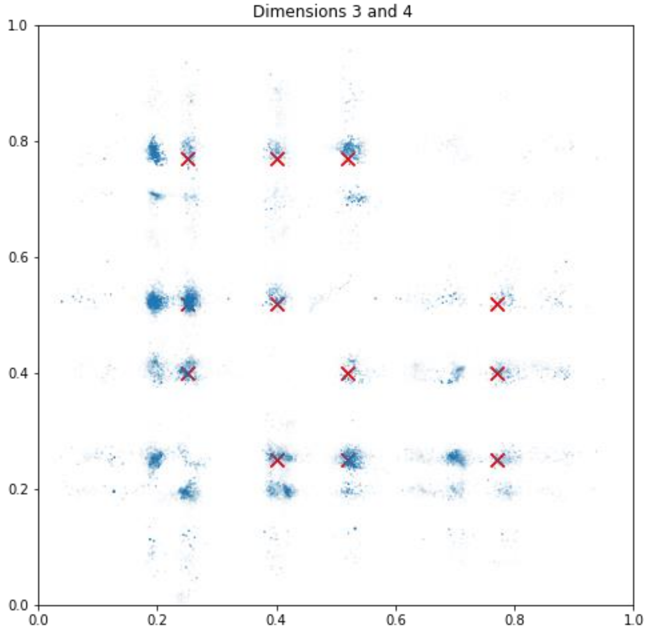
4-d squared cosine

No resampling (for reference)







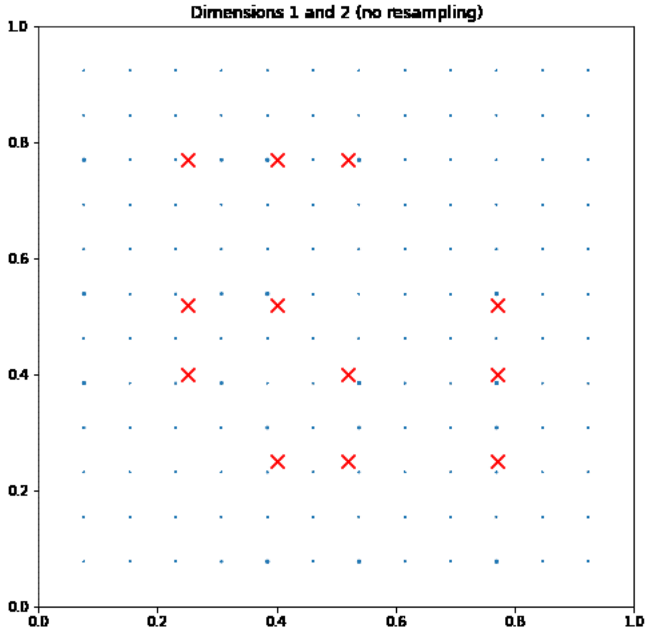


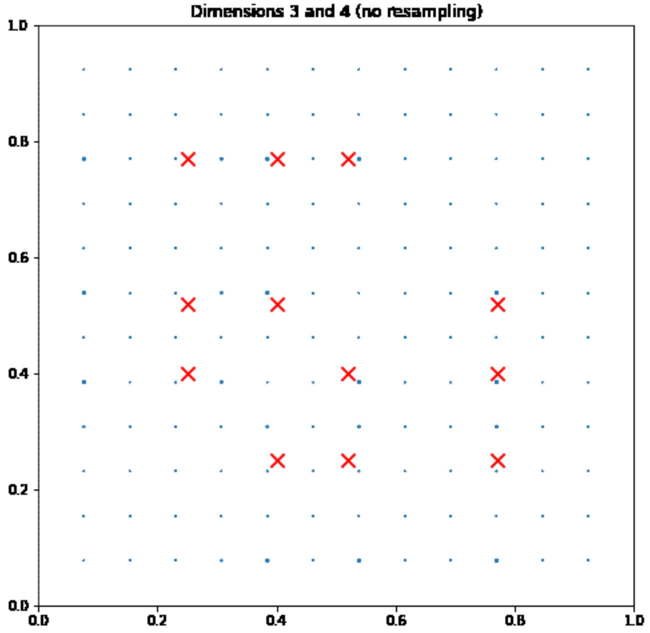
Offline estimation;
random times <= 100
HMC: M=Cov^-1, L=10, eta=0.01
MH: S=Cov, factor=0.1000
n=12^4; N=250; resampling threshold=500

* Total resampler calls: 3.
* Percentage of HMC steps: 100.0%.
* Hamiltonian Monte Carlo: 81% mean particle acceptance rate.
* Metropolis-Hastings: 39% mean particle acceptance rate.

Comparing 4-d case with Metropolis-Hastings alone

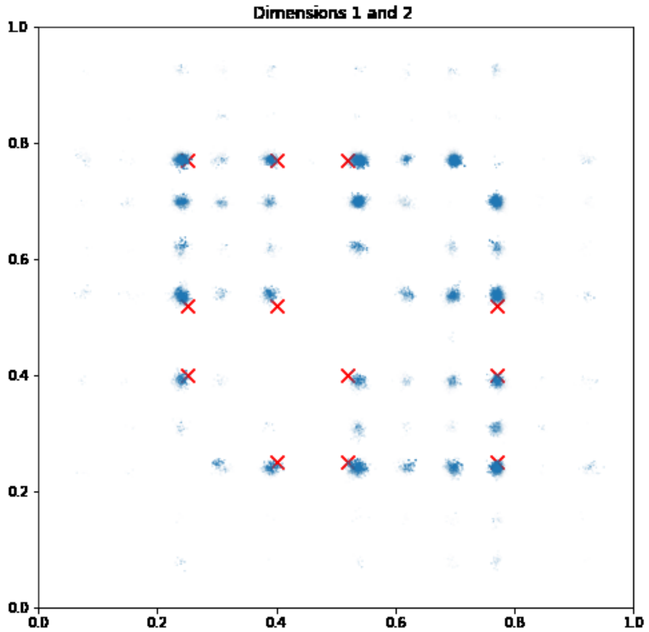
No resampling (for reference)

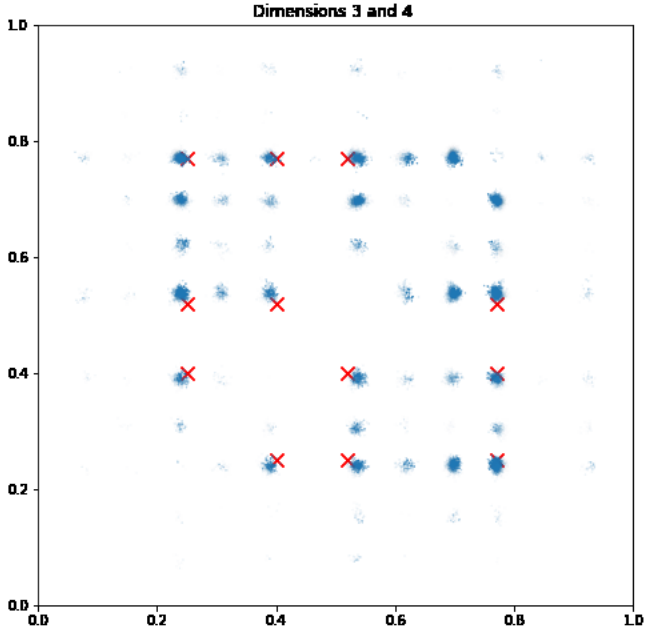




Small variance in proposals:

- Particles hardly steer away from the original lattice sites
- Tend to move towards modes, but very slowly
- High acceptance rate (though still lower than HMC), but poor variability in proposals



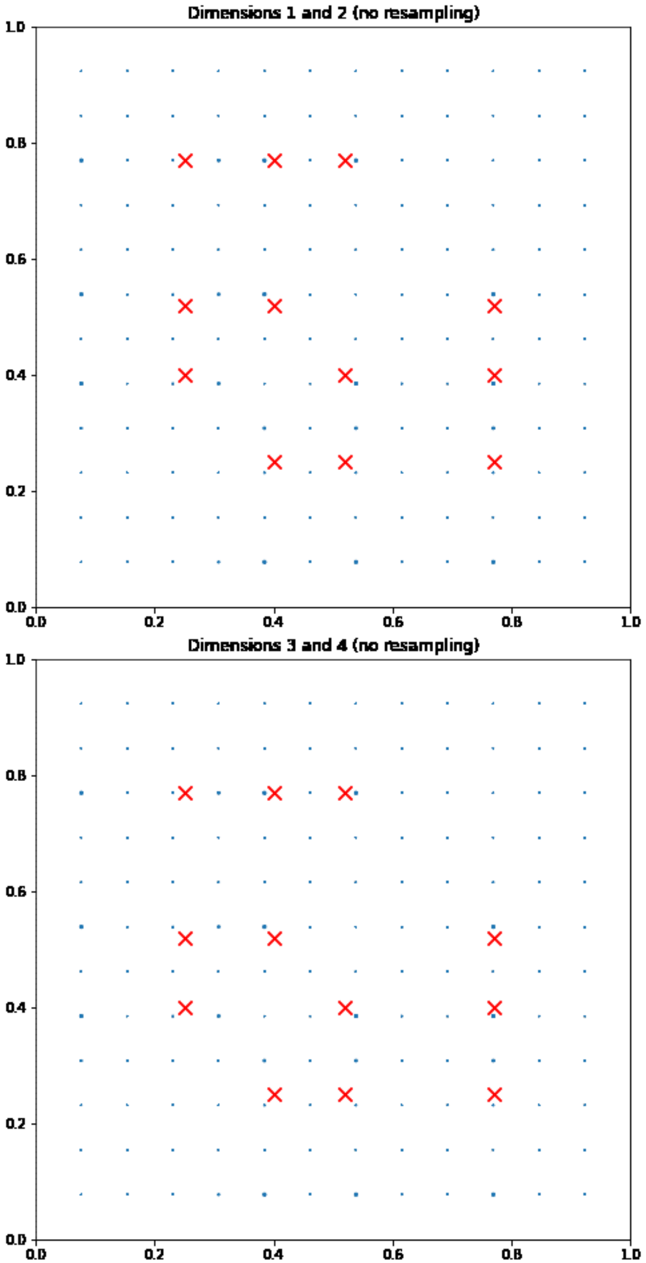


Offline estimation;
random times <= 100
MH: S=Cov, factor=0.005
n=12^4; N=250;
resampling threshold=500

* Total resampler calls: 2.
* Percentage of HMC steps: 0.0%.
* Metropolis-Hastings: 69% mean particle acceptance rate.

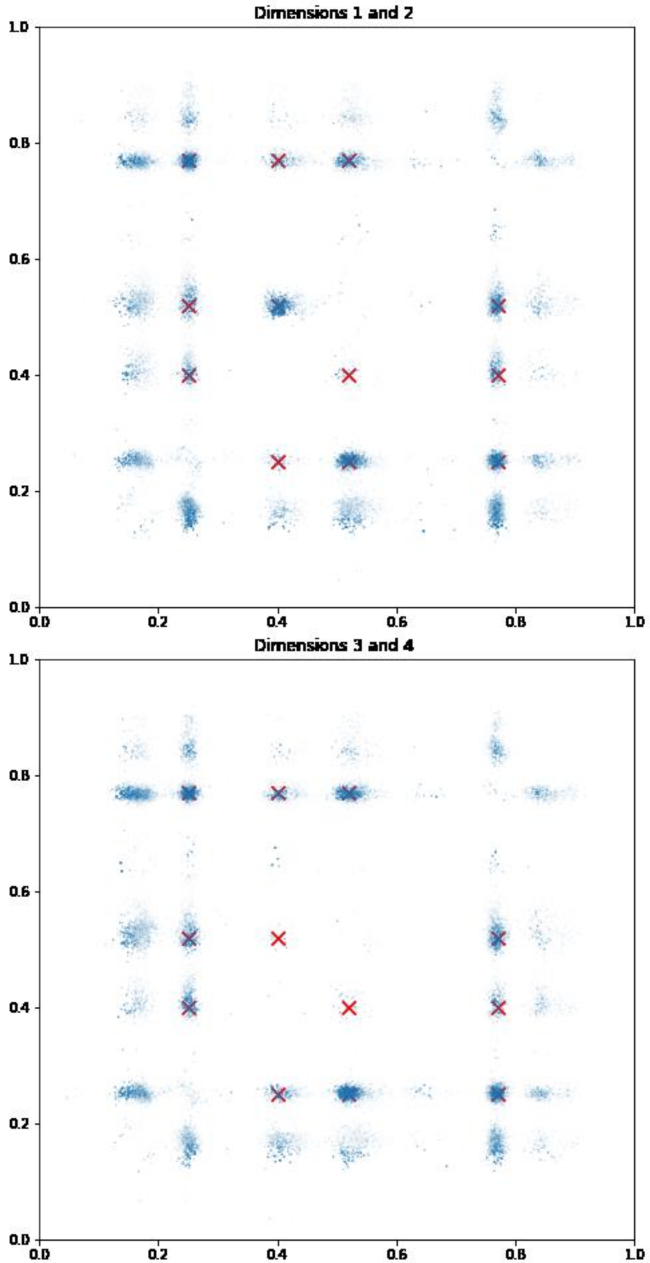
Comparing 4-d case with Metropolis-Hastings alone

No resampling (for reference)



Large variance in proposals:

- Reasonable exploration, but almost total depletion at some modes
- Very low acceptance rate
- Less effective at introducing variety (most moves are rejected), so sub-threshold ESS triggers frequent resampling steps



Offline estimation;
random times <= 100
MH: S=Cov, factor=0.03
n=12^4; N=250;
resampling threshold=500

* Total resampler calls: 30.
* Percentage of HMC steps: 0.0%.
* Metropolis-Hastings: 6% mean particle acceptance rate.