nested_fit: developments and tests

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Motivation

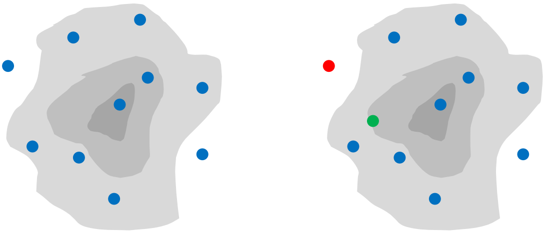
Long term: Make a quantum description of hydrogen (**electrons** + **nucleus**) in solid state matter

Quantum analysis of nucleus $\rightarrow$ increase of number of degrees of freedom

Necessary to reduce number of sampling points $\rightarrow$ Nested Sampling

Applications: analysis of experimental data, Lennard - Jones clusters

Nested Sampling: principle of exploration



Remarks

- Sampled volume at each iteration $\approx \left(\frac{K}{K+1}\right)^m$
- K: number of sampling points, m: iteration
- $E_{new} < E_m$

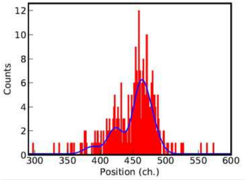
Nested Sampling: tool for fitting data

θ: parameters; $\mathcal{M}$: model; I: background information

$$\mathcal{E}(\mathcal{M}) = \mathbb{P}(\text{Data}|\mathcal{M}, I) = \int \cdots \int_{\Theta} L(\theta)\mathbb{P}(\theta|I)d\theta$$

Variable change: $X(\mathcal{L}) = \int \cdots \int_{L(\theta)>\mathcal{L}} \mathbb{P}(\theta|I)d\theta$

$\Rightarrow \mathcal{E}(\mathcal{M}) = \int_0^1 \mathcal{L}(X)dX$



Trassinelli, Ciccodicola, *Entropy*, 2020

Nested Sampling: tool for calculating the partition function

$\boldsymbol{x}$: positions; $\boldsymbol{p}$: momenta; $\beta = \frac{1}{k_b T}$

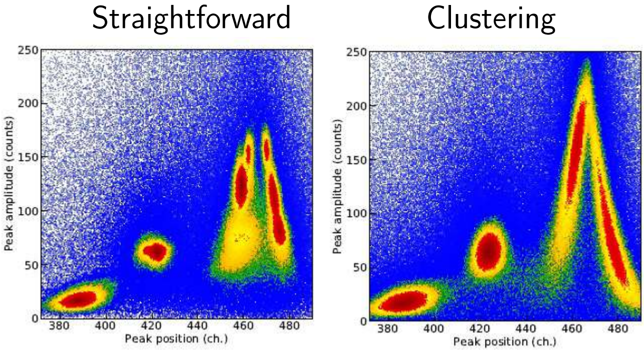
$$Z(\beta) = \int \exp(-\beta E(\boldsymbol{x}, \boldsymbol{p})) d\boldsymbol{x} d\boldsymbol{p}$$

Rewritten in function of E: $Z(\beta) = \int \rho'(E) \exp(-\beta E) dE$
$\rho'(E) \longrightarrow$ density of states between E and $E + dE$

$Z \approx \sum_m w_m \exp(-\beta E_m)$ ($w_m = \frac{1}{2}(\rho(E_{m-1}) - \rho(E_{m+1})))$

Internal energy: $U = -\frac{\partial \log(Z)}{\partial \beta}$
Heat capacity: $C_V = \frac{\partial U}{\partial T}$

Unsupervised learning: clustering data analysis



Trassinelli, Ciccodicola, *Entropy*, 2020

Computation time without clustering around eight times longer than with clustering

Without clustering: only one peak found for each run, multiple runs needed to find all peaks

Clustering methods

Mean Shift

- Two parameters: distance D + bandwidth l
- Iterative calculation of the mean of points within a given region

Density based spatial clustering for applications with noise (DBSCAN)

- Two parameters: radius ϵ + minimal number of neighbours m
- Three types of points: core, reachable, outliers

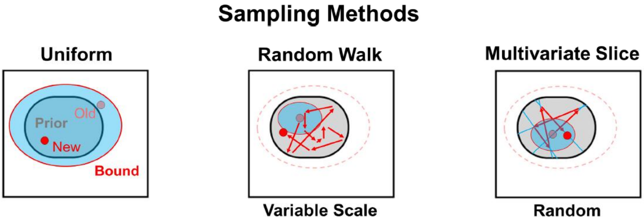
Agglomerative clustering with single linkage (Agglomerative)

- Parameter: threshold value α
- $\min_{a \in A, b \in B} d(a, b)$ (A, B: clusters; d: euclidean distance)

K nearest neighbours (KNN)

- No parameters
- Iterative on the number of neighbours k

Search methods

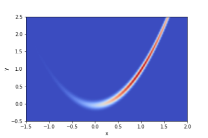


Speagle, *Montly Notices of the Royal Astronomical Society*, 2020

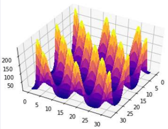
Four search methods in nested_fit: Random Walk, Uniform, Slice Sampling (size of the slice fixed) & Slice Sampling Adapt (size of the slice adaptable)

Examples studied

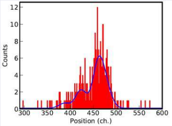
Rosenbrock 2D



Eggbox

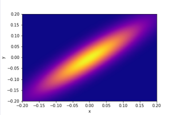


Four gaussian peaks likelihood

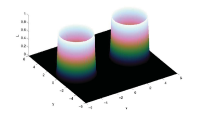


Trassinelli, Ciccodicola, *Entropy*, 2020

Gaussian with correlation



Gaussian shells

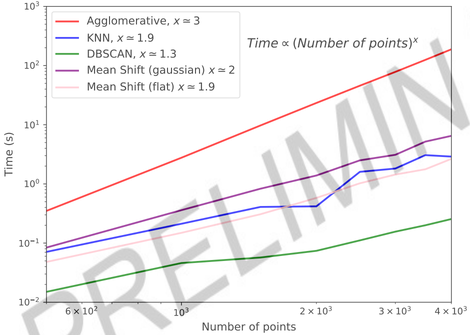


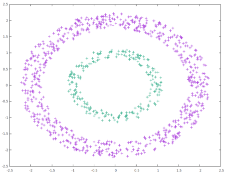
Graff, Feroz, Hobson, Lasenby, *Monthly Notices of the Royal Astronomical Society*, 2012

Other examples:

- Rosenbrock 4D
- Gaussian without correlation (5D)

Clustering methods: CPU time scaling

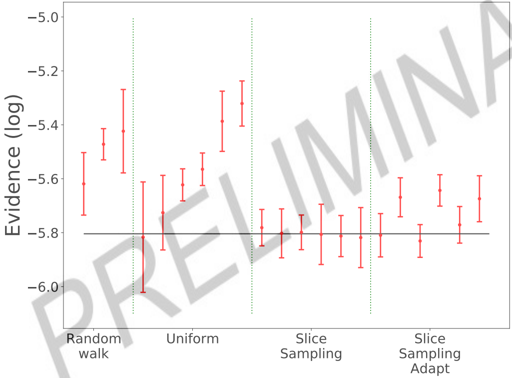


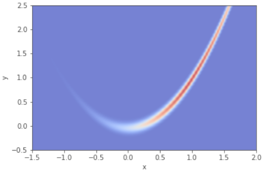


Remarks

- For a large number of points → DBSCAN preferable
- FORTRAN coded algorithms
- Tests carried out on a single processor

Search methods without clustering: Rosenbrock 2D



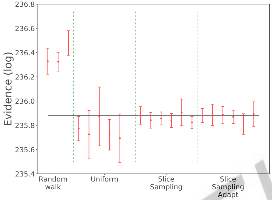


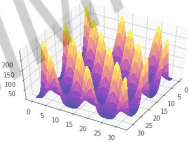
Remark

- Black line = expected value

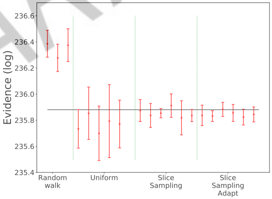
Search methods with clustering: Eggbox

Agglomerative

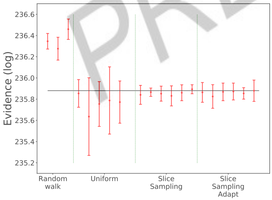




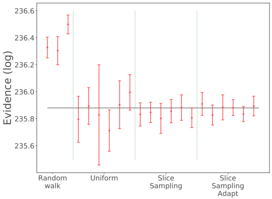
KNN



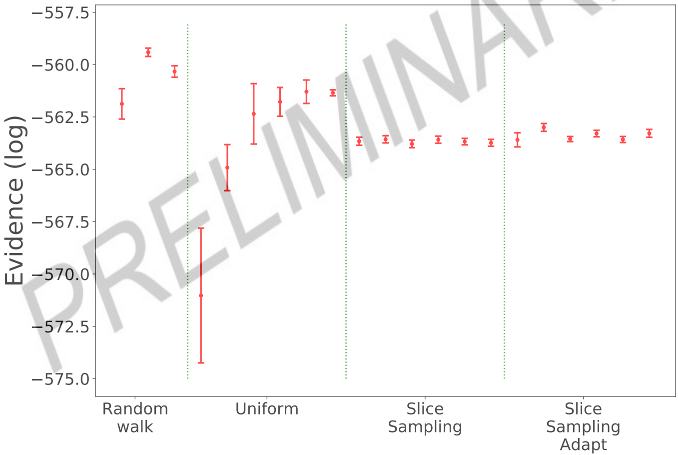
DBSCAN



Mean Shift

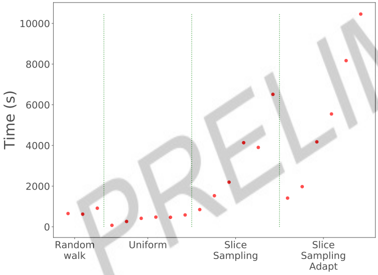


Four gaussian peaks

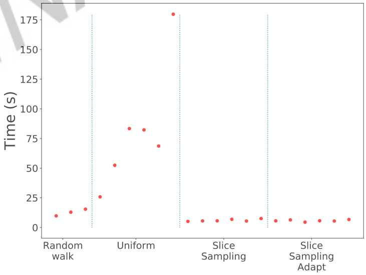


Search methods: time

Four gaussian peaks (10D)

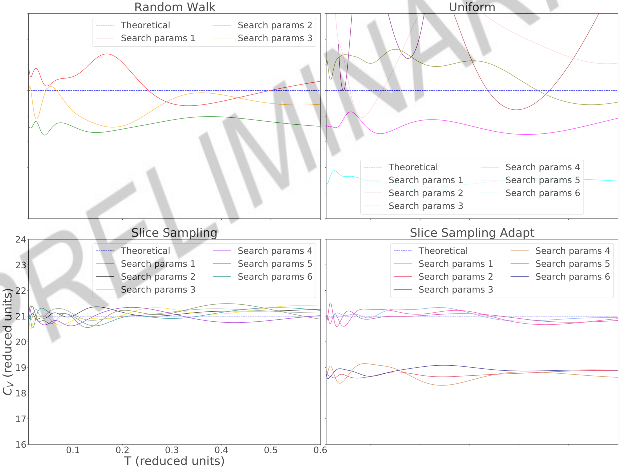


Rosenbrock 2D



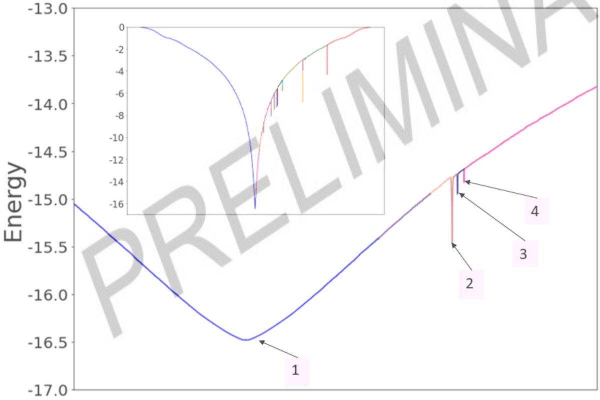
Harmonic potential

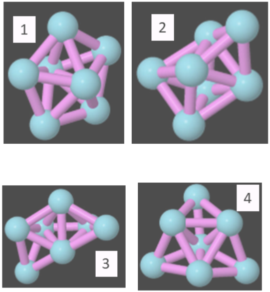
$$V_{harm}(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2),\ U = \frac{3}{2}Nk_bT,\ C_V = \frac{3}{2}Nk_b$$



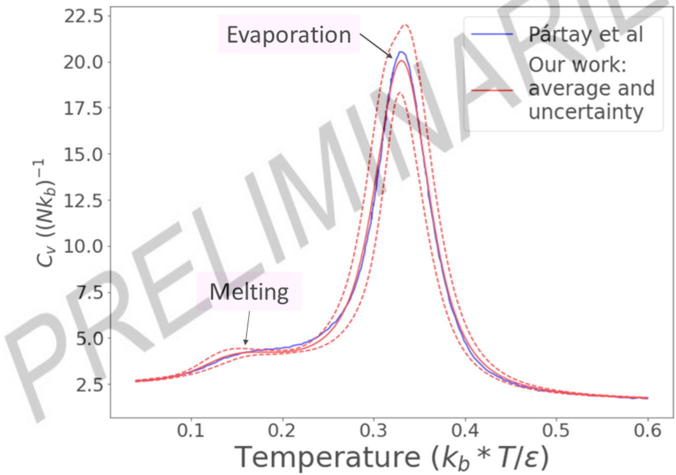
Lennard - Jones clusters I

Potential : $V_c(X) = \sum_{i<j} V_{LJ}(r_{ij})$ with $V_{LJ}(r_{ij}) = 4\epsilon \left[\left(\frac{r_0}{r_{ij}}\right)^{12} - \left(\frac{r_0}{r_{ij}}\right)^{6} \right]$, 7 atoms





Lennard - Jones clusters II



Pártay, Bartók, Csányi, *J. Phys. Chem. B*, 2010

Conclusion

Clustering

- Agglomerative: slowest method; DBSCAN: fastest method

Search methods

- Uniform search: least stable results
- Slice Sampling: best performances

Perspectives

- Extend to quantum case

- Parallelisation and better uncertainty estimation

- Neural networks with nested_fit points as input

- Reduce the numbers of degrees of freedom
  $\rightarrow$ "greedy" algorithm
  $\rightarrow$ effective Hamiltonians and Bayesian evidence calculation for their validation

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