Some Thoughts on Dynamic Quantum Clustering

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Brief review of Dynamic Quantum Clustering

In Dynamic Quantum Clustering (DQC) [1,2], one associates with each of the dataset's R d-dimensional data points a Gaussian with a common variance σ^2, and possibly a weight factor c_r, as follows

$$\mathbf{x}_r \quad \Rightarrow \quad \Phi_r(\mathbf{x}) \equiv c_r \exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big] \qquad (1 \leq r \leq R, \quad c_r \geq 0\,, \quad \sum_{r=1}^{R} c_r \neq 0)\,,$$

and then defines a probability distribution by summing over those Gaussians,

$$\Psi(\mathbf{x}) \equiv A \sum_{r=1}^{R} \Phi_r(\mathbf{x}) = A \sum_{r=1}^{R} c_r \, \exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big]\,,$$

the idea being that the cluster centers are the maxima of $\Psi(\mathbf{x})$. The constant A is a normalization factor, chosen to ensure that

$$\int d\mathbf{x}\, \Psi(\mathbf{x}) = 1\,, \text{ that is, } \; A = \frac{1}{\Big(\sigma\sqrt{2\pi}\Big)^d \sum_{r=1}^{R} c_r}\,.$$

Next, one interprets this probability distribution as a quantum probability *amplitude*, in fact, as the wave-function for the ground state of the quantum system with Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2M} + V(\hat{\mathbf{x}})\,,$$

for a certain potential function $V(\hat{\mathbf{x}})$ and mass value M. That it *is* possible for $\Psi(\mathbf{x})$ to be the *ground state*, as opposed to some excited state, is guaranteed by the fact that $\Psi(\mathbf{x})$ is

positive-definite. In fact, if it is to be a wave-function at all, then it *has* to be the one for the ground state since it has no nodes and, therefore, must have the lowest frequency (and, therefore, the lowest energy).

Then, because $\Psi(\mathbf{x})$ is the ground state, it must satisfy the time-independent Schrödinger equation with a certain energy eigenvalue $E > 0$,[1]

$$\Big[\, \frac{\hat{\mathbf{p}}^2}{2M} + V(\hat{\mathbf{x}}) \,\Big] \Psi(\mathbf{x}) = \Big[\, -\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{x}) \,\Big] \Psi(\mathbf{x}) = E\, \Psi(\mathbf{x})\,,$$

which then lets one determine what potential function gives rise to that ground state,

$$V(\mathbf{x}) = E + \frac{\hbar^2}{2M}\frac{\nabla^2\Psi(\mathbf{x})}{\Psi(\mathbf{x})}\,.$$

Noting that

$$\frac{\nabla^2\Psi(\mathbf{x})}{\Psi(\mathbf{x})} = -\frac{d}{\sigma^2} + \frac{1}{\sigma^4\,\Psi(\mathbf{x})}\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[\,-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\,\Big]\,,$$

one can rewrite the potential as

$$V(\mathbf{x}) = E - \frac{d}{2}\frac{\hbar^2}{M\sigma^2} + \frac{\hbar^2}{2M\sigma^4\,\Psi(\mathbf{x})}\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[\,-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\,\Big]\,.$$

Of course, since the mass M and Planck's constant $\hbar$ aren't meaningful in the context of data clustering, it's convenient to choose their values in order to remove extraneous constants from the analysis. Considering that the Gaussians that typically appear in quantum mechanics and those that appear in DQC are, respectively, of the forms

$$\exp(-\frac{M\omega}{2\hbar}\,x^2) \quad \text{and} \quad \exp(-\frac{1}{2\sigma^2}\,x^2)\,,$$

it's convenient to set $\hbar = 1$ and then choose $\omega = 1$ and $M = 1/\sigma^2$. Also, since the potential is defined up to an arbitrary constant, one can choose $E = d/2$. Then,

$$\hat{H} = -\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x}) \quad \text{and} \quad V(\mathbf{x}) = \frac{1}{2\sigma^2\,\Psi(\mathbf{x})}\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[\,-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\,\Big]\,.$$

Note that $V(\mathbf{x})$ is positive-definite and, more or less, resembles a weighted average of multiple harmonic oscillator potentials, each centered at a different point.

[1] E cannot be zero because of Heisenberg's uncertainty principle.

Finally, having found $V(\mathbf{x})$, one then solves the time-*de*pendent Schrödinger equation with the Hamiltonian just defined and with each data-point Gaussian $\Phi_r(\mathbf{x})$ as the initial state. Since the Hamiltonian is time-*in*dependent, the time-dependent Schrödinger equation admits the formal solution

$$| \Phi_r(\mathbf{x}, t) \rangle = \exp(-it\,\hat{H}) \, | \Phi_r(\mathbf{x}) \rangle \,.$$

Now, if the minima of the potential $V(\mathbf{x})$ are reasonably well separated, then Ehrenfest's theorem guarantees that the motion of these data-point states is nearly classical, in the sense that they follow paths close to the Newtonian ones, defined as the expectation values of the position operator in the states $\Phi_r(\mathbf{x}, t)$,

$$\langle \mathbf{x}_r(t) \rangle = \langle \Phi_r(\mathbf{x}, t) \, | \, \hat{\mathbf{x}} \, | \, \Phi_r(\mathbf{x}, t) \rangle = \langle \Phi_r(\mathbf{x}) \, | \, \exp(+it\,\hat{H}) \, \hat{\mathbf{x}} \, \exp(-it\,\hat{H}) \, | \, \Phi_r(\mathbf{x}) \rangle \,.$$

Since Newtonian paths minimize the potential function, the conclusion is that these data-point 'particles', as they were, will move towards, and very likely oscillate around, the minima of the potential. The data density, averaged over time, then tends to be maximized at these potential minima, making them good proxies for cluster centers.

Of course, actually solving for the time evolution described above is complicated. The original DQC paper uses the set $\{\Phi_r(\mathbf{x})\}$ as a basis, but I have a different suggestion, namely, to use the energy eigenstates of a d-dimensional quantum harmonic oscillator as the basis for the Hilbert space in question.[2]

Review of the 1-dimensional quantum harmonic oscillator

The Hamiltonian operator $\hat{H}$ for the 1-dimensional harmonic oscillator of mass M and angular frequency ω is given by

$$\hat{H} = \frac{\hat{p}^2}{2M} + \frac{M\omega^2}{2} \, \hat{x}^2 \,,$$

[2] I also have another idea related to DQC, which I call a 'semi-classical' approach. Since we're ultimately after the classical paths, why not solve Newton's equations directly ($m = 1/\sigma^2$),

$$\ddot{\mathbf{x}} = -\sigma^2 \, \nabla V(\mathbf{x}) \,,$$

with the quantum potential just derived, and the initial conditions $\mathbf{x}_0 = \mathbf{x}_r$ and $\dot{\mathbf{x}}_0 = 0$? Given the potential in question, this can only be done numerically. A Verlet method is probably the best kind of numerical algorithm to use here since, being a symplectic integrator, it minimizes the numerical degradation of constants of the motion such as, in this case, energy. A possible performance drawback, however, is that the numerical integration must be done anew for each data point $\mathbf{x}_r$ so the process may be too computationally expensive for very large data sets.

and is hermitian, positive-definite, and time-independent. Using the canonical commutation relation

$$[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar\,,$$

we can define two new operators,

$$\hat{a} \equiv \frac{1}{\sqrt{2M\hbar\omega}}\,(M\omega\hat{x} + i\hat{p}) \qquad \text{and} \qquad \hat{a}^\dagger \equiv \frac{1}{\sqrt{2M\hbar\omega}}\,(M\omega\hat{x} - i\hat{p})\,,$$

so that

$$\hat{H} = (\hat{a}^\dagger\hat{a} + \frac{1}{2})\,\hbar\omega\,.$$

Note that *their* commutator is 1: $[\hat{a}, \hat{a}^\dagger] = 1$. Now consider a state $|\,\alpha\,\rangle$ which is an eigenstate of the operator $\hat{a}^\dagger\hat{a}$ with eigenvalue α, that is,

$$\hat{a}^\dagger\hat{a}\,|\,\alpha\,\rangle = \alpha\,|\,\alpha\,\rangle\,.$$

Using the aforementioned commutation relation, it's easy to show that

$$\begin{aligned}\hat{a}\,|\,\alpha\,\rangle &= \sqrt{\alpha}\,|\,\alpha - 1\,\rangle \\ \hat{a}^\dagger\,|\,\alpha\,\rangle &= \sqrt{\alpha + 1}\,|\,\alpha + 1\,\rangle\,.\end{aligned}$$

The operator $\hat{a}$ thus results in a state with a *smaller* eigenvalue compared to the state it's applied to. However, the operator $\hat{a}^\dagger\hat{a}$ is hermitian and positive-*semi*-definite.[3] As a resut, its eigenvalues are necessarily *real* and *non-negative*, respectively. Then, since continually applying $\hat{a}$ to the state $|\,\alpha\,\rangle$ would eventually result in a state with a *negative* eigenvalue — which we know can't happen — we conclude that there must exist a state $|\,0\,\rangle$, the oscillator's *ground state*, such that

$$\hat{a}\,|\,0\,\rangle = 0\,|\,0\,\rangle\,.$$

Moreover, since $\hat{a}^\dagger$ increases the eigenvalue by exactly 1, we conclude that the eigenstates of $\hat{a}^\dagger\hat{a}$ have eigenvalues in the non-negative integers:

$$\hat{a}^\dagger\hat{a}\,|\,n\,\rangle = n\,|\,n\,\rangle\,, \qquad n = 0, 1, 2, \ldots\,.$$

The operator $\hat{N} \equiv \hat{a}^\dagger\hat{a}$, known as the *number operator*, then measures the number of oscillator quanta in its eigenstates. We can now build any eigenstate of $\hat{N}$ by applying

[3] Consider the squared norm of the state $\hat{a}\,|\,n\,\rangle$, where $|\,n\,\rangle$ is an eigenstate of $\hat{a}^\dagger\hat{a}$. By definition, squared norms are real non-negative numbers, so $||\,\hat{a}\,|\,n\,\rangle\,||^2 = \langle\,n\,|\,\hat{a}^\dagger\hat{a}\,|\,n\,\rangle = n\,\langle\,n\,|\,n\,\rangle = n \geq 0$.

powers of $\hat{a}^\dagger$ to the ground state:

$$\begin{aligned}
\sqrt{1}\,|\,1\,\rangle &= \hat{a}^\dagger\,|\,0\,\rangle \\
\sqrt{2}\,|\,2\,\rangle &= \hat{a}^\dagger\,|\,1\,\rangle \\
&\cdots \\
\sqrt{n}\,|\,n\,\rangle &= \hat{a}^\dagger\,|\,n-1\,\rangle\,,
\end{aligned}$$

from which we conclude that

$$|\,n\,\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|\,0\,\rangle\,.$$

Next, we can obtain the wave-function of the ground state in the position representation by making use of $\hat{a}\,|\,0\,\rangle = 0\,|\,0\,\rangle$:

$$\langle\,x\,|\,\hat{a}\,|\,0\,\rangle = \langle\,x\,|\,0\,|\,0\,\rangle = 0\,\langle\,x\,|\,0\,\rangle = 0\,.$$

In the position representation, $\hat{p} = -i\hbar\,d/dx$ and it then follows that

$$\langle\,x\,|\,\hat{a}\,|\,0\,\rangle = (M\omega x + \hbar\frac{d}{dx})\,\langle\,x\,|\,0\,\rangle = 0\,.$$

This is a differential equation for $\psi_0(x) \equiv \langle\,x\,|\,0\,\rangle$, with the normalized solution

$$\psi_0(x) = \langle\,x\,|\,0\,\rangle = \Big(\frac{M\omega}{\pi\hbar}\Big)^{1/4}\,\exp(-\frac{M\omega}{2\hbar}\,x^2)\,.$$

Then, using

$$|\,n\,\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|\,0\,\rangle$$

it's possible to show that the normalized wave-function of the n-th energy eigenstate, in the position representation, is given by [3]

$$\psi_n(x) = \langle\,x\,|\,n\,\rangle = \Big(\frac{M\omega}{\pi\hbar}\Big)^{1/4}\frac{1}{\sqrt{2^n\,n!}}\,H_n\Big(\sqrt{\frac{M\omega}{\hbar}}\,x\Big)\exp(-\frac{M\omega}{2\hbar}\,x^2)\,,$$

where H_n is the *Hermite* polynomial of order n. Moreover, since the set of Hermite polynomials $\{H_n\}$ is orthonormal according to

$$\int_{-\infty}^{+\infty} du\,H_m(u)\,H_n(u)\,e^{-u^2} = 2^n\,n!\,\sqrt{\pi}\,\delta_{m,n}\,,$$

it then follows, as expected, that the set $\{|\,n\,\rangle\}$ is orthonormal as well, that is, $\langle\,m\,|\,n\,\rangle = \delta_{m,n}$. More than that, the set $\{|\,n\,\rangle\}$ forms a basis for the Hilbert space in question.

The time-*de*pendent Schrödinger equation for a time-*in*dependent Hamiltonian

The time-dependent Schrödinger equation,

$$i\hbar \frac{d}{dt} | \, s(t) \, \rangle = \hat{H} \, | \, s(t) \, \rangle \, ,$$

admits the formal solution

$$| \, s(t) \, \rangle = \exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \, | \, s(0) \, \rangle$$

when the Hamiltonian is independent of time, where the exponential of the Hamiltonian is defined by its power series,

$$\exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \equiv \sum_{k \, = \, 0}^{\infty} \frac{(-it/\hbar)^k}{k!} \, \hat{H}^k \, .$$

Of course, if $| \, s(0) \, \rangle$ is an energy eigenstate with energy E, then

$$| \, s(t) \, \rangle = \exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \, | \, s(0) \, \rangle = \exp \Big(- \frac{it}{\hbar} \, E \Big) \, | \, s(0) \, \rangle$$

and $| \, s(0) \, \rangle$'s time evolution is trivial: only its phase changes with time.

Suppose, however, that $| \, s(0) \, \rangle$ is not an energy eigenstate. If we have a basis $\{ | \, \alpha \, \rangle \}$ for the same Hilbert space, even if it's made up of eigenstates of a different Hamiltonian in that Hilbert space, then we can use the completeness of the basis to write $| \, s(t) \, \rangle$ as a superposition of basis states:

$$| \, s(t) \, \rangle = \exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \, | \, s(0) \, \rangle = \int d\alpha \int d\alpha' \, | \, \alpha \, \rangle \langle \, \alpha \, | \, \exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \, | \, \alpha' \, \rangle \, \langle \, \alpha' \, | \, s(0) \, \rangle \, .$$

Note that $\langle \, \alpha \, | \, \exp \Big(- \frac{it}{\hbar} \, \hat{H} \Big) \, | \, \alpha' \, \rangle$ and $\langle \, \alpha' \, | \, s(0) \, \rangle$ are just complex numbers. If, in addition, the basis in question is an eigenbasis of the Hamiltonian $\hat{H}$, with corresponding eigenvalues E_α, then the above simplifies to

$$| \, s(t) \, \rangle = \int d\alpha \, | \, \alpha \, \rangle \, \exp \Big(- \frac{it}{\hbar} \, E_\alpha \Big) \, \langle \, \alpha \, | \, s(0) \, \rangle \, .$$

Of course, the integrals turn into summations when the basis is discrete.

The 1-dimensional quantum harmonic oscillator with a perturbing potential

Consider now the Hamiltonian

$$\hat{H} = \hat{H}_{\text{h.o.}} + V(\hat{x}) = \frac{\hat{p}^2}{2M} + \frac{M\omega^2}{2}\,\hat{x}^2 + V(\hat{x})\,,$$

where $V(\hat{x})$ is a 'perturbing' potential to the harmonic oscillator Hamiltonian $\hat{H}_{\text{h.o.}}$. If $|\,s(0)\,\rangle$ is some initial state of the full system, then its time evolution under the full Hamiltonian is given by the previous section's result

$$|\,s(t)\,\rangle = \exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\,s(0)\,\rangle = \int d\alpha \int d\alpha'\,|\,\alpha\,\rangle\langle\,\alpha\,|\,\exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\,\alpha'\,\rangle\,\langle\,\alpha'\,|\,s(0)\,\rangle\,,$$

with a given choice of basis states $\{|\,\alpha\,\rangle\}$.

We now choose the harmonic oscillator's energy eigenstates $\{|\,n\,\rangle\}$ as the basis to work with and, because it's a discrete set, it follows that

$$|\,s(t)\,\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}|\,m\,\rangle\langle\,m\,|\,\exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\,n\,\rangle\,\langle\,n\,|\,s(0)\,\rangle\,.$$

It would be great if we could write

$$\langle\,m\,|\,\exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\,n\,\rangle = \exp\Big(-\frac{it}{\hbar}\,E_n\Big)\,\langle\,m\,|\,n\,\rangle$$

but that's not the case because $\{|\,n\,\rangle\}$ are eigenstates of $\hat{H}_{\text{h.o.}}$, *not* of the full Hamiltonian, thanks to the non-commutation between the position and momentum operators. Nonetheless, we can make some headway by inserting the identity operator

$$\sum_{n=0}^{\infty}|\,n\,\rangle\langle\,n\,| = 1$$

between pairs of successive applications of the full Hamiltonian in

$$\begin{aligned}|\,s(t)\,\rangle &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}|\,m\,\rangle\langle\,m\,|\,\exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\,n\,\rangle\,\langle\,n\,|\,s(0)\,\rangle \\ &= \sum_{k=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(-it/\hbar)^k}{k!}|\,m\,\rangle\langle\,m\,|\,\hat{H}^k\,|\,n\,\rangle\,\langle\,n\,|\,s(0)\,\rangle\,.\end{aligned}$$

$$
\begin{aligned}
|\, s(t)\,\rangle &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} |\, m\,\rangle\langle\, m\,|\, \exp\Big(-\frac{it}{\hbar}\,\hat{H}\Big)\,|\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle \\
&= \sum_{k=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-it/\hbar)^k}{k!}|\, m\,\rangle\langle\, m\,|\,\hat{H}^k\,|\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle \\
&= \sum_{n=0}^{\infty} |\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle + \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(-it/\hbar)|\, m\,\rangle\langle\, m\,|\,\hat{H}\,|\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle \\
&+ \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{n_1=0}^{\infty} \frac{(-it/\hbar)^2}{2!}|\, m\,\rangle\langle\, m\,|\,\hat{H}\,|\, n_1\,\rangle\,\langle\, n_1\,|\,\hat{H}\,|\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle + \cdots \\
&= \sum_{n=0}^{\infty} |\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle \\
&+ \sum_{k=1}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{n_0=0}^{\infty}\cdots\sum_{n_k=0}^{\infty} \frac{(-it/\hbar)^k}{k!}|\, m\,\rangle\,\langle\, m\,|\, n_0\,\rangle\,\langle\, n_k\,|\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle \prod_{j=0}^{k-1}\langle\, n_j\,|\,\hat{H}\,|\, n_{j+1}\,\rangle\,.
\end{aligned}
$$

Since $\langle\, m\,|\, n\,\rangle = \delta_{m,n}$ for all m and n, the above simplifies to

$$
|\, s(t)\,\rangle = \sum_{n=0}^{\infty} |\, n\,\rangle\,\langle\, n\,|\, s(0)\,\rangle + \sum_{k=1}^{\infty}\sum_{n_0=0}^{\infty}\cdots\sum_{n_k=0}^{\infty} \frac{(-it/\hbar)^k}{k!}|\, n_0\,\rangle\,\langle\, n_k\,|\, s(0)\,\rangle \prod_{j=0}^{k-1}\langle\, n_j\,|\,\hat{H}\,|\, n_{j+1}\,\rangle\,.
$$

The bottom line is that it all depends on evaluating $\langle\, n_k\,|\, s(0)\,\rangle$ and the expectation values $\langle\, n_j\,|\,\hat{H}\,|\, n_{j+1}\,\rangle$. The evaluation of $\langle\, n_k\,|\, s(0)\,\rangle$ obviously depends on the choice of the initial state $|\, s(0)\,\rangle$ but we can evaluate $\langle\, n_j\,|\,\hat{H}\,|\, n_{j+1}\,\rangle$, as follows:

$$
\begin{aligned}
\langle\, n_j\,|\,\hat{H}\,|\, n_{j+1}\,\rangle &= \langle\, n_j\,|\,\hat{H}_{\text{h.o.}}\,|\, n_{j+1}\,\rangle + \langle\, n_j\,|\, V(\hat{x})\,|\, n_{j+1}\,\rangle \\
&= (n_j + \tfrac{1}{2})\,\hbar\omega\,\delta_{n_j,n_{j+1}} + \int dx\, V(x)\,\langle\, n_j\,|\, x\,\rangle\,\langle\, x\,|\, n_{j+1}\,\rangle \\
&= (n_j + \tfrac{1}{2})\,\hbar\omega\,\delta_{n_j,n_{j+1}} + \int dx\, V(x)\,\psi^*_{n_j}(x)\,\psi_{n_{j+1}}(x)\,,
\end{aligned}
$$

where, as defined earlier, $\psi_n(x)$ is the normalized wave-function of the n-th energy eigenstate, in the position representation, and $\psi^*_n(x)$ is its complex-conjugate. Since these wave-functions are real, though, the complex conjugation ends up being irrelevant here.

This is as far as we can go witout knowing the exact form of $V(\hat{x})$.

Extension to higher-dimensional spaces

Since the Hamiltonian of a d-dimensional harmonic oscillator is the sum of d *independent* 1-dimensional harmonic oscillators,

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2M} + \frac{M\omega^2}{2}\,\hat{\mathbf{x}}^2 = \sum_{j=1}^{d} \hat{H}_j = \sum_{j=1}^{d} \Big(\frac{\hat{p}_j^2}{2M} + \frac{M\omega^2}{2}\,\hat{x}_j^2 \Big)\,,$$

everything done in the previous sections carries over to the d-dimensional case, with the following extensions:

- There is a pair of $(\hat{a}, \hat{a}^\dagger)$ operators for each separate dimension, and operators from different dimensional axes commute with each other, that is, $[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$ and $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j}$, for all i and j in the integers such that $1 \le i, j \le d$;

- There are d individual number operators and one total-number operator,

$$\hat{N}_j \equiv \hat{a}_j^\dagger \hat{a}_j \quad (\,1 \le j \le d\,)$$
$$\hat{N} \equiv \sum_{j=1}^{d} \hat{N}_j\,,$$

  and the $\hat{N}_j$ operators commute with one another and, thus, also with $\hat{N}$,

$$[\hat{N}_i, \hat{N}_j] = [\hat{N}_i, \hat{N}] = 0 \quad (\,1 \le i, j \le d\,)\,.$$

  This means that it's possible to have a state that is simultaneously an eigenstate of all number operators;

- The Hamiltonian is still essentially just the number operator,

$$\hat{H} = \sum_{j=1}^{d} \hat{H}_j = \sum_{j=1}^{d} (\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2})\,\hbar\omega = \sum_{j=1}^{d} (\hat{N}_j + \frac{1}{2})\,\hbar\omega\,,$$

  and commutes with all number operators, $[\hat{H}, \hat{N}_j] = [\hat{H}, \hat{N}] = 0$. This means that it's possible to have an energy eigenstate that is simultaneously also an eigenstate of all number operators;

- A d-dimensional number and energy eigenstate now has a d-dimensional vector of non-negative integers representing it, $|\,\mathbf{n}\,\rangle \equiv |\,n_1, n_2, \ldots, n_d\,\rangle$, such that

$$\begin{aligned}
\hat{N}_j\,|\,\mathbf{n}\,\rangle &= n_j\,|\,\mathbf{n}\,\rangle \quad (\,n_j \geq 0, \quad 1 \leq j \leq d\,) \\
\hat{N}\,|\,\mathbf{n}\,\rangle &= \Big(\sum_{j=1}^{d} n_j\Big)\,|\,\mathbf{n}\,\rangle \\
\hat{H}_j\,|\,\mathbf{n}\,\rangle &= (n_j + \tfrac{1}{2})\,\hbar\omega\,|\,\mathbf{n}\,\rangle \quad (\,1 \leq j \leq d\,) \\
\hat{H}\,|\,\mathbf{n}\,\rangle &= \Big(\sum_{j=1}^{d} (n_j + \tfrac{1}{2})\,\hbar\omega\Big)\,|\,\mathbf{n}\,\rangle\,;
\end{aligned}$$

- The corresponding wave-function in the position representation is the product of the 1-dimensional wave-functions, with the appropriate indices,

$$\langle\, x\,|\,\mathbf{n}\,\rangle = \psi_{\mathbf{n}}(x) = \prod_{j=1}^{d} \langle\, x\,|\,n_j\,\rangle = \prod_{j=1}^{d} \psi_{n_j}(x)\,;$$

- The set of states $\{|\,\mathbf{n}\,\rangle\}$ is still orthonormal,

$$\langle\, \mathbf{m}\,|\,\mathbf{n}\,\rangle = \delta_{\mathbf{m},\mathbf{n}} = \prod_{j=1}^{d} \delta_{m_j,n_j}\,;$$

- The integral $\int dx$ is now d-dimensional,

$$\int d\mathbf{x} \equiv \int dx_1 \int dx_2 \ldots \int dx_d\,.$$

Using harmonic oscillator eigenstates in DQC

Our goal is to compute

$$\langle\, \mathbf{x}_r(t)\,\rangle = \langle\, \Phi_r(\mathbf{x},t)\,|\,\hat{\mathbf{x}}\,|\,\Phi_r(\mathbf{x},t)\,\rangle\,,$$

which first requires us to compute

$$|\,\Phi_r(\mathbf{x},t)\,\rangle = e^{-it\,\hat{H}}\,|\,\Phi_r(\mathbf{x})\,\rangle\,,$$

where

$$\hat{H} = -\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x}) \quad \text{and} \quad V(\mathbf{x}) = \frac{1}{2\sigma^2\,\Psi(\mathbf{x})} \sum_{r=1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big]\,.$$

Before proceeding, let's rewrite the potential in a different form. If we temporarily revert to using M in place of $1/\sigma^2$, then

$$\begin{aligned}
\Psi(\mathbf{x}) &= A\sum_{r=1}^{R} c_r\,\exp\Big[-\frac{M(\mathbf{x}-\mathbf{x}_r)^2}{2}\Big] \\
-\frac{2}{A}\,\frac{\partial\Psi(\mathbf{x})}{\partial M} &= \sum_{r=1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[-\frac{M(\mathbf{x}-\mathbf{x}_r)^2}{2}\Big] \\
V(\mathbf{x}) &= \frac{M}{2\,\Psi(\mathbf{x})}\sum_{r=1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[-\frac{M(\mathbf{x}-\mathbf{x}_r)^2}{2}\Big] = -\frac{M}{A}\,\frac{1}{\Psi(\mathbf{x})}\,\frac{\partial\Psi(\mathbf{x})}{\partial M}\,.
\end{aligned}$$

Thus,

$$V(\mathbf{x}) = -\frac{1}{A\sigma^2}\,\frac{\partial\ln\Psi(\mathbf{x})}{\partial(1/\sigma^2)}\,.$$

We now define a new potential,

$$U(\mathbf{x}) \equiv V(\mathbf{x}) - \frac{1}{2\sigma^2}\,\mathbf{x}^2 = -\frac{1}{2\sigma^2}\,\Big(\frac{2}{A}\,\frac{\partial\ln\Psi(\mathbf{x})}{\partial(1/\sigma^2)} + \mathbf{x}^2\Big)\,,$$

so that

$$\hat{H} = -\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x}) = \Big(-\frac{\sigma^2}{2}\nabla^2 + \frac{1}{2\sigma^2}\,\mathbf{x}^2\Big) + U(\mathbf{x})\,.$$

In other words, the Hamiltonian is the sum of the Hamiltonian for a d-dimensional harmnonic oscillator (with $M = 1/\sigma^2$, $\omega = 1$, and $\hbar = 1$) and a perturbing potential $U(\mathbf{x})$.

Next, we make use of the result from a previous section, properly extended to d dimensions, and write

$$\begin{aligned}
|\,\Phi_r(\mathbf{x},t)\,\rangle &= \sum_{\mathbf{n}} |\,\mathbf{n}\,\rangle\,\langle\,\mathbf{n}\,|\,\Phi_r(\mathbf{x})\,\rangle \\
&\quad + \sum_{k=1}^{\infty}\sum_{\mathbf{n}_0}\cdots\sum_{\mathbf{n}_k}\frac{(-it)^k}{k!}|\,\mathbf{n}_0\,\rangle\,\langle\,\mathbf{n}_k\,|\,\Phi_r(\mathbf{x})\,\rangle\prod_{j=0}^{k-1}\langle\,\mathbf{n}_j\,|\,\hat{H}\,|\,\mathbf{n}_{j+1}\,\rangle\,.
\end{aligned}$$

Moreover, similarly to the earlier result,

$$\langle\, \mathbf{n}_j \,|\, \hat{H} \,|\, \mathbf{n}_{j+1} \,\rangle = \sum_{\ell=1}^{d} [\, (\mathbf{n}_j)_\ell + \frac{1}{2} \,]\, \delta_{\mathbf{n}_j,\mathbf{n}_{j+1}} + \int d\mathbf{x}\, U(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x})\,.$$

The next goals, then, are to evaluate $\langle\, \mathbf{n}_k \,|\, \Phi_r(\mathbf{x}) \,\rangle$ and $\int d\mathbf{x}\, U(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x})$.

Evaluating $\langle\, \mathbf{n}_k \,|\, \Phi_r(\mathbf{x}) \,\rangle$

$$\begin{aligned}
\langle\, \mathbf{n}_k \,|\, \Phi_r(\mathbf{x}) \,\rangle &= \int d\mathbf{y}\, \langle\, \mathbf{n}_k \,|\, \mathbf{y} \,\rangle\, \langle\, \mathbf{y} \,|\, \Phi_r(\mathbf{x}) \,\rangle \\
&= \int d\mathbf{y}\, \langle\, \mathbf{n}_k \,|\, \mathbf{y} \,\rangle\, \delta(\mathbf{y}-\mathbf{x})\, \langle\, \mathbf{x} \,|\, \Phi_r(\mathbf{x}) \,\rangle \\
&= \langle\, \mathbf{n}_k \,|\, \mathbf{x} \,\rangle\, \langle\, \mathbf{x} \,|\, \Phi_r(\mathbf{x}) \,\rangle \\
&= \psi^*_{\mathbf{n}_k}(\mathbf{x})\, \Phi_r(\mathbf{x})\,.
\end{aligned}$$

Evaluating $\int d\mathbf{x}\, U(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x})$

$$\begin{aligned}
\int d\mathbf{x}\, U(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) &= -\frac{1}{2\sigma^2} \int d\mathbf{x} \left(\frac{2}{A}\, \frac{\partial \ln \Psi(\mathbf{x})}{\partial(1/\sigma^2)} + \mathbf{x}^2 \right) \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) \\
&= -\frac{1}{A\sigma^2}\, \frac{\partial}{\partial(1/\sigma^2)} \int d\mathbf{x}\, \ln \Psi(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) \\
&\quad - \frac{1}{2\sigma^2} \int d\mathbf{x}\, \mathbf{x}^2\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x})
\end{aligned}$$

$$\begin{aligned}
\int d\mathbf{x}\, \mathbf{x}^2\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) &= \int \Big(\sum_{s=1}^{d} x_s^2 \Big) \Big(\prod_{\ell=1}^{d} dx_\ell\, \psi^*_{(\mathbf{n}_j)_\ell}(x_\ell)\, \psi_{(\mathbf{n}_{j+1})_\ell}(x_\ell) \Big) \\
&= \sum_{s=1}^{d} \int dx_s\, x_s^2\, \psi^*_{(\mathbf{n}_j)_s}(x_s)\, \psi_{(\mathbf{n}_{j+1})_s}(x_s) \Big(\prod_{\substack{\ell=1 \\ \ell \neq s}}^{d} \int dx_\ell\, \psi^*_{(\mathbf{n}_j)_\ell}(x_\ell)\, \psi_{(\mathbf{n}_{j+1})_\ell}(x_\ell) \Big) \\
&= \sum_{s=1}^{d} \int dx_s\, x_s^2\, \psi^*_{(\mathbf{n}_j)_s}(x_s)\, \psi_{(\mathbf{n}_{j+1})_s}(x_s) \Big(\prod_{\substack{\ell=1 \\ \ell \neq s}}^{d} \delta_{(\mathbf{n}_j)_\ell,(\mathbf{n}_{j+1})_\ell} \Big)
\end{aligned}$$

Using [4]

$$\int dx\, x^2\, H_m(x)\, H_n(x)\, e^{-x^2} = \sqrt{\pi}\; 2^n\, n!\, \Big((n+\frac{1}{2})\, \delta_{m,n} + (n+2)(n+1)\, \delta_{n+2,m} + \frac{1}{4}\, \delta_{n-2,m} \Big)\,,$$

we find

$$\begin{aligned} \int d\mathbf{x}\, \mathbf{x}^2\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) \;&=\; \sqrt{\pi} \sum_{s=1}^{d} 2^{(\mathbf{n}_j)_s}\, (\mathbf{n}_j)_s! \\ \times \quad \Big(((\mathbf{n}_j)_s + \tfrac{1}{2})\, \delta_{(\mathbf{n}_{j+1})_s,(\mathbf{n}_j)_s} &+ ((\mathbf{n}_j)_s + 2)((\mathbf{n}_j)_s + 1)\, \delta_{(\mathbf{n}_j)_s+2,(\mathbf{n}_{j+1})_s} + \tfrac{1}{4}\, \delta_{(\mathbf{n}_j)_s-2,(\mathbf{n}_{j+1})_s} \Big) \\ &\times \Big(\prod_{\substack{\ell=1 \\ \ell\neq s}}^{d} \delta_{(\mathbf{n}_j)_\ell,(\mathbf{n}_{j+1})_\ell} \Big)\,. \end{aligned}$$

Evaluating $\int d\mathbf{x}\, \ln \Psi(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x})$

$$\int d\mathbf{x}\, \ln \Psi(\mathbf{x})\, \psi^*_{\mathbf{n}_j}(\mathbf{x})\, \psi_{\mathbf{n}_{j+1}}(\mathbf{x}) \;=\; \prod_{s=1}^{d} \int dx_s\, \ln \Psi(\mathbf{x})\, \psi^*_{(\mathbf{n}_j)_s}(x_s)\, \psi_{(\mathbf{n}_{j+1})_s}(x_s)\,.$$

Consider one particular component of $\mathbf{x}$, say, the s-th component x_s. The product of 1-dimensional wave-functions for that particular direction in d-space can be written as

$$\psi^*_m(x_s)\, \psi_n(x_s) = \Big(\frac{1}{\pi\sigma^2}\Big)^{1/2} \frac{1}{\sqrt{2^m\, m!}}\, \frac{1}{\sqrt{2^n\, n!}}\, H_m(\frac{x_s}{\sigma})\, H_n(\frac{x_s}{\sigma})\, e^{-x_s^2/\sigma^2}$$

and, so,

$$\begin{aligned} \int dx_s\, \ln \Psi(\mathbf{x})\, \psi^*_m(x_s)\, \psi_n(x_s) \;&=\; \Big(\frac{1}{\pi\sigma^2}\Big)^{1/2} \frac{1}{\sqrt{2^m\, m!}}\, \frac{1}{\sqrt{2^n\, n!}} \\ &\times \int dx_s\, \ln \Psi(\mathbf{x})\, H_m(\frac{x_s}{\sigma})\, H_n(\frac{x_s}{\sigma})\, e^{-x_s^2/\sigma^2} \\ &= \Big(\frac{1}{\pi\sigma^2}\Big)^{1/2} \frac{1}{\sqrt{2^m\, m!}}\, \frac{1}{\sqrt{2^n\, n!}} \\ &\times \int \sigma\, du_s\, \ln G(\mathbf{u})\, H_m(u_s)\, H_n(u_s)\, e^{-u_s^2} \\ &= \frac{1}{\sqrt{\pi}}\, \frac{1}{\sqrt{2^m\, m!}}\, \frac{1}{\sqrt{2^n\, n!}} \int du_s\, \ln G(\mathbf{u})\, H_m(u_s)\, H_n(u_s)\, e^{-u_s^2}\,, \end{aligned}$$

where

$$\begin{aligned} G(\mathbf{u}) = \Psi(\sigma\,\mathbf{u}) &= A\sum_{r=1}^{R} c_r\,\exp\Big[-\frac{(\sigma\,\mathbf{u}-\mathbf{x}_r)^2}{2\sigma^2}\Big] = A\sum_{r=1}^{R} c_r\,\exp\Big[-\frac{(\mathbf{u}-\mathbf{x}_r/\sigma)^2}{2}\Big] \\ &= A\sum_{r=1}^{R} c_r \prod_{\ell=1}^{d}\exp\Big[-\frac{(u_\ell-(\mathbf{x}_r)_\ell/\sigma)^2}{2}\Big] \\ &= A\sum_{r=1}^{R} c_r\Big(\prod_{\substack{\ell=1\\ \ell\neq s}}^{d}\exp\Big[-\frac{(u_\ell-(\mathbf{x}_r)_\ell/\sigma)^2}{2}\Big]\Big)\,\exp\Big[-\frac{(u_s-(\mathbf{x}_r)_s/\sigma)^2}{2}\Big]. \end{aligned}$$

Hmm... this isn't going to work well, or maybe not even at all. Maybe a power-series expansion of the logarithm? Even then, we'll have powers of the sum over r. I suppose I could then use the binomial expansion theorem to get powers of the exponential on u_s and then we'd be left with having to evaluate

$$\int du_s\,\Big(\exp\Big[-\frac{(u_s-(\mathbf{x}_r)_s/\sigma)^2}{2}\Big]\Big)^k\,H_m(u_s)\,H_n(u_s)\,e^{-u_s^2}.$$

Expanding *that* exponential into a power series and then applying the binomial theorem yet again would result in the need to evaluate

$$\int du_s\,u_s^k\,H_m(u_s)\,H_n(u_s)\,e^{-u_s^2}.$$

And *that* I think is something for which there are analytical results. Still, it's a ton of power expansions and index juggling, very complicated and easy to screw up. It's doable and might be worth it, though. The end result would be lots of sums and powers of the components of $\mathbf{x}_r$ multiplied by Kronecker deltas on various indices $(\mathbf{n}_j)_s$ of energy eigenstates $\mathbf{n}_j$. I need Mathematica...

The semi-classical approach to DQS

As I mentioned earlier, it occurred to me that since the goal of DQS is to find the classical path of a data point by computing the expectation values of the position operator in a time-dependent state whose initial value is the data point's Gaussian extension, then why not simply numerically solve Newton's equations for the quantum potential derived in DQC, with appropriate initial conditions?

Newton's law of motion states that the acceleration of a particle of mass $m = 1/\sigma^2$ under the influence of a potential function $V(\mathbf{x})$ is given by

$$\ddot{\mathbf{x}} = -\sigma^2\,\nabla V(\mathbf{x}).$$

With the DQC potential derived earlier,

$$V(\mathbf{x}) = \frac{1}{2\sigma^2\,\Psi(\mathbf{x})}\,\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big]\,,$$

we find

$$\ddot{\mathbf{x}} = -\frac{1}{2}\,\nabla\Big(\frac{1}{\Psi(\mathbf{x})}\,\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,E_r(\mathbf{x})\Big)\,,$$

where

$$E_r(\mathbf{x}) \equiv \exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big]\,.$$

Then,

$$\begin{aligned} 2\Psi(\mathbf{x})\,\ddot{\mathbf{x}} \,=\, & \frac{1}{\Psi(\mathbf{x})}\,\nabla\Big(\Psi(\mathbf{x})\Big)\,\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,E_r(\mathbf{x}) \\ & -\,\sum_{r\,=\,1}^{R} c_r\nabla\Big((\mathbf{x}-\mathbf{x}_r)^2\Big)E_r(\mathbf{x}) - \sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,\nabla\Big(E_r(\mathbf{x})\Big)\,. \end{aligned}$$

Since

$$\Psi(\mathbf{x}) = A\,\sum_{r\,=\,1}^{R} c_r\,\exp\Big[-\frac{(\mathbf{x}-\mathbf{x}_r)^2}{2\sigma^2}\Big] = A\,\sum_{r\,=\,1}^{R} c_r\,E_r(\mathbf{x})$$

and

$$\nabla\Big(E_r(\mathbf{x})\Big) = -\frac{(\mathbf{x}-\mathbf{x}_r)}{\sigma^2}\,E_r(\mathbf{x})\,,$$

we have

$$\nabla\Psi(\mathbf{x}) = -\frac{A}{\sigma^2}\,\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)\,E_r(\mathbf{x})\,,$$

and, thus,

$$\begin{aligned} 2\Psi(\mathbf{x})\,\ddot{\mathbf{x}} \,=\, & -\frac{A}{\sigma^2}\,\frac{1}{\Psi(\mathbf{x})}\,\Big(\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)\,E_r(\mathbf{x})\Big)\,\Big(\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)^2\,E_r(\mathbf{x})\Big) \\ & -\,2\Big(\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)\,E_r(\mathbf{x})\Big) + \frac{1}{\sigma^2}\Big(\sum_{r\,=\,1}^{R} c_r\,(\mathbf{x}-\mathbf{x}_r)\,(\mathbf{x}-\mathbf{x}_r)^2\,E_r(\mathbf{x})\Big)\,. \end{aligned}$$

If we now define

$$\begin{aligned}
\mathbf{B}(\mathbf{x}) &\equiv \sum_{r=1}^{R} c_r \,(\mathbf{x}-\mathbf{x}_r)\, E_r(\mathbf{x}) \\
C(\mathbf{x}) &\equiv \sum_{r=1}^{R} c_r \,(\mathbf{x}-\mathbf{x}_r)^2\, E_r(\mathbf{x}) \\
\mathbf{D}(\mathbf{x}) &\equiv \sum_{r=1}^{R} c_r \,(\mathbf{x}-\mathbf{x}_r)\,(\mathbf{x}-\mathbf{x}_r)^2\, E_r(\mathbf{x})
\end{aligned}$$

then

$$\ddot{\mathbf{x}} = \frac{\Big(\mathbf{D}(\mathbf{x}) - 2\sigma^2\,\mathbf{B}(\mathbf{x})\Big)\,\Psi(\mathbf{x}) - A\,\mathbf{B}(\mathbf{x})\,C(\mathbf{x})}{2\sigma^2\,\Big(\Psi(\mathbf{x})\Big)^2}\,.$$

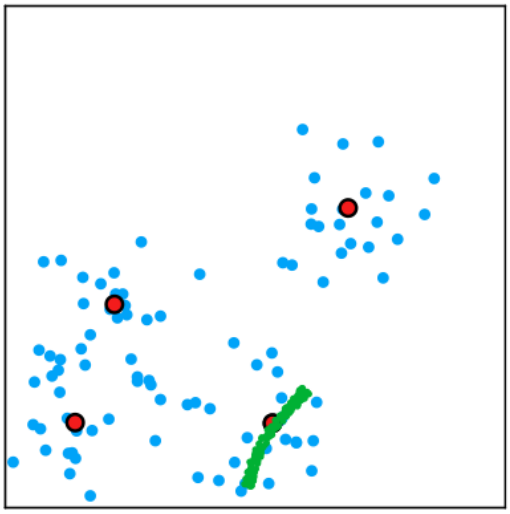
Note that, although $E_r(\mathbf{x}) > 0$ for any value of its argument, it is possible to have it equal zero in a numerical computation, because of limited precision. This would lead to a $0/0$ scenario, which can be avoided by keeping $E_r(\mathbf{x})$ above a minimum tiny value, say, 10^{-9}.

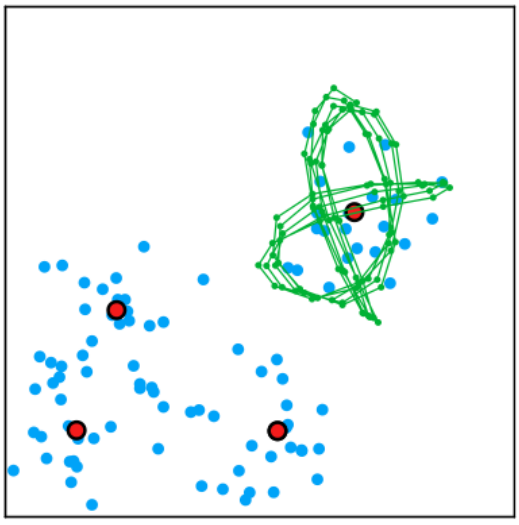
Also, even in an efficient computation of the acceleration, where all four quantities $\mathbf{B}(\mathbf{x}), C(\mathbf{x}), \mathbf{D}(\mathbf{x})$, and $\Psi(\mathbf{x})$ are computed in a single pass of the entire data set, it's still the case that a full pass over the data set is required for the evaluation of the acceleration at a given point. That's expensive but unavoidable.

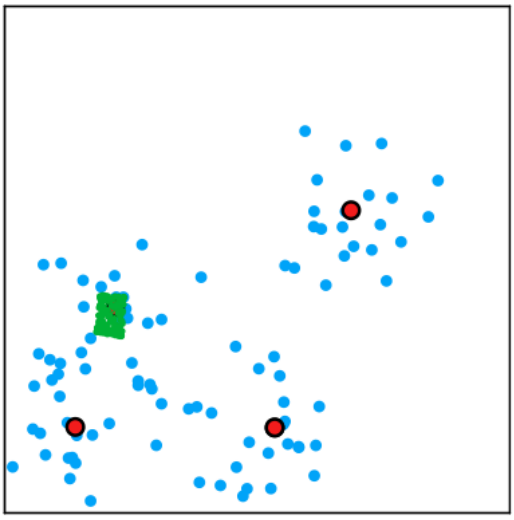
The numerical integration of the acceleration defined above may typically involve hundreds of function evaluations, hence hundreds of passes over the data set, *per choice of initial condition*. If, in addition, we're performing the integration for every data point as the initial condition, the entire process takes time that is *quadratic* in the size R of the data set, with a large multiplying constant C:

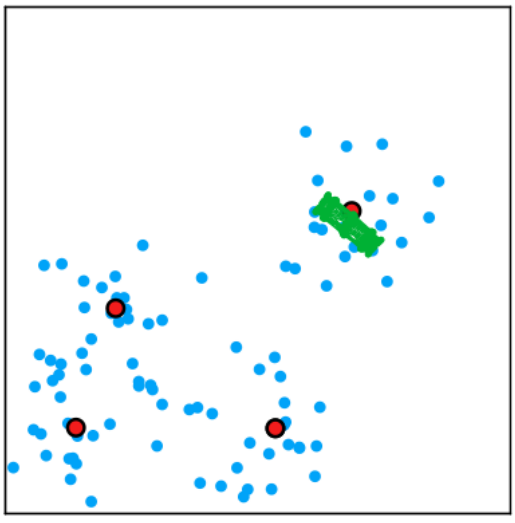
$$\text{running time } \approx CR^2\,.$$

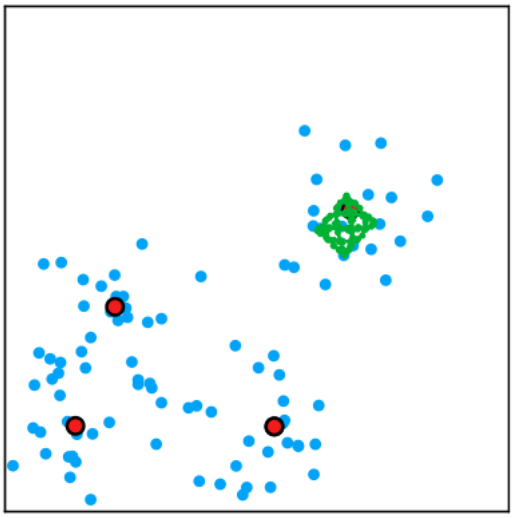
What follows is the result of a quick-and-dirty implementation of a velocity-Verlet integrator [5] running on randomly generated sample data: 100 points (blue) around 4 clusters (red). The green lines represent the path of a single data point, from its initial position, towards a local potential minimum. Note the oscillatory behavior around a minimum (as expected from the potential being a kind of weighted average of harmonic oscilator potentials) and the occasional wanderer trajectory, due either to the crude implementation of the integrator (which is prone to numerical anomalies) or to the possibly meta-stable nature of some of the potential minima.

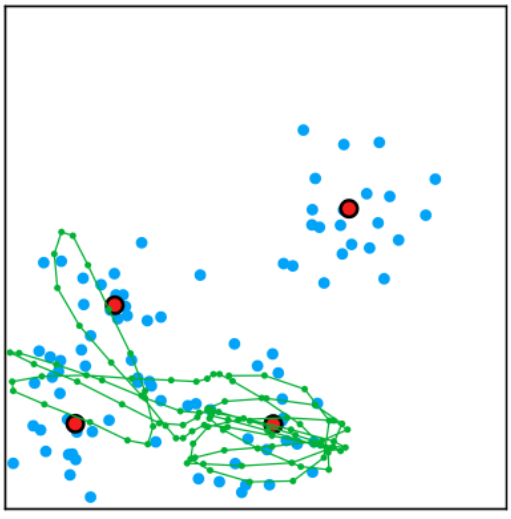


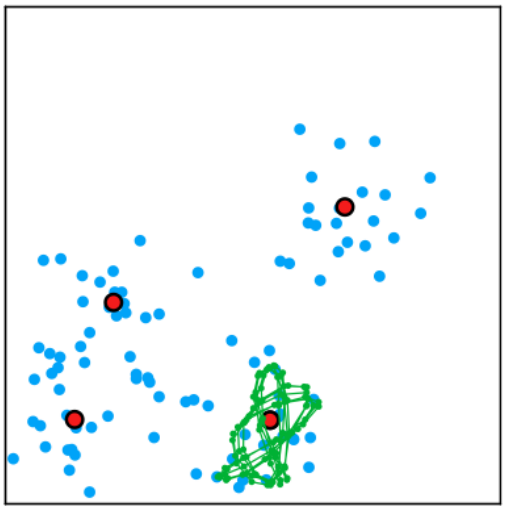


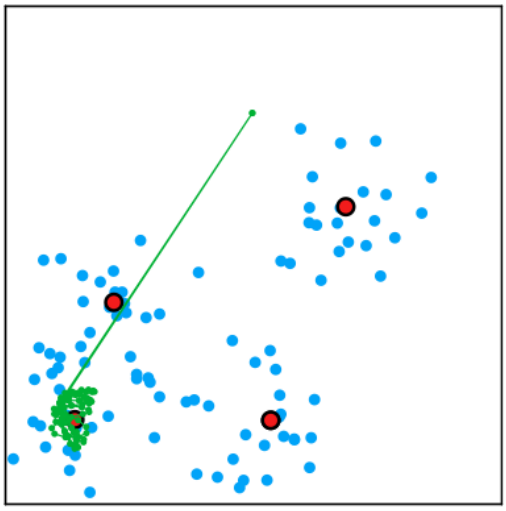


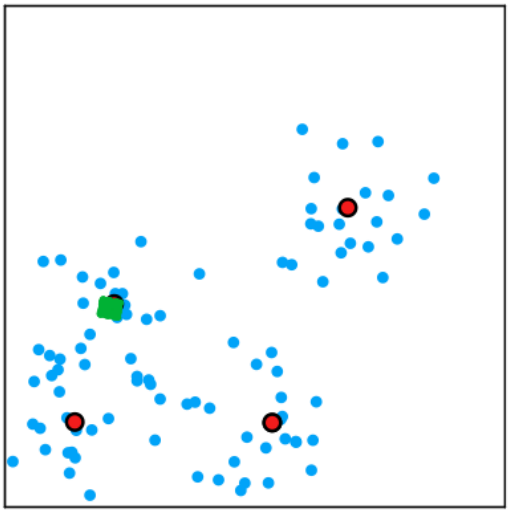


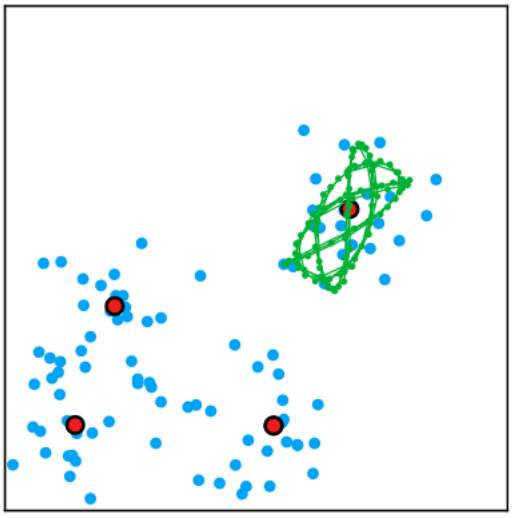


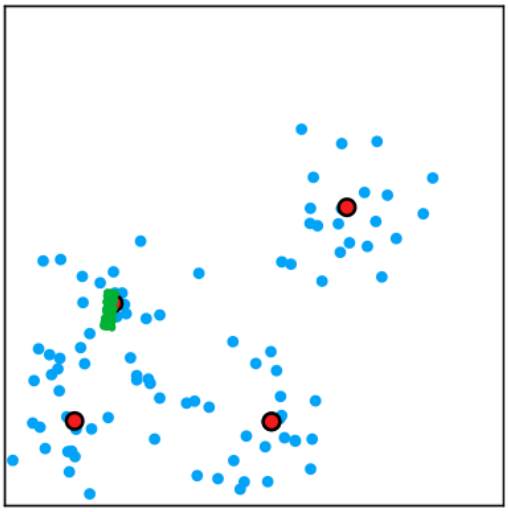


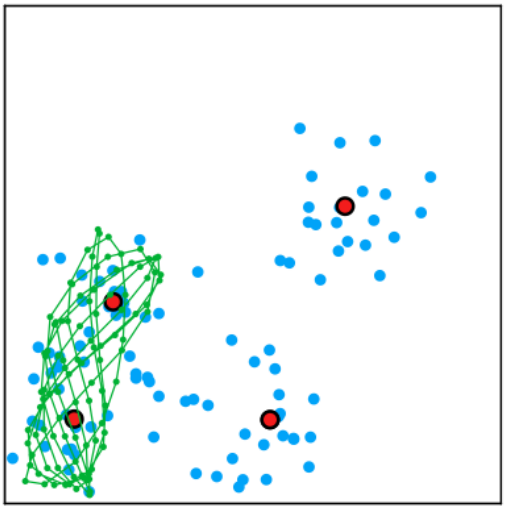


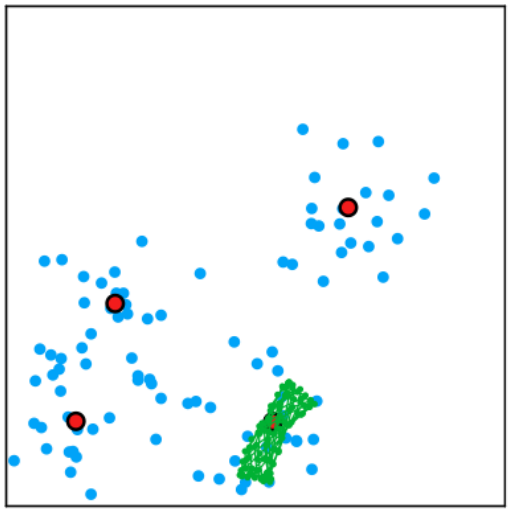


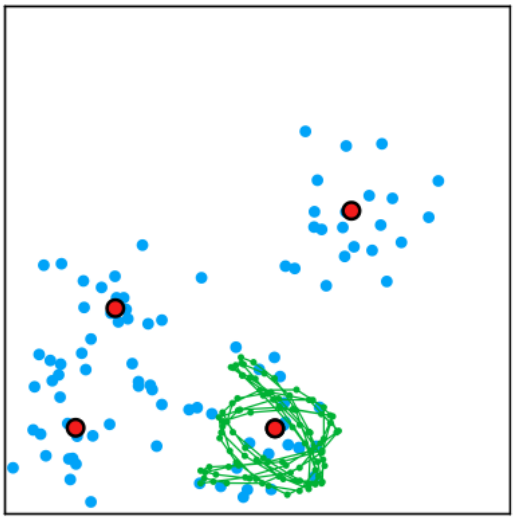


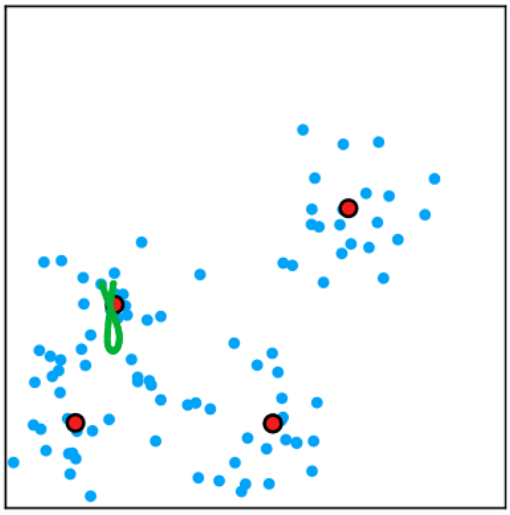


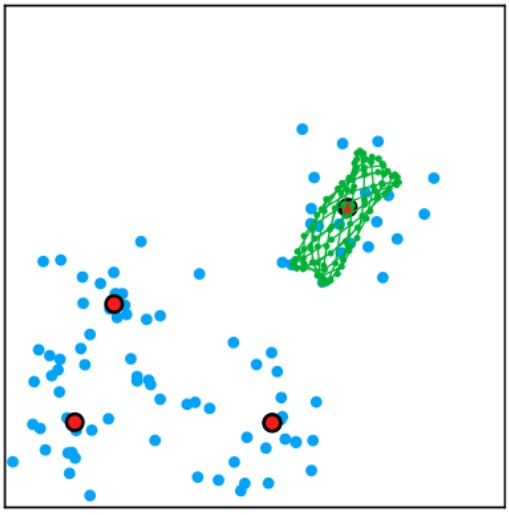












Using a better integrator

The results in the previous section were obtained by integrating

$$\ddot{\mathbf{x}} = -\sigma^2 \, \nabla V(\mathbf{x})$$

using a simple velocity-Verlet algorithm [5], with no step-size control and just some ad-hoc measures to prevent the acceleration from blowing up. The results were ok some of the time but there were several instances where severe instabilities creeped in. I next tried a better integrator, using a Beeman update rule [6], with a step-size control algorithm of my own, described next.

Suppose we go from x_n to x_{n+1} by means of a *single* step in time, of length Δt. The result, using a Beeman update, is

$$\begin{aligned} x_{n+1}^{(1)} &= x_n + v_n \, \Delta t + \frac{1}{6} \, (4a_n - a_{n-1}) \, (\Delta t)^2 + \mathcal{O}(\Delta t)^3 \\ v_{n+1}^{(1)} &= v_n + \frac{1}{6} \, (2a_{n+1} + 5a_n - a_{n-1}) \, \Delta t + \mathcal{O}(\Delta t)^2 \, . \end{aligned}$$

But we could, instead, go from x_n to x_{n+1} by means of *two* successive steps, of length $\Delta t/2$ each. The result would then be

$$\begin{aligned} x_{n+1}^{(2)} &= x_n + v_n \, \Delta t + \frac{1}{8} \, (5a_n - a_{n-1}) \, (\Delta t)^2 + \mathcal{O}(\Delta t)^3 \\ v_{n+1}^{(2)} &= v_{n+1}^{(1)} + \mathcal{O}(\Delta t)^2 \end{aligned}$$

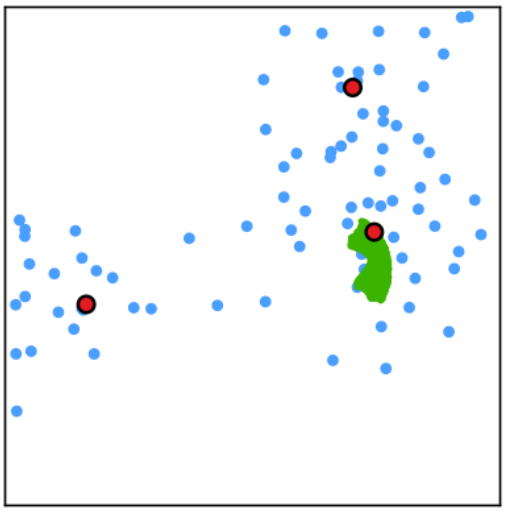
We can use the absolute difference

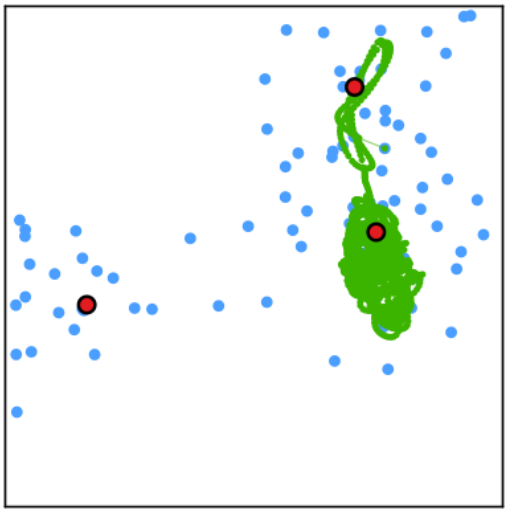
$$| \, x_{n+1}^{(2)} - x_{n+1}^{(1)} \, | = \frac{| \, a_n - a_{n-1} \, | \, (\Delta t)^2}{24}$$

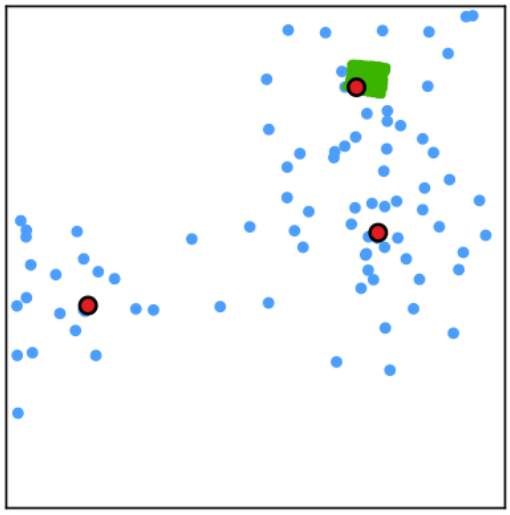
as a measure of the local truncation error and impose that it be limited by some prescribed value ε of our choosing, thereby setting a limit to how large Δt can be at any given iteration step:

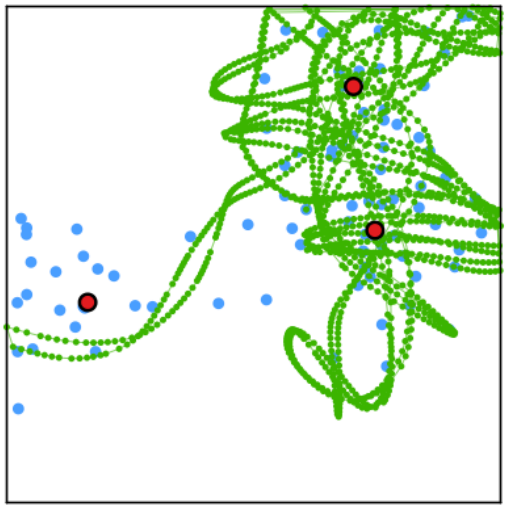
$$| \, x_{n+1}^{(2)} - x_{n+1}^{(1)} \, | \, \leq \, \varepsilon \quad \Rightarrow \quad (\Delta t_n)^2 \leq \frac{24 \, \varepsilon}{| \, a_n - a_{n-1} \, |} \, .$$

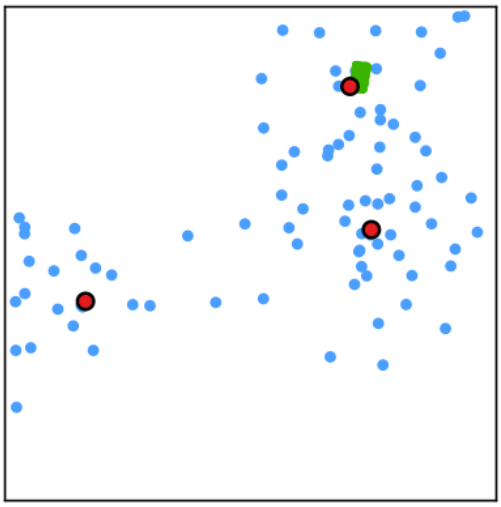
The results that follow were obtained using the update rules above on a randomly generated data set of 100 points and 3 cluster centers, with 2,000 iteration steps per data point. Not a single instability creeped in this time (after several trials), but some of the trajectories are still of the wanderer type, possibly due to the potential minima being metastable for some initial conditions.

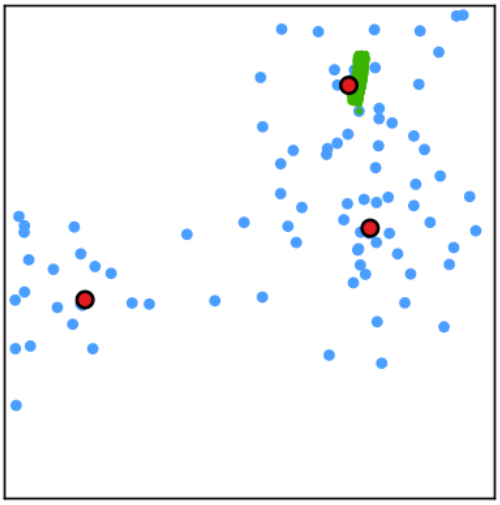


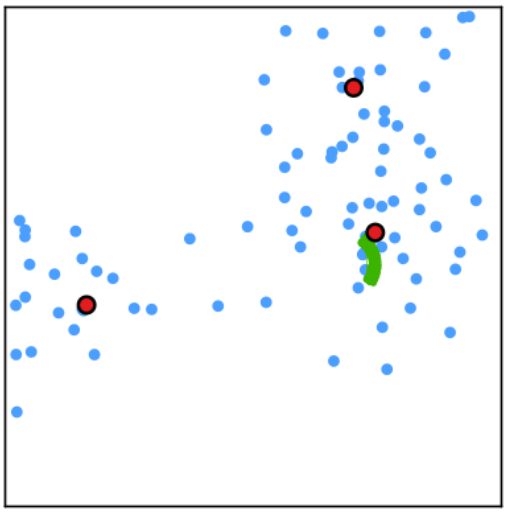


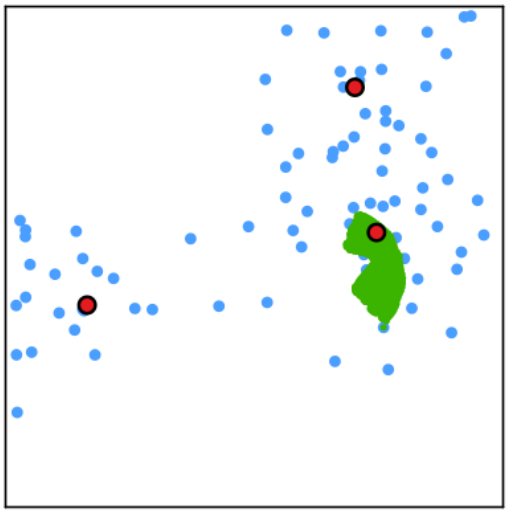


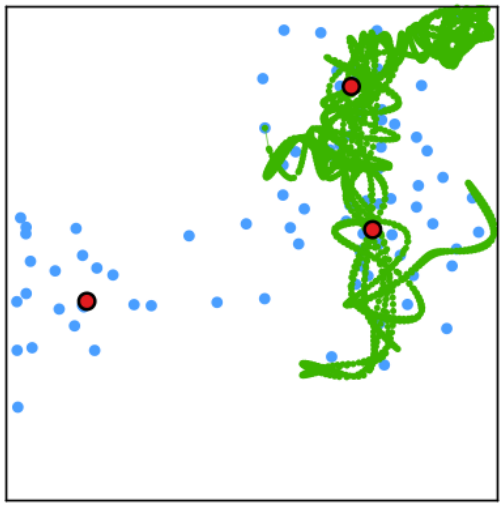


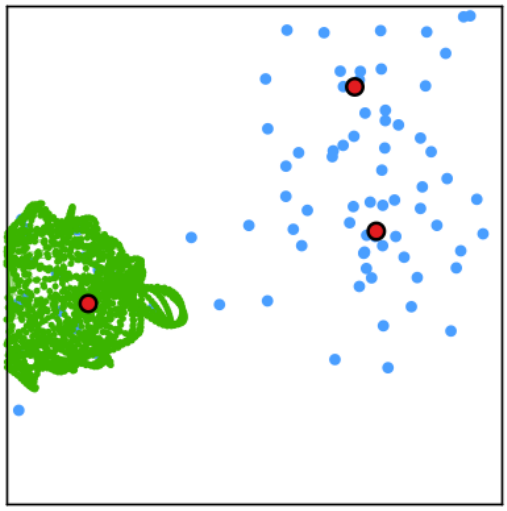












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