Stochastic evaluation of traces

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Background:

On a microscopic level the behavior of most physical systems, like their thermodynamics or response to external probes, depends on the distribution of the eigenvalues and the properties of the eigenfunctions of a Hamilton operator or dynamical matrix. In numerical approaches the latter correspond to Hermitian matrices of finite dimension D, which can become large already for a moderate number of particles, lattice sites, or gridpoints. The calculation of eigenvalues and eigenvectors turns into an intractable task.

An altanative way is to use numerical Chebyshev expansion and kernal polynomial method (KPM). In many situations we concerns the physical quantity related to the Hamiltonian matrix *H*. The Chebyshev expansion moments have their depencences on *H*, One type of such moments are the traces of the first kind Chebyshev exapansion term $T_n(H)$ and the given operator *A*.

$$\mu_n = Tr[AT_n(H)]$$

Here first kind Chebyshev expansion term $T_n(H)$ has the properties:

$$T_0(H) = 1, T_1(H) = T_{-1}(H) = H$$
$$T_{n+1}(H) = 2HT_n(H) - T_{n-1}(H)$$

Instead of calculating the trace on the whole Hilbert space directly which is time-consuming, we could try a effecient approximation method.

Stochastic evaluation:

Approximate the trace μ_n with only a small number of randomly chosen states.

$$\mu_n = Tr[AT_n(H)] \approx \frac{1}{R}\sum_{r=0}^{R}\langle r|AT_n(H)|r\rangle$$

In above equation, $R \ll D. |r\rangle = \sum_{i=0}^{D-1}\xi_{ri}|i\rangle$, $\{|i\rangle\}$ is the base vector set of the *D* dimensional Hilbert space. ξ_{ri} is the random variable has some following statistical propeties.

requirements:

1. objective matrix $AT_n(H)$ is Hermian.

2. $\lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N}\xi_{\mathrm{ri}} = \langle \xi_{\mathrm{ri}}\rangle = 0$.

3. $\langle \xi_{\mathrm{ri}}\xi_{r'j}\rangle = 0$.

4. $\langle \xi_{ri}^{*}\xi_{r'j}\rangle = \delta_{\mathrm{rr'}}\delta_{\mathrm{ij}}$.

Implementation:

Setting parameters and build the Hamiltonian-like Hermitian matrix:

```
D = 10000;
R = 30;
off = 1*rand(D-1,1)+1i*rand(D-1,1);
matA = diag(2*rand(D,1))+diag(off,1)+diag(conj(off),-1);
```

Use built-in function to calculate the trace of such matrix:

```
Tr1 = trace(matA);
disp(Tr1)
```

```
9.8228e+03
```

To meet the requirements, here I choose $\xi_{\mathrm{ri}} = e^{i\phi} = \cos(\phi) + i\sin(\phi), \phi \in [0, 2\pi]$ is random phase.

```
theta = rand([R,D])*2*pi;
xi_ri = cos(theta)+1i*sin(theta);
tmp = zeros(R,1);
for i = 1:R
    tmp(i) = xi_ri(i,:)*matA*xi_ri(i,:)';
end
Tr2 = real(sum(tmp)/R);
disp(Tr2)
```

```
9.8212e+03
```

Now discuss the error: theoretically the analytic relative error: $\delta\mu_n/\mu_n \sim O\left(\frac{1}{\sqrt{\mathrm{RD}}}\right)$.

```
err_analytic = 1/sqrt(R*D);
err_real = abs(Tr1-Tr2)/abs(Tr1);
fprintf('the real relative error is: %2.5f, the analytic relative error is %2.5f\n', err_real,e
```

```
the real relative error is: 0.00016, the analytic relative error is 0.00183
```