Automatically Differentiable Unitary Coupled-Cluster

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github.com/kottmanj/stc2022

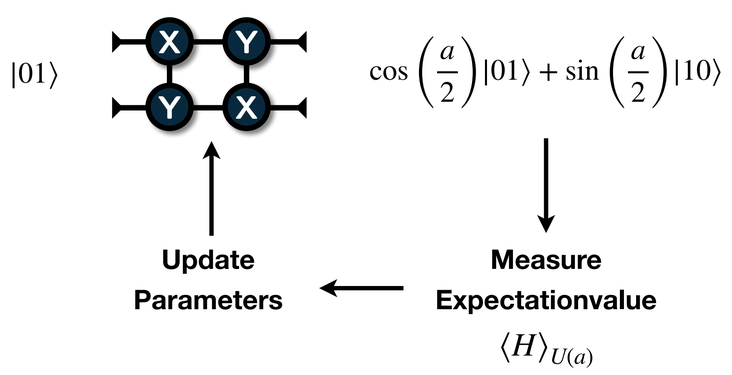
Variational Quantum Algorithms

Quantum Circuits:

$U(a) = \prod_k e^{-i\frac{a_k}{2}G_k}$ **with Generators:** G_k

Example:

$U(a,b) = e^{-i\frac{a}{2}\sigma_x\otimes\sigma_y}e^{-i\frac{a}{2}\sigma_y\otimes\sigma_x}$



Unitary Coupled-Cluster

$G_f = a_n^\dagger a_n a_v^\dagger a_w \ldots - h.c.$

$a_m^\dagger \rightarrow \sigma_+(m)\prod_{k<m}\sigma_z(k)$

Differentiability

Shift-Rule (Schuld et. al.)

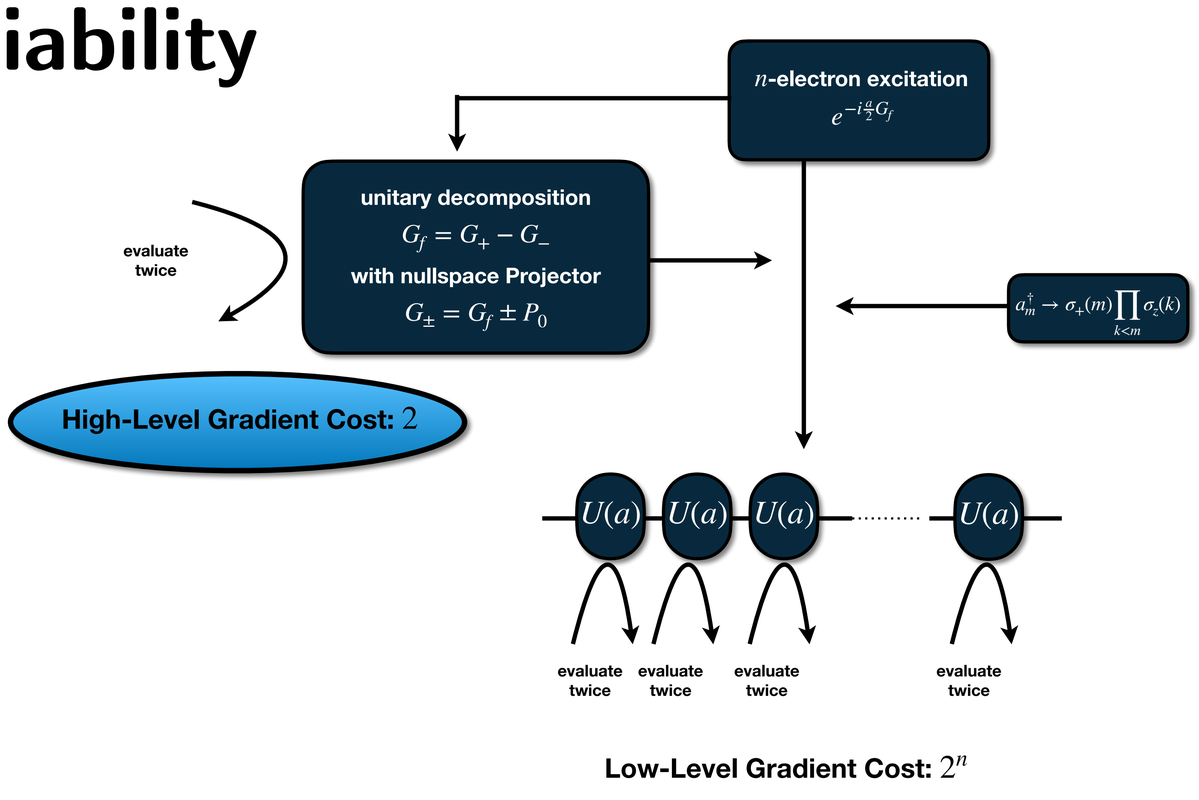
$$\frac{\partial\langle H\rangle_{U(a)}}{\partial a} \propto \langle H\rangle_{U(a+s)} - \langle H\rangle_{U(a-s)}$$

Condition: Generator is unitary

For UCC this does not hold

Cost can be reduced to 2

(same cost as finite-differences)



Tequila Framework

```
a = Variable("a")
f = (-a**2).apply(exp)
U = Ry(f,0) + CNOT(0,1)

H = X(0)*X(1) + 0.5*Z(0) + Y(1)
E = ExpectationValue(H=H, U=U)
dE = grad(E, "a")

F = E + (-dE**2).apply(exp)
```

```
L = tq.compile(F)
```

```
eval = L({"a":1.0})
```

$$H = \sigma_x(0)\sigma_x(1) + \frac{1}{2}\sigma_z(0) + \sigma_y(1)$$

$$L = \langle H\rangle_{U(a)} + e^{-\left(\frac{\partial}{\partial a}\langle H\rangle_{U(a)}\right)^2}$$

$e^{-i\frac{f(a)}{2}\sigma_y}$

$f(a) = e^{-a^2}$

Examples

more on: github.com/kottmanj/stc2022

Standard Quantum Chemistry

```
mol = Molecule("beh2.xyz", basis_set="sto-3g")
```

Krylov Methods

```
m = QTensor(shape=[x,y])
m[i,j] = braket(U1,U2,H)
M = tq.compile(m)
```

Basis-Set-Free Quantum Chemistry

```
mol = Molecule("beh2.xyz")
```

UCC Gates

```
U = mol.make_excitation_gate([(0,2)], angle="a")
```

Excited States

```
S2 = ExpectationValue(H=Q,U=U2+U.dagger())
f = E - c*S2
result = minimize(f)
```

Ground States

```
H = mol.make_hamiltonian()
E = ExpectationValue(H=H, U=U)
result = minimize(E)
```

Defined Methods

```
UCCSD, k-UpCCGSD, SPA, ADAPT
```

Orbital Optimization

```
opt = optimize_orbitals(mol, circuit=U)
```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Tequila

Recent Developments

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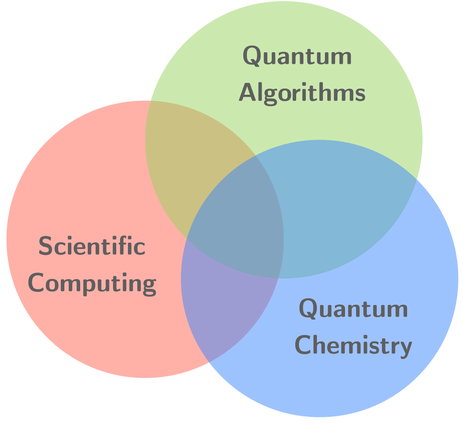
Initial Team

Sumner Alperin Lea, Alba Cervera-Lierta, Teresa Tamayo-Mendoza, Cyrillle Lavigne

Dependencies

Qulacs (or Qiskit/Cirq/PyQuil/Qibo), OpenFermion, PySCF, Madness, SciPy, Jax (or Autograd)



Interested?

Positions (E13 100%) available

(PhD & Postdoc)

starting Nov. 2022

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