Online PCA in Converging Self-consistent Field Equations

Xihan Li[1], Xiang Chen[2], Rasul Tutunov[3], Haitham Bou Ammar[3], Lei Wang[4], Jun Wang[1]

[1]University College London

[2]Huawei Noah's Ark Lab

[3]Huawei R&D U.K.

[4]Institute of Physics, Chinese Academy of Sciences

Speaker: Xihan Li

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Problem Setting

Eigen Decomposition

An $n \times n$ matrix

A scalar (eigenvalue)

$$Av = \lambda v$$

Eigen decomposition: given matrix A, find a vector v (eigenvector) and a scalar λ (eigenvalue) to satisfy the above equation

E.g., given $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$, we can do standard eigen decomposition to get a vector $v = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and a scalar $\lambda = 3$ so that

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 3 \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Problem Setting

What will happen if matrix A is not directly given, but A is a given function of v?

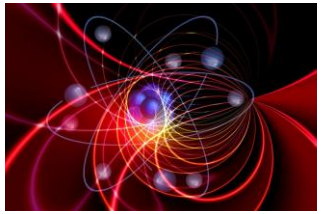
F is given

$$A \doteq F(v)$$

An $n \times n$ matrix

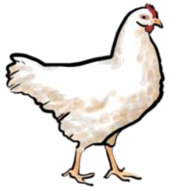
A scalar (eigenvalue)

$$\boxed{F(v)}v = \lambda v$$



Self-consistent Field Equation
(Important in Quantum Physics!)
$H|\Psi\rangle = E|\Psi\rangle$

Eigen decomposition cannot be directly applied anymore!



To obtain v, eigen decomposition needs $A \rightarrow A$ comes from $F(v) \rightarrow$ we need to obtain v

Traditional Methods

Self-consistent Field method (fixed point iteration) for solving $F(v)v = \lambda v$

Eigen decomposition

Assign an initial $v_0 \xrightarrow{F_0 = F(v_0)} F_0 \xrightarrow{F_0 v_1 = \lambda v_1} v_1 \longrightarrow F_1 \longrightarrow v_2 \longrightarrow$ … (until convergence)

Problem: easily fails to converge (**infinite oscillation** between two or more states)

$$\cdots \longrightarrow \underbrace{v' \longrightarrow F' \longrightarrow v'' \longrightarrow F'' \longrightarrow v'}_{\text{Repeat infinitely}} \longrightarrow \cdots$$

Two current main research directions:

1. Generate a better initial solution v_0
2. Mix F_t with those in previous iterations $F_{t-1}, F_{t-2}, \ldots$ to stabilize the iteration

We propose a third direction with the aid of machine learning techniques

Motivation

We find a connection between two very different problems in different fields

- Self-consistent Field Equation

An $n \times n$ matrix

A scalar (eigenvalue)

$$\boxed{F(v)}v = \lambda v$$

Infinite oscillation

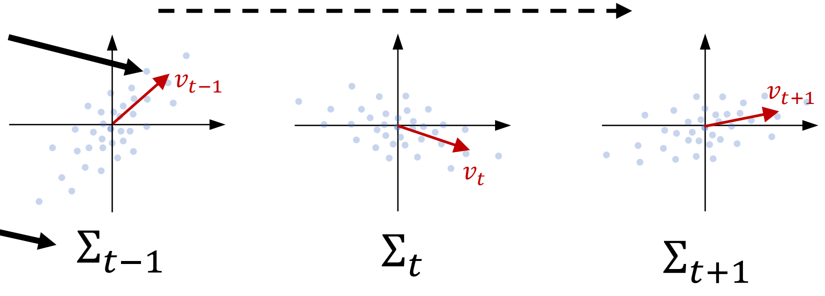
Task: finding v
Features:
1. Involves eigen decomposition
2. $F(v)$, the matrix to be decomposed, is not determined during the decomposition

- Online PCA

Time-variant data distribution in an online, non-stationary environment

Top principal component

Covariance matrix of the data distribution

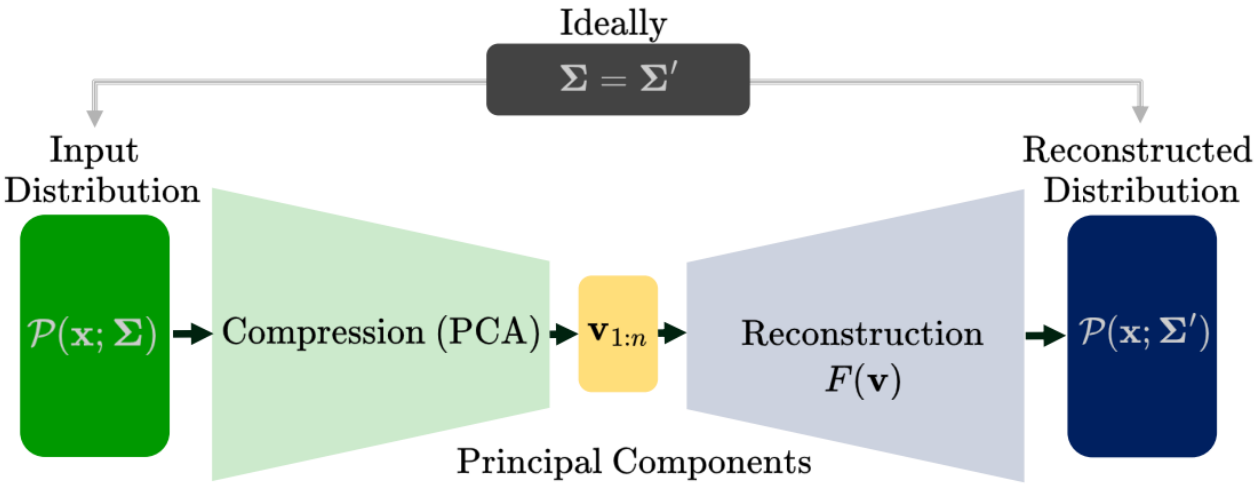


Incrementally Updated

Task: finding v
Features:
1. Involves eigen decomposition
2. Σ_t, the matrix to be decomposed, is not determined during the decomposition

Can we use Online PCA to resolve the infinite oscillation issue of SCF equation solving?

Our Method



- $F(v)v = \lambda v$ is to say, if we have a matrix Σ, then
    1. Decompose Σ to get its top eigenvector v
    2. Compute a new matrix $\Sigma' = F(v)$

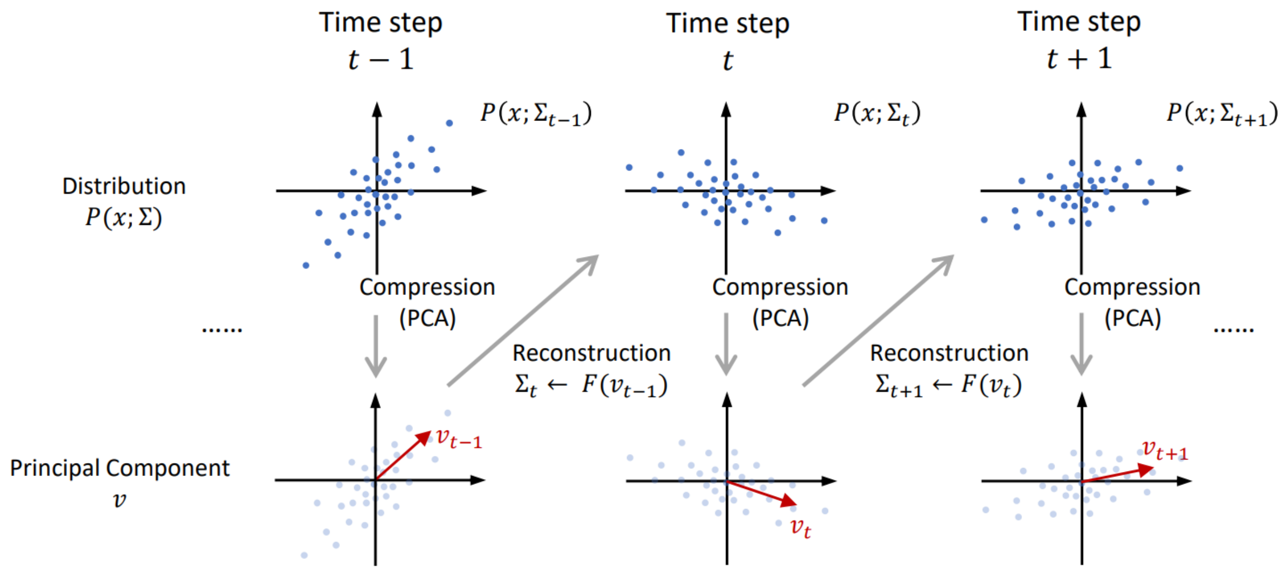
Then we will have $\Sigma' = \Sigma$

New interpretation:

"compress" Σ with PCA to have v

"reconstruct" Σ from v with $F(\cdot)$

Our Method



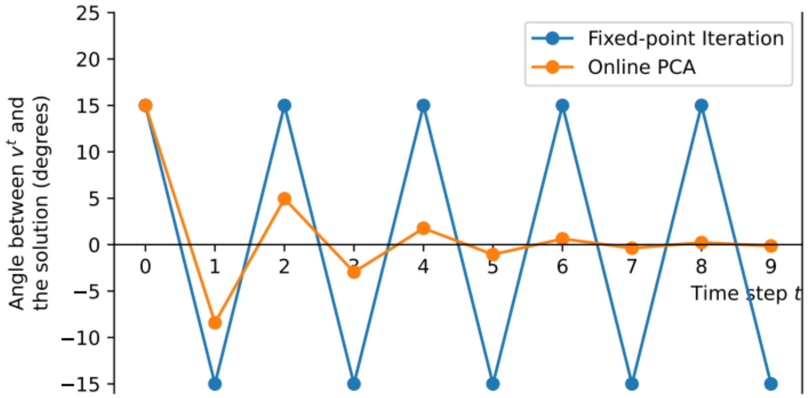
Then, the fixed-point iteration $v_0 \rightarrow F_0 \rightarrow v_1 \rightarrow F_1 \rightarrow \cdots$ can be regarded as

Compress (PCA) → reconstruct → compress (PCA) → reconstruct → …

We are continuously running PCA in a non-stationary environment!

Now we can apply Online PCA to **update v incrementally** to avoid **infinite oscillation**

Our Method



Then, the fixed-point iteration $v_0 \to F_0 \to v_1 \to F_1 \to \cdots$ can be regarded as

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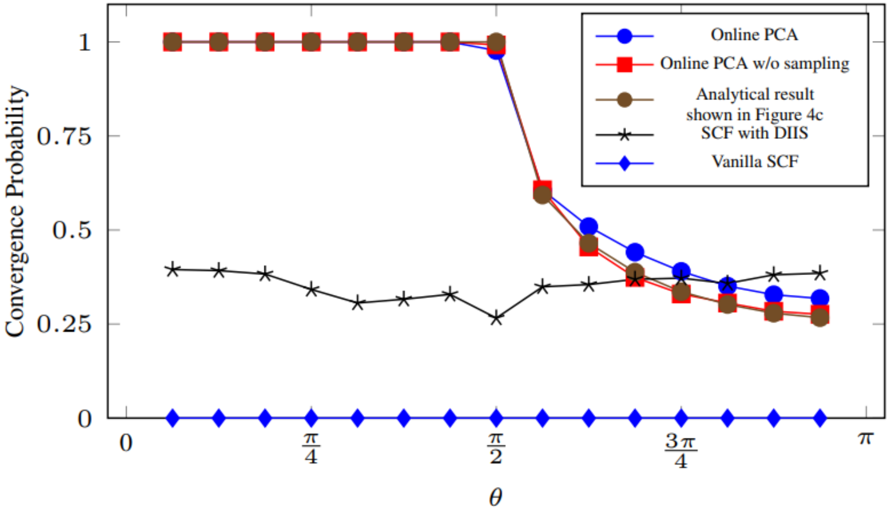
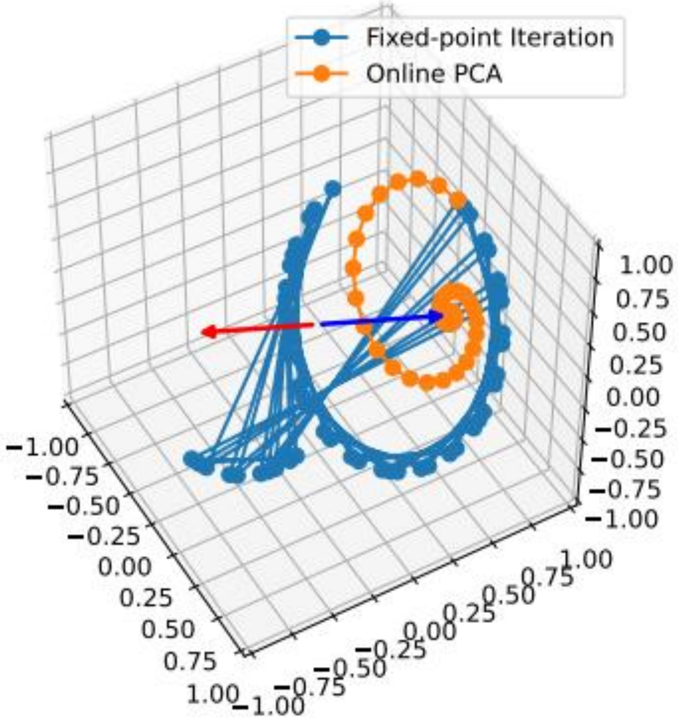
Experiment



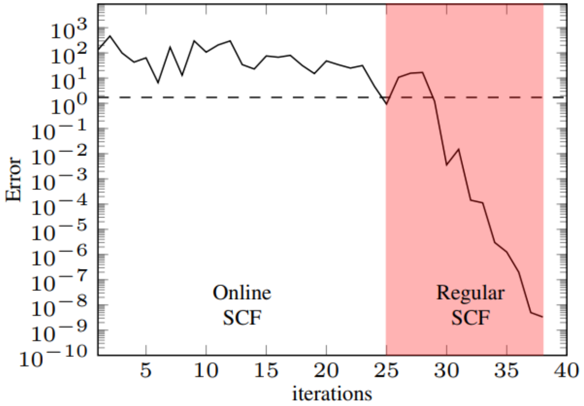
(a) Convergence ratio

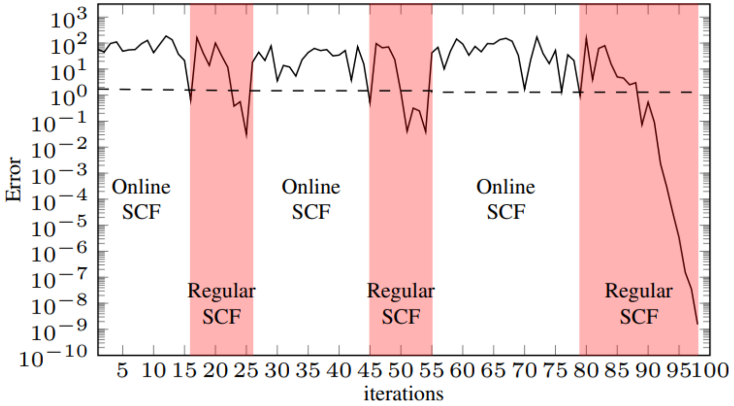


- Case study: solve $(Avv^\top A^\top)v = \lambda v$
  - Vanilla fixed-point method: does not work at all (0% convergence ratio)
  - DIIS: ~40% convergence ratio
  - Online PCA: the top curves, half has 100% convergence ratio

Experiment

Methods	Hartree-Fock #(Nonconverged molecules)		Hartree-Fock Average #(iterations)	DFT with B3LYP #(Nonconverged molecules)		DFT with B3LYP Average #(iterations)
Regular SCF	124	(9.27%)	25.49	407	(30.42%)	21.09
Full Online SCF	13	(0.97%)	584.68	217	(16.22%)	1835.24
Adaptive Online SCF	0	(0%)	42.97	0	(0%)	60.58





- For real-world SCF equations such as Hartree-Fock and DFT, our proposed method with adaptations (Online SCF) can also achieve high convergence ratio with a moderate increase of iterations.
- We also proposed an adaptive switching mechanism between online and regular mode, to balance efficiency and convergency.

Thank you!

Xihan Li

Department of Computer Science, University College London

Email: xihan.li@cs.ucl.ac.uk

Webpage: https://snowkylin.github.io