1 DIIS method (Anderson mixing)

1.1 simple mixing

input ($\rho^{(n)}$) $\rightarrow$ some calculation $\rightarrow$ output ($F^{(n)}$) $\rightarrow$ next input ($\rho^{(n+1)}$)
In the simple mixing, the (optimized) next input is

$$\rho^{(n+1)} = (1-\alpha)\rho^{(n)} + \alpha F^{(n)}$$

1.2 scheme

iteration 1,2,...,n,...
input $\rho^{(1)}$,$\rho^{(2)}$,...,$\rho^{(n)}$,...
output $F^{(1)}$,$F^{(2)}$,...,$F^{(n)}$,...

define optimized input and output
input $\bar{\rho}^{(1)}$,$\bar{\rho}^{(2)}$,...,$\bar{\rho}^{(n)}$,...
output $\bar{F}^{(1)}$,$\bar{F}^{(2)}$,...,$\bar{F}^{(n)}$,...

$$\begin{aligned} \bar{\rho}^{(n)} &= (1-\theta^{(n)})\rho^{(n-1)} + \theta^{(n)}\rho^{(n)} & (1) \\ \bar{F}^{(n)} &= (1-\theta^{(n)})F^{(n-1)} + \theta^{(n)}F^{(n)} & (2) \end{aligned}$$

Minimize $||\bar{\rho}^{(n)} - \bar{F}^{(n)}||^2 = \langle \bar{\rho}^{(n)} - \bar{F}^{(n)} | \bar{\rho}^{(n)} - \bar{F}^{(n)} \rangle$ to find $\theta^{(n)}$. Then

$$\theta^{(n)} = -\frac{\langle \Delta\mathcal{F}^{(n)} | \mathcal{F}^{(n-1)} \rangle}{\langle \Delta\mathcal{F}^{(n)} | \Delta\mathcal{F}^{(n)} \rangle}$$

where

$$\begin{aligned} \mathcal{F}^{(n)} &= F^{(n)} - \rho^{(n)} & (3) \\ \Delta\mathcal{F}^{(n)} &= \mathcal{F}^{(n)} - \mathcal{F}^{(n-1)} & (4) \end{aligned}$$

Anderson mixing uses n-1 and n to calculate optmized n. It is straightforward to generalize this method, like

$$\begin{aligned} \bar{\rho}^{(n)} &= \theta_m^{(n)}\rho^{(n-m)} + \cdots + \theta_1^{(n)}\rho^{(n-1)} + \theta_0^{(n)}\rho^{(n)} & (5) \\ 1 &= \theta_m^{(n)} + \cdots + \theta_1^{(n)} + \theta_0^{(n)} & (6) \end{aligned}$$

1.3 Note

Equation (4) says that the breakdown occurs in the calculation if $\mathcal{F}^{(n)} = \mathcal{F}^{(n-1)}$, i.e., ρ or F is the completely converged. Stop the calculation if the error is below the criterion.

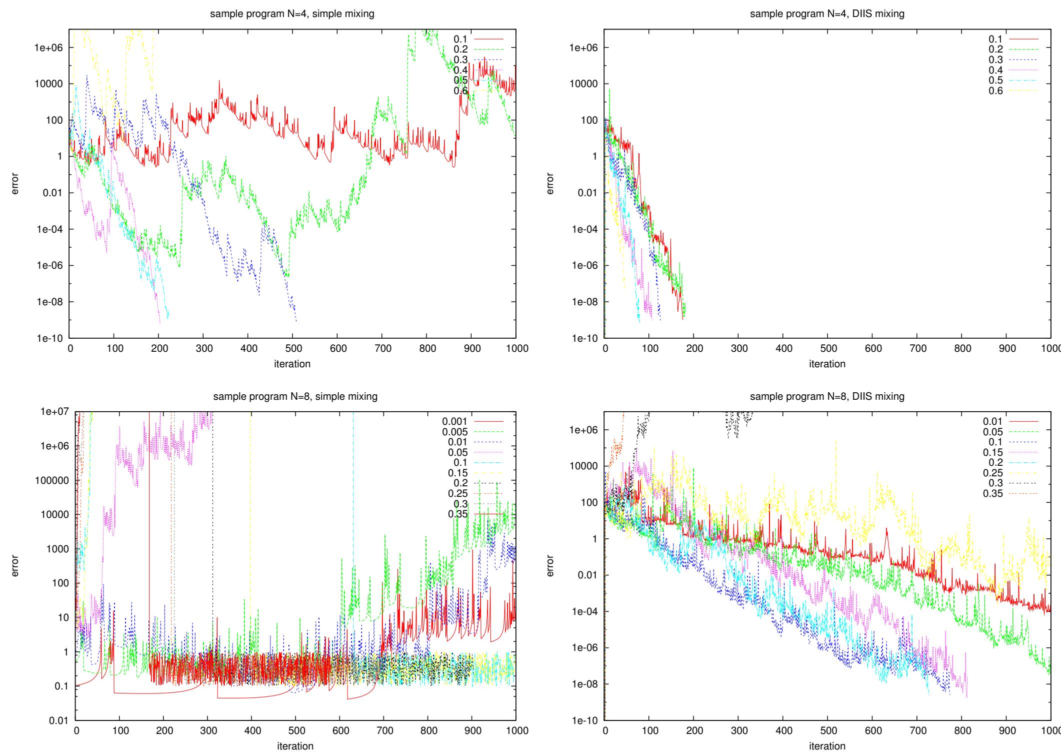

Figure 1: left: simple mixing, right: DIIS mixing. The simple mixing can not make the system of N=8 converged, while the DIIS mixing can converge it.