

DIIS Acceleration of Fixed-Point Iteration

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Background: Electronic Structure Problem

Physics problem: Find the ground state energy and electron wave functions for a many-electron system.

Express as ...

Minimization problem: Minimize $E(X)$ subject to $X^T X = I_p$, where the columns of $X \in \mathbb{R}^{n \times p}$ are the electron wave functions and $E(X)$ is the total energy.

Recast as ...

Nonlinear eigenvalue problem: $H(X)X = X\Lambda$, where $X^T X = 1$ and the diagonal elements of Λ are the p smallest eigenvalues of $H(X)$.

Background: Self-Consistent Field Iteration

SCF Iteration: Given an initial X .

Iterate:

Evaluate $H(X)$ and solve $H(X)X_+ = X_+\Lambda_+$.

Update $X \leftarrow X_+$.

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Recast in terms of the *electron charge density* $\rho \equiv \text{diag}(XX^T) \in \mathbb{R}^n$.

Assume: $H(X) = H(\rho)$. Then an SCF iteration sequence looks like

$$\dots \rightarrow X \rightarrow \rho \rightarrow H(\rho) \rightarrow X_+ \rightarrow \rho_+ \rightarrow \dots$$

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DIIS: Direct Inversion on the Iterative Subspace.

Suppose we have a fixed-point iteration $\rho_+ = G(\rho)$, $G : \mathbb{R}^n \rightarrow \mathbb{R}^n$.

DIIS Acceleration: Given $m \geq 2$ and ρ_0 .

Set $\rho_1 = G(\rho_0)$.

Iterate: For $k = 1, 2, \dots$

Set $m_k = \min\{m, k + 1\}$.

Set $D_k = (d_1, \dots, d_{m_k})$, where $d_i = G(\rho_{k-m_k+i}) - \rho_{k-m_k+i}$.

Solve $\min_{\alpha \in \mathbb{R}^{m_k}} \|D_k \alpha\|_2$ s. t. $\sum_{i=1}^{m_k} \alpha_i = \mathbf{1}$.

Set $\rho_{k+1} = \sum_{i=1}^{m_k} \alpha_i G(\rho_{k-m_k+i})$.

Suppose $G(\rho) = A\rho + b$ for $A \in \mathbf{R}^{n \times n}$ and $b \in \mathbf{R}^n$.

Then $\rho_{k+1} = \sum_{i=1}^{m_k} \alpha_i G(\rho_{k-m_k+i}) = G(\sum_{i=1}^{m_k} \alpha_i \rho_{k-m_k+i})$. Thus

$$\rho_{k+1} = G(\rho_{min})$$

where $\rho_{min} = \sum_{i=1}^{m_k} \alpha_i \rho_{k-m_k+i}$ has minimal residual within the affine subspace containing $\{\rho_{k-m_k+i}\}_{i=1, \dots, m_k}$ (the *iterative subspace*).

Can show: For the “untruncated” method ($m_k = k$),

$$\rho_{k+1} = G(\rho_k^{GMRES})$$

where ρ_k^{GMRES} is the k th iterate of GMRES applied to $(A - I)\rho = -b$.

The DIIS Least-Squares Problem

The problem is

$$\min_{\alpha \in \mathbb{R}^{m_k}} \|D_k \alpha\|_2 \quad \text{s.t.} \quad \sum_{i=1}^{m_k} \alpha_i = 1.$$

Note:

- D_{k+1} is obtained from D_k by adding a column on the right and, if $k \geq m$, also dropping a column on the left.
- In practice, additional columns may be dropped on the left to maintain acceptable conditioning.

Solving the LS Problem: the Lagrange-Multiplier Method

Set $\Phi(\alpha, \lambda) \equiv \frac{1}{2} \|D_k \alpha\|_2^2 - \lambda(\sum \alpha_i - 1)$. Then

$$\nabla \Phi(\alpha, \lambda) = 0 \iff \begin{pmatrix} D_k^T D_k & -\vec{1} \\ -\vec{1}^T & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \lambda \end{pmatrix} = \begin{pmatrix} \vec{0} \\ -1 \end{pmatrix},$$

where $\vec{1} = (1, \dots, 1)^T$ and $\vec{0} = (0, \dots, 0)^T$. It follows that

$$\alpha = \frac{1}{\vec{1}^T (D_k^T D_k)^{-1} \vec{1}} (D_k^T D_k)^{-1} \vec{1}$$

Forming $(D_k^T D_k)$ followed by Cholesky factorization costs $O(m_k^2 n) + O(m_k^3)$ flops.

But updating the QR decomposition of D_{k-1} to obtain $D_k = QR$ costs only $O(m_k n)$ flops. Then $D_k^T D_k = (QR)^T (QR) = R^T R$.

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Either way, *the condition number is* $\kappa(D_k^T D_k) = \kappa(D_k)^2$.

Solving the LS Problem: the Method of Elimination

General idea: Use the constraint to express some variables in terms of others to obtain a lower-dimensional unconstrained problem.

Kresse–Furthmüller (1996): Introduce $\bar{\alpha} = (\bar{\alpha}_1, \dots, \bar{\alpha}_{m_k-1})^T$ such that

$$\begin{aligned}D_k \alpha &= \sum_{i=1}^{m_k} \alpha_i d_i \\&= \bar{\alpha}_1 (d_2 - d_1) + \bar{\alpha}_2 (d_3 - d_2) + \dots + \bar{\alpha}_{m_k-1} (d_{m_k} - d_{m_k-1}) + d_{m_k} \\&= D_k W \bar{\alpha} + d_{m_k},\end{aligned}$$

where $W = \begin{pmatrix} -1 & & & & \\ 1 & -1 & & & \\ & & \ddots & \ddots & \\ & & & 1 & -1 \\ & & & & 1 \end{pmatrix} \in \mathbf{R}^{m_k \times (m_k-1)}.$

Solving the LS Problem: the Method of Elimination (cont.)

Then the problem is

$$\min_{\bar{\alpha} \in \mathbb{R}^{m_k-1}} \|D_k W \bar{\alpha} + d_{m_k}\|_2.$$

Kresse–Furthmüller: Solve the normal equation $(D_k W)^T (D_k W) \bar{\alpha} = -(D_k W)^T d_{m_k}$.

Better:

- ▶ Update the QR decomposition of D_{k-1} to obtain $D_k = QR$ with $O(m_k n)$ flops.
- ▶ Update the factorization $D_k W = QRW$ to obtain $D_k W = \bar{Q} \bar{R}$ with an additional $O(m_k n)$ flops.
- ▶ Solve $\bar{R} \bar{\alpha} = -\bar{Q}^T d_{m_k}$.
- ▶ Obtain $\alpha = W \bar{\alpha} + (0, \dots, 0, 1)^T$.

Note: $\kappa(\bar{R}) = \kappa(\bar{Q} \bar{R}) = \kappa(D_k W) \leq \kappa(D_k) \kappa(W)$.

Numerically, $\kappa(W) \approx 2m_k/\pi$ for all but the smallest values of m_k .

Solving the LS Problem: the Null-Space Method

General idea:

- ▶ Write the solution as a sum of a vector that satisfies the constraint and a vector in the null-space of the constraint matrix.
- ▶ Choose a basis of the null-space to obtain a lower-dimensional, unconstrained least-squares problem for the null-vector.

Here, write $\alpha = \nu + \beta$, where $\vec{1}^T \nu = 1$ and $\vec{1}^T \beta = 0$.

Let $V \in \mathbf{R}^{m_k \times (m_k - 1)}$ be full rank and such that $\vec{1}^T V = 0$.

Write $\beta = V\gamma$ for $\gamma \in \mathbf{R}^{m_k - 1}$.

Then the problem is

$$\min_{\gamma \in \mathbf{R}^{m_k - 1}} \|D_k \nu + D_k V \gamma\|_2.$$

Solving the LS Problem: the Null-Space Method (cont.)

Useful choices:

- ▶ $\nu = (0, \dots, 0, 1)^T$, so $D_k \nu = d_{m_k}$.
- ▶ $V = (v_1, \dots, v_{m_k-1})$, where

$$v_j = \begin{pmatrix} -1/\sqrt{j(j+1)} \\ \vdots \\ -1/\sqrt{j(j+1)} \\ \sqrt{j/(j+1)} \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \left. \vphantom{\begin{pmatrix} -1/\sqrt{j(j+1)} \\ \vdots \\ -1/\sqrt{j(j+1)} \\ \sqrt{j/(j+1)} \\ 0 \\ \vdots \\ 0 \end{pmatrix}} \right\} j \text{ components}, \quad j = 1, \dots, m_k - 1,$$

so $\vec{1}^T V = 0$, $V^T V = I$, and V is upper-Hessenberg.

Solving the LS Problem: the Null-Space Method (cont.)

Then:

- ▶ Update the QR decomposition of D_{k-1} to obtain $D_k = QR$ with $O(m_k n)$ flops.
- ▶ Update the factorization $D_k V = QRV$ to obtain $D_k V = \bar{Q}\bar{R}$ with an additional $O(m_k n)$ flops.
- ▶ Solve $\bar{R}\gamma = -\bar{Q}^T d_{m_k}$.
- ▶ Obtain $\alpha = d_{m_k} + V\gamma$.

Note: $\kappa(\bar{R}) = \kappa(D_k V) \leq \kappa(D_k)\kappa(V) = \kappa(D_k)$.

Numerical Experiments

We applied SCF+DIIS with these LS solution methods using data from various materials (with thanks to Chao Yang.)

We observed the maximum condition numbers that occurred with varying values of m .

The table shows typical results.

m	Lagrange Multipliers	Null-Space Method	Method of Elimination
1	1.000e+000	1.000e+000	1.000e+000
2	3.377e+002	1.000e+000	1.000e+000
3	6.096e+004	3.965e+001	3.750e+001
4	9.640e+005	1.725e+002	1.386e+002
5	4.467e+007	1.489e+003	1.015e+003
6	1.839e+010	2.028e+004	1.546e+004
7	7.703e+012	3.861e+005	2.795e+005
8	1.599e+014	8.838e+005	5.123e+005

Maximum Observed Condition Numbers with Water Molecule Data