Inexact Restoration Method

with application to Hartree-Fock equations

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0. Introduction

Introduction

Electronic structure

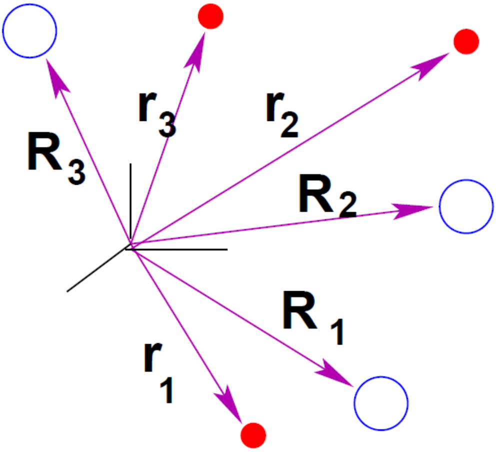

Figure: Electronic structure scheme - source: SAAD, Y., CHELIKOWSKY, J. R., SCHONTZ, S. M., Numerical Methods for Electronic Structure of Materials

System of N electrons described by the antisymmetric wave function

$$\psi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right), \tag{1}$$

Stationary Schrödinger equation

$$\hat{H}\psi = E\psi \tag{2}$$

with Hamiltonian

$$\hat{H} = \hat{T}_e + V_{ee} + V_{en}. \tag{3}$$

where

$$\hat{T}_e = -\sum_{i=1}^{N} \frac{\Delta_{e_j}}{2}, \quad V_{ee} = \frac{1}{2} \sum_{\substack{i,j \in \{1,\ldots,N\} \\ i \neq j}} \frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|}, \tag{4}$$

$$V_{en} = -\sum_{i=1}^{M} \sum_{j=1}^{N} \frac{Z_i}{\|\mathbf{R}_i - \mathbf{r}_j\|}, \tag{5}$$

We search the smallest eigenvalue E and corresponding eigenfunction ψ (ground state).

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Hartree-Fock method transforms $(3N)$D problem into system of N 3D problems (although with an approximation).

1. Hartree-Fock method

Consider a wave function in a special form:

$$\psi\left(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\right) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1\left(\mathbf{x}_1\right) & \chi_1\left(\mathbf{x}_2\right) & \cdots & \cdots & \chi_1\left(\mathbf{x}_N\right) \\ \chi_2\left(\mathbf{x}_1\right) & \chi_2\left(\mathbf{x}_2\right) & \cdots & \cdots & \chi_2\left(\mathbf{x}_N\right) \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ \chi_N\left(\mathbf{x}_1\right) & \chi_N\left(\mathbf{x}_2\right) & \cdots & \cdots & \chi_N\left(\mathbf{x}_N\right) \end{vmatrix}, \tag{6}$$

where

$$\chi_i\left(\mathbf{x}_i\right) = \phi_i\left(\mathbf{r}_i\right) \sigma_i\left(s_i\right) \;\; i = 1, 2, \ldots, N \tag{7}$$

Antisymmetry is guaranteed.

Let's minimize the energy functional $\left\langle \psi | \hat{H} | \psi \right\rangle$ subject to ψ as Slater determinant. We can write the Lagrangian as

$$L = \left\langle \psi | \hat{H} | \psi \right\rangle - \sum_{i,j} \lambda_{ij} \left(\langle \chi_i | \chi_j \rangle - \delta_{ij} \right) \tag{8}$$

By variation of the Lagrangian we obtain Hartree-Fock equations.

$$\forall k \in \{1, \ldots, N\}:$$

$$\left(\underbrace{-\frac{1}{2}\Delta_{e_k}}_{\hat{T}} \underbrace{-\sum_{i=1}^{M} \frac{Z_i}{\|\mathbf{R}_i - \mathbf{r}\|}}_{V_{en}} + \underbrace{\sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{|\phi_i(\mathbf{r}')|^2}{\|\mathbf{r}' - \mathbf{r}\|} \mathrm{d}^3\mathbf{r}'}_{V_H} \right) \phi_k(\mathbf{r}) -$$

$$- \sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{\phi_i(\mathbf{r}')\,\phi_k(\mathbf{r}')}{\|\mathbf{r}' - \mathbf{r}\|} \mathrm{d}^3\mathbf{r}' \; \delta_{\sigma_i \sigma_k} \; \phi_i(\mathbf{r}) = \lambda_k \phi_k(\mathbf{r}), \qquad (9)$$

Consider a closed shell system (system without unpaired electrons) of $2N$ electrons. Each orbital is occupied by two electrons with different spins. We can rewrite the HF equation to

$$\forall k \in \{1, \ldots, N\}:$$

$$\left(\underbrace{-\frac{1}{2}\Delta_{e_k}}_{\hat{T}} \underbrace{- \sum_{i=1}^{M} \frac{Z_i}{\|\mathbf{R}_i - \mathbf{r}\|}}_{V_{en}} + \underbrace{2 \sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{|\phi_i(\mathbf{r}')|^2}{\|\mathbf{r}' - \mathbf{r}\|} \mathrm{d}^3\mathbf{r}'}_{V_H} \right) \phi_k(\mathbf{r}) - \sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{\phi_i(\mathbf{r}')\phi_k(\mathbf{r}')}{\|\mathbf{r}' - \mathbf{r}\|} \mathrm{d}^3\mathbf{r}' \; \phi_i(\mathbf{r}) = \lambda_k \phi_k(\mathbf{r}), \tag{10}$$

- Representation of the Hartree–Fock equation in a non orthonormal basis set (plane wave basis, localized orbitals):

$$\phi_i(\mathbf{r}) = \sum_{j=1}^{N_b} c_{ji}\mu_j(\mathbf{r}) \tag{11}$$

- Choosing μ_j as test functions we can rewrite the system (10) as a generalized eigenvalue problem

$$\begin{cases} \mathbf{F}(\mathbf{C})\,\mathbf{C} & = & \mathbf{SC}\Lambda, \\ \mathbf{C}^T\mathbf{SC} & = & \mathbf{I} \end{cases} \tag{12}$$

with coefficient matrix $\mathbf{C} \in \mathbb{R}^{N_b \times N}$, $(\mathbf{C})_{ij} = c_{ij}$, overlap matrix $\mathbf{S} \in \mathbb{R}^{N_b \times N_b}$, $(\mathbf{S})_{ij} = \int_{\mathbb{R}^3} \mu_i(\mathbf{r})\,\mu_j(\mathbf{r})\,\mathrm{d}^3\mathbf{r}$, diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$ and Fock matrix $\mathbf{F} \in \mathbb{R}^{N_b \times N_b}$.

Hartree-Fock method

Roothaan Equation $\mathbf{F}(\mathbf{C})\,\mathbf{C} = \mathbf{S}\mathbf{C}\Lambda$.

$$\mathbf{F}(\mathbf{C}) = \mathbf{H} + \mathbf{J}(\mathbf{C}) + \mathbf{K}(\mathbf{C}) \tag{13}$$

Density matrix

$$\mathbf{Z} = \mathbf{C}\mathbf{C}^T \tag{14}$$

Then

$$(\mathbf{J}(\mathbf{Z}) + \mathbf{K}(\mathbf{Z}))_{ij} = \sum_{k,l=1}^{N_b} (2g_{ijkl} - g_{ilkj})\,(\mathbf{Z})_{lk}\,, \tag{15}$$

where

$$g_{ijkl} = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\mu_i(\mathbf{r})\,\mu_j(\mathbf{r})\,\mu_k(\mathbf{r}')\,\mu_l(\mathbf{r}')}{\|\mathbf{r}-\mathbf{r}'\|}\mathrm{d}^3\mathbf{r}\;\mathrm{d}^3\mathbf{r}' \tag{16}$$

Standard approach - the problem is solved by iteration of a self-consistent field (SCF)

$$\mathbf{F}(\mathbf{C}_{k-1})\,\mathbf{C}_k = \mathbf{SC}_k\Lambda. \tag{17}$$

To ensure the convergence one may use the DIIS iteration (a new coefficient matrix is computed as a combination of previous iterations).

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To ensure the convergence one may use the DIIS iteration (a new coefficient matrix is computed as a combination of previous iterations).
Alternative - an optimization approach.

Hartree-Fock Energy functional

$$E(\mathbf{Z}) = \mathrm{Trace}\left[2\mathbf{HZ} + (\mathbf{J}(\mathbf{Z}) + \mathbf{K}(\mathbf{Z}))\mathbf{Z}\right] \tag{18}$$

with gradient

$$\nabla E(\mathbf{Z}) = 2(\mathbf{H} + \mathbf{J}(\mathbf{Z}) + \mathbf{K}(\mathbf{Z})) = 2\mathbf{F}(\mathbf{Z}) \tag{19}$$

Quadratic programming problem

$$\min E(\mathbf{Z}) \tag{20}$$

with equality constraints:

$$\mathbf{Z} = \mathbf{Z}^T, \tag{21}$$

$$\mathbf{ZSZ} = \mathbf{Z} \tag{22}$$

$$\mathrm{Trace}(\mathbf{ZS}) = N. \tag{23}$$

Let's define matrix $\mathbf{X} = \mathbf{S}^{1/2}\mathbf{Z}\mathbf{S}^{1/2}$ and function $f(\mathbf{X}) = E\left(\mathbf{S}^{-1/2}\mathbf{X}\mathbf{S}^{-1/2}\right)$. We can rewrite our optimization problem to

$$\min f(\mathbf{X}) \tag{24}$$

subject to

$$\mathbf{X} = \mathbf{X}^T, \tag{25}$$

$$\mathbf{X}\mathbf{X} = \mathbf{X}, \tag{26}$$

$$\mathrm{Trace}(\mathbf{X}) = N. \tag{27}$$

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Once we have obtained a solution $\mathbf{X}$, we can get a coefficient matrix as:

$$\mathbf{C} = \mathbf{S}^{-\frac{1}{2}}\mathbf{Q},$$

where columns of $\mathbf{Q} \in \mathbb{R}^{N_B \times N}$ are an orthonormal basis of the null space of $\mathbf{X} - \mathbf{I}$.

2. Inexact Restoration method

Let $f : \mathbb{R}^n \to \mathbb{R}$, $h : \mathbb{R}^n \to \mathbb{R}^m$ be differentiable and ∇f, ∇h Lipschitz-continuous on convex and closed polytope Ω. Consider the nonlinear optimization problem

$$\min f(x) \text{ subj. to } h(x) = 0, \; x \in \Omega. \tag{28}$$

Lagrangian of the problem:

$$L(x, \lambda) = f(x) + h(x)^T \lambda. \tag{29}$$

$\left(\overline{x}, \overline{\lambda}\right) \in \Omega \times \mathbb{R}^m$ is a critical pair, if

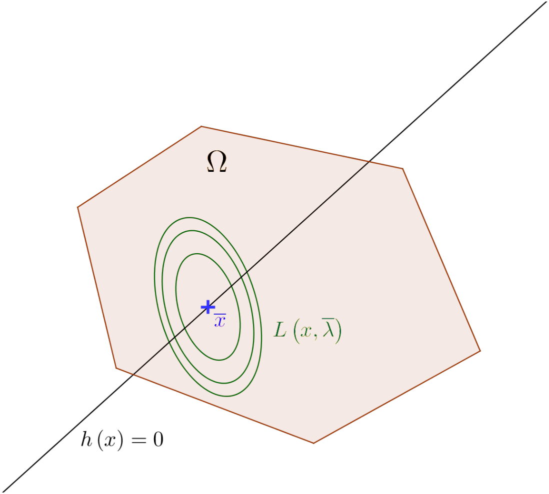
$$h(\overline{x}) = 0 \tag{30}$$

and

$$P_\Omega\left(\overline{x} - \nabla L\left(\overline{x}, \overline{\lambda}\right)\right) - \overline{x} = 0; \tag{31}$$

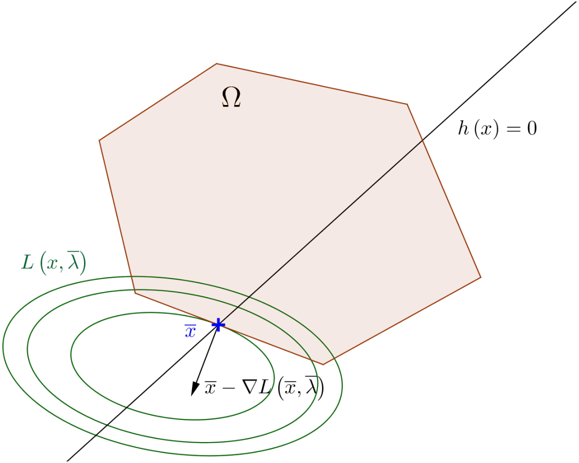
Inexact Restoration method

Critical pair scheme



Inexact Restoration method

Critical pair scheme



Let us define :

- Merit function ($x \in \Omega, \theta \in [0,1]$):

$$\Phi(x,\theta) = \theta f(x) + (1-\theta)\|h(x)\| \tag{32}$$

- Tangent set ($y \in \mathbb{R}^n$):

$$T(y) = \left\{ z \in \Omega | \nabla h(y)^T (z-y) = 0 \right\} \tag{33}$$

Algorithmic parameters: $r \in [0,1), \beta, \gamma, \tau > 0$. We assume that $r_k \in [0, r]$ for every iteration nr. $k \in \mathbb{N}$.

0. Initialization Choose arbitrarily $x_0 \in \Omega$, initialize $\theta_{-1} \in (0,1)$ and $k = 0$.

1. Restoration step Compute $y^k \in \Omega$ such that:

$$\left\| h\left(y^k\right) \right\| \leq r_k \left\| h\left(x^k\right) \right\| \tag{34}$$

and

$$\left\| y^k - x^k \right\| \leq \beta \left\| h\left(x^k\right) \right\| \tag{35}$$

Get closer to $h(x) = 0$ and stay in Ω.

2. Penalty parameter Compute θ_k - first element of sequence $\left\{\frac{\theta_{k-1}}{2^j}\right\}_{j\in\mathbb{N}}$ such that

$$\Phi\left(y^k,\theta\right) \leq \Phi\left(x^k,\theta\right) + \frac{1}{2}\left(\left\|h\left(y^k\right)\right\| - \left\|h\left(x^k\right)\right\|\right) \tag{36}$$

3. Tangent descent direction Compute $d^k \in \mathbb{R}^n$ such that $y^k + d^k \in \Omega$,

$$f\left(y^k + td^k\right) \leq f\left(y^k\right) - \gamma t\left\|d^k\right\|^2 \tag{37}$$

for all $t \in [0,\tau]$ and

$$\nabla h\left(y^k\right)^T d^k = 0. \tag{38}$$

4. Acceptance of the step Compute t_k as the first element t of the sequence $\left\{\frac{1}{2^j}\right\}_{j\in\mathbb{N}_0}$ such that

$$\Phi\left(y^k + td^k, \theta_k\right) \leq \Phi\left(x^k, \theta_k\right) + \frac{1-r}{2}\left(\left\|h\left(y^k\right)\right\| - \left\|h\left(x^k\right)\right\|\right) \quad (39)$$

and

$$f\left(y^k + t_k d^k\right) \leq f\left(y^k\right) - \gamma t_k \left\|d^k\right\|^2 \quad (40)$$

Set $x^{k+1} = y^k + t_k d^k$, $k \leftarrow k+1$ and go to **1**.

- Restoration step

  How to get closer to $h(x) = 0$? For example

$$y^k = x^k - \beta \frac{\nabla \left\| h\left(x^k\right) \right\|}{\left\| \nabla \left\| h(x^k) \right\| \right\|} = x^k - \beta \frac{\nabla h\left(x^k\right)^T h\left(x^k\right)}{\left\| \nabla h(x^k)^T h(x^k) \right\|} \tag{41}$$

- Tangent descent direction

  Optimal direction in the tangent set $T\left(y^k\right)$?

  Solution: Approximately minimize the lagrangian $L\left(y^k + d, \lambda^k\right)$.
  Alternative: Let V be a matrix, which columns form an orthogonal basis of $\ker\left(-\nabla h\left(y^k\right)\right)$. Then the direction of the local steepest descent in the tangent set is

$$d^k = VV^T \nabla f\left(y^k\right) \tag{42}$$

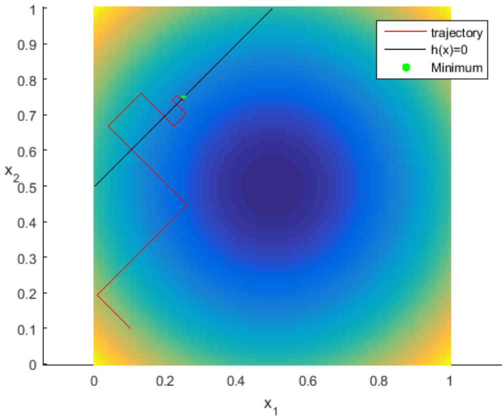
(projection of -gradient of f onto tangent set).

Inexact Restoration method

Matlab example

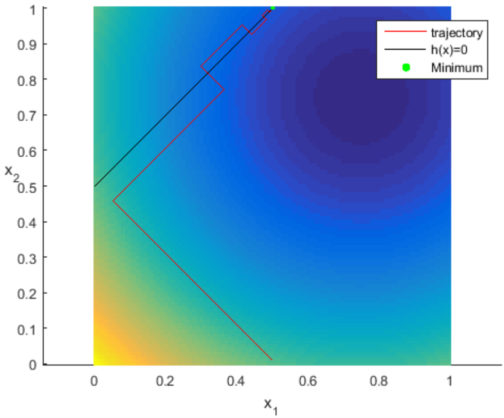
Example

$$f(x) = (x_1 - 1/2)^2 + (x_2 - 1/2)^2, \; h(x) = x_2 - x_1 - 1/2, \; \Omega = \langle 0, 1\rangle \times \langle 0, 1\rangle$$



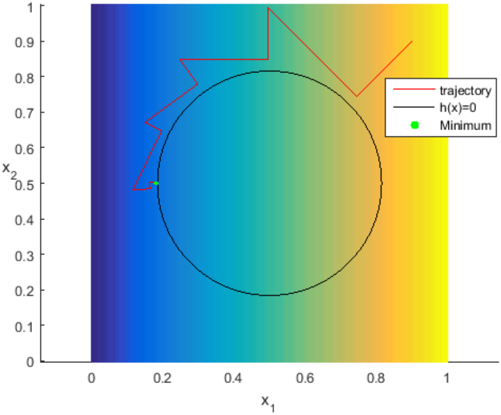
Example

$$f(x) = (x_1 - 3/4)^2 + (x_2 - 3/4)^2 \,,\ h(x) = x_2 - x_1 - 1/2,\ \Omega = \langle 0,1\rangle \times \langle 0,1\rangle$$



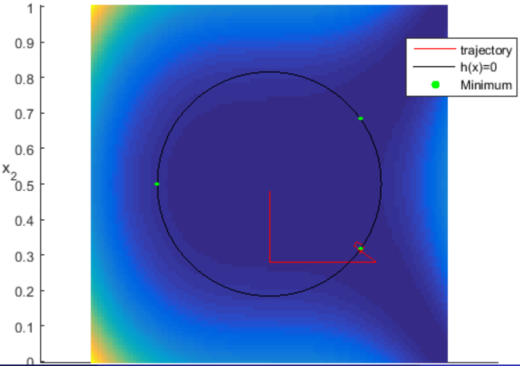
Example

$$f(x) = x_1,\ \ h(x) = (x_1 - 1/2)^2 + (x_2 - 1/2)^2 - 1/10,\ \ \Omega = \langle 0, 1\rangle \times \langle 0, 1\rangle$$



Example

$f(x) = 100\left((2x_1-1)^3 - (2x_2-1)^2\right)^2 + (1-(2x_1-1))^2, \; h(x) = (x_1-1/2)^2 + (x_2-1/2)^2 - 1/10, \; \Omega = \langle 0,1\rangle \times \langle 0,1\rangle$



Let $f : \mathbb{R}^{K\times K} \to \mathbb{R}$; $K, N \in \mathbb{N}$, $N < K$. Assume that f has continuous first derivatives for all $\mathbf{X} \in \mathbb{R}^{K\times K}$. The optimization problem can be written as

$$\min f(\mathbf{X}) \ \text{subj. to} \ \mathbf{X} \in \mathcal{G} \tag{43}$$

where

$$\mathcal{G} = \left\{ \mathbf{X} \in \mathbb{R}^{K\times K} \middle| \ \mathbf{X} = \mathbf{X}^T, \ \mathbf{X}^2 = \mathbf{X}, \ \mathrm{Trace}(\mathbf{X}) = N \right\} \tag{44}$$

(known as Grassmann manifold)

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(known as Grassmann manifold)
Number of equality constraints exceeds the number of variables! (It is necessary to show (using special techniques), that the minimizer satisfies KKT conditions).

Inexact Restoration method - matrix problem

Problem definition

We define similarly to general algorithm (minimization with equality constraint, convex set, lagrangian):

- Convex set

$$\Omega = \left\{ \mathbf{X} \in \mathbb{R}^{K \times K} | \mathbf{X} = \mathbf{X}^T, \mathrm{Trace}\left(\mathbf{X}\right) = N \right\} \tag{45}$$

- Lagrangian

$$L\left(\mathbf{X}, \Lambda\right) = f\left(\mathbf{X}\right) + \left\langle \mathbf{X}^2 - \mathbf{X}, \Lambda \right\rangle, \ \Lambda \in \mathbb{R}^{K \times K}, \tag{46}$$

with gradient

$$\nabla_{\mathbf{X}} L\left(\mathbf{X}, \Lambda\right) = \nabla f\left(\mathbf{X}\right) + \mathbf{X}\Lambda + \Lambda\mathbf{X} - \Lambda. \tag{47}$$

- Critical pair $\left(\overline{\mathbf{X}}, \overline{\Lambda}\right)$ satisfies

$$\overline{\mathbf{X}}^2 - \overline{\mathbf{X}} = \mathbf{O}, \ P_\Omega\left(\overline{\mathbf{X}} - \nabla_{\mathbf{X}} L\left(\overline{\mathbf{X}}, \overline{\Lambda}\right)\right) - \overline{\mathbf{X}} = \mathbf{O} \tag{48}$$

Algorithmic parameters: $\gamma \in (0, 1/4)\,, \tau, \mu > 0$.

0. Initialization Choose an initial symmetric matrix $\mathbf{X_0} \in \mathbb{R}^{N_b \times N_b}$ such that $\mathrm{Trace}\,(\mathbf{X}_0) = N$, initialize $\theta_{-1} \in (0, 1)$ and $k = 0$.

1. Restoration step Compute $\mathbf{Y}_k \in \mathcal{G}$ as a solution of:

$$\min \|\mathbf{X}_k - \mathbf{Y}\|_F \ \text{subj. to } \mathbf{Y} \in \mathcal{G} \tag{49}$$

Projection to the feasible set. *"Exact restoration"*.

2. **Penalty parameter** Compute θ_k - first element of sequence $\left\{ \frac{\theta_{k-1}}{2^j} \right\}_{j \in \mathbb{N}}$ such that

$$\theta f(\mathbf{Y}_k) \leq \theta f(\mathbf{X}_k) + \left(1 - \theta - \frac{1}{2}\right) \left\| \mathbf{X}_k^2 - \mathbf{X}_k \right\|_F \tag{50}$$

3. **Tangent descent direction** Compute $\mathbf{E}_k \in S(\mathbf{Y}_k)$ such that

$$f(\mathbf{Y}_k + t\mathbf{E}_k) \leq f(\mathbf{Y}_k) - \gamma t \|\mathbf{E}_k\|_F^2 \tag{51}$$

for all $t \in [0, \tau]$ and

$$\|\mathbf{E}_k\|_F \geq \mu \left\| P_{S(\mathbf{Y}_k)} [\nabla f(\mathbf{Y}_k)] \right\|_F . \tag{52}$$

4. Acceptance of the step Compute t_k as the first element t of the sequence $\left\{\frac{1}{2^j}\right\}_{j\in\mathbb{N}_0}$ such that

$$\theta_k f(\mathbf{Y}_k + t\mathbf{E}_k) + (1-\theta_k)\left\|(\mathbf{Y}_k + t\mathbf{E}_k)^2 - (\mathbf{Y}_k + t\mathbf{E}_k)\right\|_F \leq$$

$$\leq \theta_k f(\mathbf{X}_k) + \left(1 - \theta_k - \frac{1}{2}\right)\left\|\mathbf{X}_k^2 - \mathbf{X}_k\right\|_F \tag{53}$$

and

$$f(\mathbf{Y}_k + t_k\mathbf{E}_k) \leq f(\mathbf{Y}_k) - \gamma t_k \|\mathbf{E}_k\|_F^2 \tag{54}$$

Set $\mathbf{X}_{k+1} = \mathbf{Y}_k + t_k\mathbf{E}_k$, $k \leftarrow k+1$ and go to **1**.

Let $\mathbf{X} \in \mathcal{G}$. Then it can be written as

$$\mathbf{X} = \mathbf{C}\mathbf{C}^T, \tag{55}$$

where $\mathbf{C} \in \mathbb{R}^{K \times N}$ has orthonormal columns which form a basis of the N-dimensional subsp. $\mathcal{R}(\mathbf{X})$. Therefore, $\mathbf{X}$ has N eigenvalues equal to 1 and $K - N$ eigenvalues equal to 0.

Denote $S(\mathbf{Y})$ parallel subspace to the subset $T(\mathbf{Y})$.

Theorem

Assume that $\mathbf{Y} \in \mathcal{G}$. *Then*

$$S(\mathbf{Y}) = \left\{ \mathbf{E} \in \mathbb{R}^{K \times K} \middle| \; \mathbf{E} = \mathbf{E}^T, \; \mathbf{YE} + \mathbf{EY} - \mathbf{E} = \mathbf{0} \right\} \tag{56}$$

and

$$T(\mathbf{Y}) = \left\{ \mathbf{Z} \in \mathbb{R}^{K \times K} \middle| \; \mathbf{Z} = \mathbf{Z}^T, \; \mathbf{Y}(\mathbf{Z} - \mathbf{Y}) + (\mathbf{Z} - \mathbf{Y})\mathbf{Y} - (\mathbf{Z} - \mathbf{Y}) = \mathbf{0} \right\}. \tag{57}$$

The dimension of $S(\mathbf{Y})$ *is* $N(K - N)$

How to find a projection of symmetric matrix $\mathbf{A}$ onto $S(\mathbf{Y})$?

How to find a projection of symmetric matrix $\mathbf{A}$ onto $S(\mathbf{Y})$?

Theorem

Assume that $\mathbf{Y} \in \mathcal{G}$. *Let* $\mathbf{A} \in \mathbb{R}^{K \times K}$ *be a symmetric matrix. The the Frobenius projection of* $\mathbf{A}$ *onto* $S(\mathbf{Y})$, *respectively* $T(\mathbf{Y})$ *is given by*

$$P_{S(\mathbf{Y})}(\mathbf{A}) = \mathbf{YA} + \mathbf{AY} - 2\mathbf{YAY}, \tag{58}$$

resp.

$$P_{T(\mathbf{Y})}(\mathbf{A}) = \mathbf{Y} + \mathbf{Y}(\mathbf{A} - \mathbf{Y}) + (\mathbf{A} - \mathbf{Y})\mathbf{Y} - 2\mathbf{Y}(\mathbf{A} - \mathbf{Y})\mathbf{Y}. \tag{59}$$

Lemma

Let $\mathbf{Y} \in \mathcal{G}$ *and* $\mathbf{B} \in T(\mathbf{Y})$ $(K \geq 2N)$*. Then the eigenvalues of* $\mathbf{B}$ *are given by*

$$\left\{ -\varepsilon_N, -\varepsilon_{N-1}, \dots, -\varepsilon_1, \underbrace{0, \dots, 0}_{K-2N}, 1+\varepsilon_1, 1+\varepsilon_2, \dots, 1+\varepsilon_N \right\}, \qquad (60)$$

where $\varepsilon_i \geq 0$ *for all* $i = 1, \dots, N$*.*

In the restoration phase we want to find the Frobenius projection of $\mathbf{X}_k$ onto $\mathcal{G}$, which can be written as

$$\mathbf{Y}_k = \arg\min \|\mathbf{X}_k - \mathbf{Y}\|_F \text{ where } \mathbf{Y} \in \mathcal{G}. \tag{61}$$

To find it we can use the following theorem

Theorem

Let $\mathbf{Z} \in \mathbb{R}^{K\times K}$ *be symmetric. The spectral decomposition of the matrix* $\mathbf{Z}$ *is* $\mathbf{Z} = \mathbf{QDQ}^T$*, where diagonal elements of the matrix* $\mathbf{D}$ *are in non-increasing order. Define*

$$\overline{\mathbf{S}} = diag(\underbrace{1,\ldots,1}_{N},\underbrace{0,\ldots,0}_{K-N}). \tag{62}$$

Then $\mathbf{Q}\overline{\mathbf{S}}\mathbf{Q}^T$ *is a solution of*

$$\arg\min \|\mathbf{Z} - \mathbf{Y}\|_F \text{ where } \mathbf{Y} \in \mathcal{G}. \tag{63}$$

Restoration phase require expensive diagonalization of matrix $\mathbf{X}_k$. But this computation can be replaced by an iterative process

$$\mathbf{Y}_k^{j+1} = \mathbf{Y}_k^j - \left(2\mathbf{Y}_k^j - \mathbf{I}\right)^{-1} \left[\left(\mathbf{Y}_k^j\right)^2 - \mathbf{Y}_k^j\right]. \tag{64}$$

(It is application of Newton method to each eigenvalue of the matrix $\mathbf{Y}_k^j = \mathbf{Q}\mathbf{D}_k^j\mathbf{Q}^T$ for solving the equation $d_i^2 - d_i = 0$). For $d_i \in \{0, 1\}\, \forall i$ following equation holds:

$$\left(2\mathbf{Y}_k^j - \mathbf{I}\right)^{-1} = \left(2\mathbf{Y}_k^j - \mathbf{I}\right). \tag{65}$$

We have obtained a new iteration process

$$\mathbf{Y}_k^{j+1} = 3\left(\mathbf{Y}_k^j\right)^2 - 2\left(\mathbf{Y}_k^j\right)^3. \tag{66}$$

"Purification step".

Inexact Restoration method - matrix problem

Tangent descent direction

How to find an optimal direction in the tangent set?
Consider the subproblem

$$\arg\min Q_k(\mathbf{E}) \text{ subj. to } \mathbf{E} \in S(\mathbf{Y}_k) \tag{67}$$

where $Q_k(\mathbf{E}) = L(\mathbf{Y}_k + \mathbf{E}, \Lambda_k)$. Suppose we have an approximation of Lagrange multiplier matrix Λ_k. We can use Conjugate gradient approach to minimize $Q_k(\mathbf{E})$. Instead of the gradient direction we use the projection of the gradient to the tangent set. After finding the minimum we have to test the condition

$$\left\langle \mathbf{E}_k, P_{S(\mathbf{Y}_k)}[\nabla f(\mathbf{Y}_k)] \right\rangle \leq -10^{-6} \|\mathbf{E}_k\|_F \left\| P_{S(\mathbf{Y}_k)}[\nabla f(\mathbf{Y}_k)] \right\|_F \tag{68}$$

If not fulfilled, we choose $\mathbf{E}_k = P_{S(\mathbf{Y}_k)}[-\nabla f(\mathbf{Y}_k)]$.

Inexact Restoration method - matrix problem

Tangent descent direction

Consider the Lagrangian

$$L(\mathbf{X}, \Lambda) = f(\mathbf{X}) + \sum_{i,j=1}^{K} \lambda_{ij} \left(\mathbf{X}^2 - \mathbf{X}\right)_{ij} \tag{69}$$

Lagrange multiplier matrix $\Lambda \in \mathbb{R}^{K \times K}$ can be approximated as

$$\Lambda_k = -\frac{1}{2} \left((2\mathbf{Y}_k - \mathbf{I}) \nabla f(\mathbf{Y}_k) + [(2\mathbf{Y}_k - \mathbf{I}) \nabla f(\mathbf{Y}_k)]^T \right) \tag{70}$$

Example

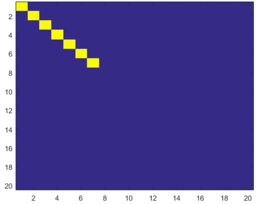
$f(\mathbf{X}) = \text{Trace}\,(\mathbf{TX})\,, \nabla f(\mathbf{X}) = \mathbf{T}$

$$\mathbf{T} = \text{Diag}(\underbrace{-1, \ldots, -1}_{N}, \underbrace{0, \ldots, 0}_{K-N})$$

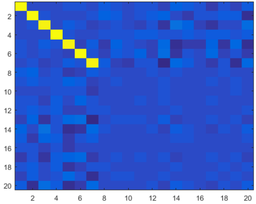
Solution:

$$\mathbf{X}^* = \text{Diag}(\underbrace{1, \ldots, 1}_{N}, \underbrace{0, \ldots, 0}_{K-N})$$

.



(a) Accurate solution



(b) Solution by IRM

Figure: $K = 20$ (matrix size 20×20), $N = 7$

$\|\mathbf{X}^* - \mathbf{X}\| = 0.5346, f(\mathbf{X}^*) = -7.0000, f(\mathbf{X}) = -6.8571$, 214 iterations.

Inexact Restoration method - matrix problem

Matlab experiments - example

Example

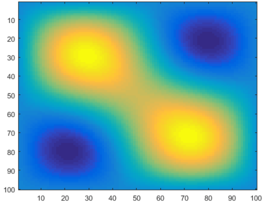
$f(\mathbf{X}) = \text{Trace}(\mathbf{TX}), \nabla f(\mathbf{X}) = \mathbf{T}$

$$\mathbf{T} = \begin{pmatrix} 2 & -1 & & & 0 \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ 0 & & & -1 & 2 \end{pmatrix}$$

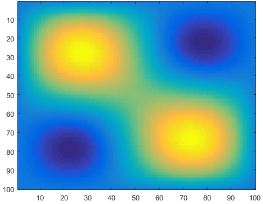
Solution: Projection matrix onto the subspace generated by the N smallest eigenvalues of the matrix $\mathbf{T}$.

Inexact Restoration method - matrix problem

Matlab experiments - solution



(a) Accurate solution



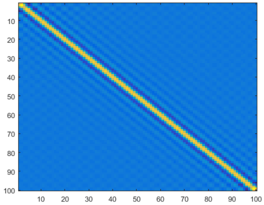
(b) Solution by IRM

Figure: $K = 100$ (matrix size 100×100), $N = 2$

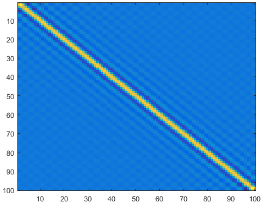
$\|\mathbf{X}^* - \mathbf{X}\| = 0.1701, f(\mathbf{X}^*) = 0.0048, f(\mathbf{X}) = 0.0050$, 3 iterations.

Inexact Restoration method - matrix problem

Matlab experiments - solution



(a) Accurate solution



(b) Solution by IRM

Figure: $K = 100$ (matrix size 100×100), $N = 40$

$\|\mathbf{X}^* - \mathbf{X}\| = 0.1701, f(\mathbf{X}^*) = 19.7845, f(\mathbf{X}) = 19.7844$, 4 iterations.

Thank you for attention

References

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- **Hartree-Fock method**: SAAD, Yousef, James R. CHELIKOWSKY a Suzanne M. SHONTZ. Numerical Methods for Electronic Structure Calculations of Materials. *SIAM Review*. 2010, DOI: 10.1137/060651653. ISSN 0036-1445. Available at: http://epubs.siam.org/doi/abs/10.1137/060651653