Inexact Restoration approach for minimization with inexact evaluation of the objective function

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$$\min_{x \in \mathbb{R}^n} f(x)$$

- $f(x)$ can be computed with different levels of accuracy $\{1, 2 \ldots, N\}$
- $f_J(x)$ - the functional value when f is computed at the J-th level of accuracy
- no error bound for inexact evaluation

$$\min f_N(x). \tag{1}$$

- Sample Average Approximation

$$f(x) = E[F(x,\xi)], \ f_J = \sum_{i=1}^{J} F(x,\xi^i)$$

- Data fitting methods

$$f_N(x) = \sum_{i=1}^{N} F(x,y^i)$$

- Electronic Structure Calculation
  - f is computed iteratively, $f_J(x)$ - the inexact functional value after J iterations

$$\min f_N(x)$$

- Cheaper evaluations $f_J(x), J < N$ whenever possible

Schedule sequence

$$\{N_0, N_1, N_2, \dots\}$$

$$N_k \in \{1, \dots, N\} \text{ - accuracy level at iteration } k$$

The dynamics of the schedule sequence - Inexact Restoration

The dynamics of the schedule sequence:

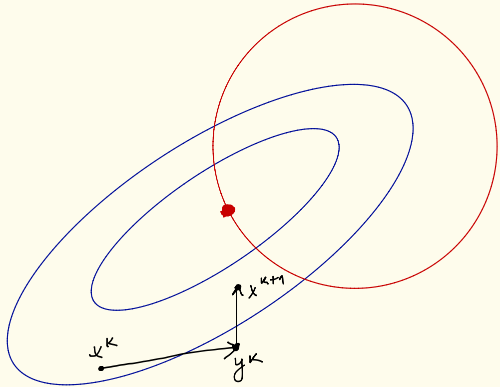
- SAA problem: Shapiro, Ruszczynski 2003, Shapiro, Wardi 1996, Spall 2003, Polak, Royset 2008, Pasupathy 2010, Homen-de-Mello 2003
- Bastin 2004, Bastin, Cirillo, Toint 2006, NK, Krklec 2013, NK, Krklec-Jerinkic 2014
- Data fitting: Friedlander, Schmidt 2012, Byrd et al 2011,2012,2014
- Distributed optimization: Bajović, Jakovetić, NK, Krklec Jerinkić, 2016

$$\min f_N(x)$$

$$\min z \text{ s.t. } z = f_N(x)$$

Inexact Restoration

- Restoration phase - y_k improved feasibility w.r.t. x_k
- Optimality phase - $y_k + \alpha d_k$ - improved optimality w.r.t. y_k
- IR + trust region Martínez 2001, Martínez, Pillota 2000, IR + filter Gonzaga, Karas, Vanti 2003, IR + line search Fischer, Friedlander 2010



x^{k+1}
x^k
y^k

Infeasibility measure (z, x, M)

$$h(z,x,M) = |z - f_M(x)| + g(M)$$

$g(M)-$ decreasing and $g(N) = 0$.
Feasible point $(z, x, M) : M = N, \ z = f_N(x)$

Merit function

$$\phi(z,x,M,\theta) = \theta z + (1-\theta)h(z,x,M), \ \theta \in [0,1]$$

$$\min z \text{ s.t. } z = f_N(x)$$

$$(z_k, x_k, N_k) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{N}$$

Algorithm 1 Given $z_0 \in \mathbb{R}, x_0 \in \mathbb{R}^n$, $N_0 \in \{1, 2, \dots, N\}, r \in (0, 1), \tau, \theta_0 \in (0, 1)$, and $\beta, \gamma, \bar{\gamma} > 0$, set $k \leftarrow 0$.

Step 1. (Restoration phase)
If $N_k < N$ find $\tilde{N}_{k+1} > N_k$ and $(u_k, y_k) \in \mathbb{R} \times \mathbb{R}^n$ such that

$$\tilde{N}_{k+1} \leq N, \; h(u_k, y_k, \tilde{N}_{k+1}) \leq rh(z_k, x_k, N_k), \tag{2}$$

and

$$\|(u_k, y_k) - (z_k, x_k)\| \leq \beta h(z_k, x_k, N_k). \tag{3}$$

If $N_k = N$ set $\tilde{N}_{k+1} = N$ and find (u_k, y_k) such that (2) and (3) hold.

Step 2. (Updating the penalty parameter)
If

$$\begin{aligned} &\phi(u_k, y_k, \tilde{N}_{k+1}, \theta_k) - \phi(z_k, x_k, N_k, \theta_k) \\ \leq \;& \frac{1-r}{2}\left(h(u_k, y_k, \tilde{N}_{k+1}) - h(z_k, x_k, N_k)\right) \end{aligned} \qquad (4)$$

set $\theta_{k+1} = \theta_k$.
Else compute

$$\theta_{k+1} = \frac{(1+r)\left(h(z_k, x_k, N_k) - h(u_k, y_k, \tilde{N}_{k+1})\right)}{2\left[u_k - z_k + h(z_k, x_k, N_k) - h(u_k, y_k, \tilde{N}_{k+1})\right]} \qquad (5)$$

Step 3 (Optimization Phase)

Step 3.1 Choose $p_k \in \mathbb{R}^n$ and an integer valued function $N_{k+1}(\alpha)$ such that, for all $\alpha \in (0, \tau]$, we have that $N_{k+1}(\alpha) \leq \tilde{N}_{k+1}$,

$$f_{N_{k+1}(\alpha)}(y_k + \alpha p_k) - f_{\tilde{N}_{k+1}}(y_k) \leq -\gamma\alpha\|p_k\|^2, \tag{6}$$

and

$$h(u_k + d_k(\alpha), y_k + \alpha p_k, N_{k+1}(\alpha)) \leq h(u_k, y_k, \tilde{N}_{k+1}) + \bar{\gamma}\alpha^2\|p_k\|^2, \tag{7}$$

where

$$d_k(\alpha) = [-f_{\tilde{N}_{k+1}}(y_k) + f_{N_{k+1}(\alpha)}(y_k + \alpha p_k)]. \tag{8}$$

Step 3.2. Find $\alpha_k \in (0, 1]$ as large as possible such that (6) and (7) hold for $\alpha = \alpha_k$ and

$$\phi(u_k + d_k(\alpha_k), y_k + \alpha_k p_k, N_{k+1}(\alpha_k), \theta_{k+1}) \leq \phi(z_k, x_k, N_k, \theta_{k+1}) + \frac{1-r}{2}\Big(h(u_k, y_k, \tilde{N}_{k+1}) - h(z_k, x_k, N_k)\Big). \tag{9}$$

Step 4. Set $x_{k+1} = y_k + \alpha_k p_k, z_{k+1} = u_k + d_k(\alpha_k), N_{k+1} = N_{k+1}(\alpha_k), k \leftarrow k + 1$ and go to Step 1

Convergence results

Assumption A1 For all $k = 0, 1, 2, \ldots$, it is possible to compute sequences $\{N_k\}$ and $\{(u_k, y_k)\}$ such that (2)-(3) are satisfied.

$$|f_{N_k}(x_k) - f_N(x_k)| \leq (\beta - 1)g(N_k),$$

- The algorithm is well defined
- The penalty parameters are positive, nonincreasing and $\lim_{k\to\infty} \theta_k = \theta^* > 0$

Theorem

Assume that A1 is satisfied, f_N is Lipschitz continuous, the functions f_M are continuous for $M \leq N$ and that the sequences $\{z_k\} \in \mathbb{R}, \{x_k\} \in \mathbb{R}^n$ generated by Algorithm 1 are bounded. Then, there exists $k_0 \in \mathbb{N}$ such that $N_k = \tilde{N}_{k+1} = N$ for $k \geq k_0$. Furthermore $\lim_{k\to\infty} \|p_k\| = 0$.

Electronic Structure Calculation

- Originates from the time-dependent Schrödinger equation
- Fixed nuclei coordinates, an ESC consists of finding the wave function from which the spatial electronic distribution the system can be derived
- Simplifications
- C - coefficient matrix, $2 \times nocc$ - the number of electrons, K - the number of basis elements, $P = CC^T$ - density matrix
- Fixed Point Self-Consistent Field (SCF) Method: Given P_c solve (10) to get P_{new}

$$\text{Minimize } Trace(\nabla E(P_c)P)$$

$$\text{subject to } P = P^T, P^2 = P, Trace(P) = nocc, P \in \mathbb{R}^{K \times K}. \tag{10}$$

Birgin, Martínez, Martínez, Rocha, J. Chem. Theor. Comput. 2013

$$\min_x f(x)$$

$$f(x) = (Trace[B(x)] - nocc)^2, \; B \in \mathbb{R}^{K \times K}$$

- Evaluation of f is based on the application of the projective gradient method to solve (10)
- Max number of iterations for the projective gradient method in practice is N
- $x_k \in (\lambda_{nocc}, \lambda_{nocc+1}), \; Trace(B_k) \approx nocc$
- Otherwise many PG iterations are wasted

The level of accuracy (max number of PG iterations) - the schedule sequence

Assume that $\varepsilon > 0$ and $N_k \in \{1, \ldots, N\}$.
Step 1 Compute $B_{start} = c(-A - xI) + \frac{1}{2} I_{K \times K}$ in such a way that all the eigenvalues of B_{start} are between 0 and 1.
Step 2 Consider

$$\text{Minimize } \|B^2 - B\|_F^2 \text{ s.t. } B = B^t$$

with the sparsity pattern constraint and obtain an approximate solution $B(x)$ as the result of applying the Projected Gradient method with convergence stopping criterion ε on the ∞-norm of the projected gradient and a maximum of N_k projected gradient iterations.
Step 3 Define $f_{N_k}(x) = (Trace[B(x)] - nocc)^2$.

Implementation

- $N = 1000$.
- The accuracy measure $g(M)$ is given by
$$g(M) = \frac{N - M}{M}.$$
- $$x_0 = \frac{[K - (nocc + 0.5)]a + (nocc + 0.5)b}{K}$$
where a and b are lower and upper bounds for the eigenvalues of $\nabla E(P_c)$ computed using the Gershgorin Theorem.
- $N_0 = 10$ and $z_0 = f_{N_0}(x_0)$.
- $r = 0.5$, $\beta = 10^3$, $\gamma = 10^{-4}$, $\bar{\gamma} = 100$, $\theta_0 = 0.9$, $\tau = 10^{-2}$.
- $\tilde{N}_{k+1} = 2N_k$ and $u_k = f_{\tilde{N}_{k+1}}(y_k)$
- $z_0 = f_{N_0}(x_0)$

- $Trace[B(x)]$ is non-decreasing as a function of x and we wish to find x such that $Trace[B(x)] = nocc$, we keep approximate upper and lower bounds of the solution. The first trial for p_k is based on safeguarded regula-falsi and bisection. If this direction satisfies (6) and (7) for $\alpha = 1$ we adopt this choice for p_k and set $N_{k+1}(1) = \tilde{N}_{k+1}/2$. Otherwise we choose $p_k = -\nabla f_{\tilde{N}_{k+1}}(x_k)$ and $N_{k+1}(1) = \tilde{N}_{k+1}$.
- The value of α_k that satisfies (9) is obtained by backtracking (with factor 0.5) using $\alpha = 1$ as first trial. If $\alpha < 1$ we define $N_{k+1}(\alpha) = \tilde{N}_{k+1}$.
- $\|B(x)^2 - B(x)\| \leq 10^{-8}$ and $|Trace[B(x)] - nocc| \leq 0.4$ or $k > 1000$

Test examples

- Family A - $\nabla E(P_c)$ - diagonal
- Family B - $\nabla E(P_c)$ - tridiagonal
- Family C - $\nabla E(P_c)$ - band sparse

Family A: $\nabla E(P_c)$ Diagonal						
Problem	nocc	K	Pseudo-gap	$\|\|B^2 - B\|\|$	Iterations	CPU Time (seconds)
1	500,000	1,000,000	8.E-8	7.E-16 | 7.E-16	3 | 5	5.51 | 7.57
2	250,000	1,000,000	4.E-6	4.E-14 | 1.E-8	4 | 1	5.41 | 5.80
3	5,000,000	10,000,000	4.E-9	4.E-15 | 5.E-16	9 | 9	100.4 | 110.5
4	2,500,000	10,000,000	2.E-7	1.E-9 | 1.E-9	3 | 4	52.1 | 86.7
Family B: $\nabla E(P_c)$ Tridiagonal						
Problem	nocc	K	Pseudo-gap	$\|\|B^2 - B\|\|$	Iterations	CPU Time
5	500,000	1,000,000	3.25	9.E-7 | 9.E-7	4 | 4	22.0 | 172.2
6	250,000	1,000,000	3.25	5.E-7 | 9.E-7	2 | 7	4.07 | 154.0
7	5,000,000	10,000,000	3.35	9.E-7 | 9.E-11	1 | 0	51.9 | 6.89
8	2,500,000	10,000,000	3.35	6.E-8 | 6.E-8	4 | 4	121.1 | 1082.8
Family C: $\nabla E(P_c)$ Band Sparse						
Problem	nocc	K	Pseudo-gap	$\|\|B^2 - B\|\|$	Iterations	CPU Time
9. diags = 21	24,000	36,000	12.5	2.E-9 | 2.E-9	7 | 7	3.7 | 124.2
10, diags = 41	24,000	36,000	17.2	2.E-10 | 2.E-10	1 | 1	11.5 | 284.1
11, diags = 81	24,000	36,000	30.0	6.E-11 | 6.E-11	1 | 1	33.9 | 1057.6
12, diags = 161	24,000	36,000	60.0	2.E-9 | 2.E-9	1 | 1	231.6 | 7753.2

Conclusions

- Unconstrained optimization problem with expensive function evaluation
- IR Merit function combines the accuracy of function evaluation and optimality
- Infeasibility is defined without calculation the (expensive) true functional value
- The schedule sequence and the penalty parameters depend on internally computed quantities
- Max precisssion is eventually reached
- Good numerical results