半光滑牛顿算法

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Outline

广义雅可比的定义

假定$\Omega \subseteq \mathbb{R}^n$是开集，$F:\Omega \to \mathbb{R}^m$是局部李普希兹连续的，根据Rademacher定理，F是几乎处处可微的，因此我们可以引入广义微分的概念。

定义

设$F:\Omega \to \mathbb{R}^m$是局部李普希兹连续, D_F是F是可微点组成的集合, F在x的B-微分可以被定义为

$$\partial_B F(x) := \left\{ \lim_{k\to\infty} F'(x^k) | x^k \in D_F, x^k \to x \right\}.$$

克拉克广义雅可比定义为所有B-微分的凸包

$$\partial F(x) = \mathrm{co}(\partial_B F(x))$$

其中co为凸包。

For a monotone and Lipschitz continuous mapping $F:\mathbb{R}^n \to \mathbb{R}^n$ and any $x \in \mathbb{R}^n$, each element of $\partial_B F(x)$ is positively semidefinite.

Proof: We first show that, at a differentiable point $\bar{x}$, $F'(\bar{x})$ is positively semidefinite. Suppose that there exist $a > 0$ and $d \in \mathbb{R}^n$ with $\|d\|_2 = 1$ such that $\langle d, F'(\bar{x})d\rangle = -a$. For any $t > 0$, let

$$\Phi(t) := F(\bar{x} + td) - F(\bar{x}) - tF'(\bar{x})d.$$

Since F is differentiable at $\bar{x}$, we have $\|\Phi(t)\|_2 = o(t)$ as $t \to 0$. The monotonicity of F indicates that

$$\begin{aligned} 0 & \le \langle td, F(\bar{x} + td) - F(\bar{x})\rangle = \langle td, tF'(\bar{x})d + \Phi(t)\rangle \\ & \le -at^2 + t\|d\|_2\|\Phi(t)\|_2 = -at^2 + o(t^2), \end{aligned}$$

which leads to a contradictory.

For any $x \in \mathbb{R}^n$ and each $J \in \partial_B F(x)$, there exists a differentiable point sequence $x^k \to x$ such that $F'(x^k) \to J$. Since every $F'(x^k)$ is positively semidefinite, we have that J is also positively semidefinite.

- 设g 是$\mathbb{R}^n$ 上适当的闭凸函数，g^* 为其共轭函数，则

$$\begin{aligned}\partial_{\mathrm{B}}(\mathbf{prox}_{\gamma g^*}(x)) &= \{J = I - Q | Q \in \partial_{\mathrm{B}}(\mathbf{prox}_{g/\gamma}(x/\gamma))\}, \\ \partial(\mathbf{prox}_{\gamma g^*}(x)) &= \{J = I - Q | Q \in \partial(\mathbf{prox}_{g/\gamma}(x/\gamma))\}.\end{aligned} \tag{1}$$

证明：利用Moreau 分解我们有

$$\mathbf{prox}_{\gamma g^*}(x) = x - \gamma\mathbf{prox}_{g/\gamma}(x/\gamma). \tag{2}$$

利用上式以及定义立即得到第一个等式（因为这里我们将$\mathbf{prox}_{\gamma g^*}$ 表示成两个连续可导函数的差）。再由

$$co\{I - Q | Q \in \partial_{\mathrm{B}}(\mathbf{prox}_{g/\gamma}(x/\gamma))\} = I - \mathbf{conv}(\partial_{\mathrm{B}}(\mathbf{prox}_{g/\gamma}(x/\gamma))), \tag{3}$$

我们就得到第二个等式

广义雅可比例子

- 设超平面$D=\{x|Ax=b\}$，其中$A\in\mathbb{R}^{m\times n}$。其投影映射$\Pi_D(x)=x-A^\dagger(Ax-b)$，其中$A^\dagger$为$A$的Moore-Penrose广义逆。显然$\Pi_D$是线性映射，因此其处处可导，故

$$\partial(\Pi_D(x))=\partial_{\mathrm{B}}(\Pi_D(x))=\nabla\Pi_D(x)=\{I-A^\dagger A\}. \tag{4}$$

- 记$x_+=\max\{0,x\}$。对于半空间$D=\{x|a^\top x\le b\}$，我们有

$$\Pi_D(x)=x-\left(\frac{(a^\top x-b)_+}{\|a\|_2^2}\right)a, \tag{5}$$

以及

$$\partial(\Pi_D(x))=\begin{cases}\{I-\frac{aa^\top}{\|a\|_2^2}\}, & \text{若 } a^\top x>b,\\ \{I\}, & \text{若 } a^\top x<b,\\ \mathrm{co}\{I, I-\frac{aa^\top}{\|a\|_2^2}\}, & \text{若 } a^\top x=b.\end{cases} \tag{6}$$

广义雅可比例子

- 设$B = \{x \mid \|x\|_2 = 1\}$ 为单位球，则其投影映射

$$\Pi_B(x) = \begin{cases} x/\|x\|_2, & 若\ \|x\|_2 > 1, \\ x, & 若\ \|x\|_2 \le 1. \end{cases} \tag{7}$$

若定义$w = x/\|x\|_2^2$，则我们有

$$\partial(\Pi_B)(x) = \begin{cases} \{\frac{I - ww^\top}{\|x\|_2}\}, & 若\ \|x\|_2 > 1, \\ \{I\}, & 若\ \|x\|_2 < 1, \\ \mathrm{co}\{\frac{I - ww^\top}{\|x\|_2}, I\}, & 若\ \|x\|_2 = 1. \end{cases} \tag{8}$$

广义雅可比例子

- 设$(t,x) \in \mathbb{R} \times \mathbb{R}^n$，定义二次锥$K = \{(t,x) \mid \|x\|_2 \le t\}$。则对任意$(t,x) \in \mathbb{R} \times \mathbb{R}^n$，若

$$V \in \partial_{\mathsf{B}}(\Pi_K)((t,x)), \tag{9}$$

则或者$V = 0$，或者$V = I_{n+1}$，或者V 可以表示成

$$V = \begin{pmatrix} 1 & w \\ w & H \end{pmatrix}, \tag{10}$$

其中$w \in \mathbb{R}^n$ 为单位向量，而$H \in \mathbb{R}^{n\times n}$ 有如下形式

$$H = (1+\alpha)I_n - \alpha w w^\top, \quad |\alpha| \le 1. \tag{11}$$

- 设$g = \|x\|_2$，则

$$\mathbf{prox}_{\gamma g}(x) = \begin{cases} (1 - \gamma/\|x\|_2)x, & \text{若 } \|x\|_2 \geq \gamma, \\ 0, & \text{若 } \|x\|_2 < \gamma. \end{cases} \tag{12}$$

注意到$\mathbf{prox}_{\gamma g}(x)$ 是分片光滑的，故其B-次微分可以通过分片求其雅可比矩阵得到，特别地，若令$w = x/\|x\|_2$，则

$$\partial_{\mathrm{B}}(\mathbf{prox}_{\gamma g}(x)) = \begin{cases} \{I - \gamma/\|x\|_2(I - ww^\top)\}, & \text{若 } \|x\|_2 \geq \gamma, \\ \{0\}, & \text{若 } \|x\|_2 < \gamma, \\ \{I - \gamma/\|x\|_2(I - ww^\top), 0\}, & \text{若 } \|x\|_2 = \gamma. \end{cases} \tag{13}$$

- 设$g = \|x\|_1$，则

$$\mathbf{prox}_{\gamma g}(x)_i = (\mathrm{sign}(x_i)(|x_i| - \gamma)_+)_i, \quad 1 \le i \le n. \tag{14}$$

注意到$\mathbf{prox}_{\gamma g}(x)$ 是可分的，因此$\partial_{\mathrm{B}}(\mathbf{prox}_{\gamma g}(x))$ 中的每个元素均为对角矩阵，
设$\alpha = \{i||x_i| > \gamma\}$，$\beta = \{i||x_i| = \gamma\}$，$\delta = \{i||x_i| < \gamma\}$，
若$J \in \partial_{\mathrm{B}}(\mathbf{prox}_{\gamma g}(x))$，则我们有

$$J_{ii} = \begin{cases} 1, & \text{若 } i \in \alpha, \\ \in \{0,1\}, & \text{若 } i \in \beta, \\ 0, & \text{若 } i \in \delta. \end{cases} \tag{15}$$

广义雅可比例子

- 谱函数: $G(X) = h(\lambda(X))$, $X \in \mathbb{S}^n$, 其中$\mathbb{S}^n$ 表示所有n 阶实对称矩阵组成的集合，$\lambda : \mathbb{S}^n \to \mathbb{R}^n$ 特征值按从大到小的顺序排列。$h : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ 是一个适当的闭凸函数，且它是关于变量对称的，即h 的值在任意调换变量顺序下保持不变。
- 谱函数G 继承了h 的许多性质，例如

$$\mathbf{prox}_{\gamma G}(X) = Q\mathbf{diag}(\mathbf{prox}_{\gamma h}(\lambda(X)))Q^\top, \tag{16}$$

其中$X = Q\mathbf{diag}(\lambda(X))Q^\top$ 是实对称矩阵X 的谱分解。

- 对于任意$X \in \mathbb{S}^n$ 和$P \in \partial_\mathrm{B}(\mathbf{prox}_{\gamma G})(X)$，有

$$P(S) = Q(\Omega \circ (Q^\top SQ))Q^\top, \quad \forall S \in \mathbb{S}^n, \tag{17}$$

其中$\circ$ 表示Hadamard 积，而矩阵$\Omega \in \mathbb{R}^{n\times n}$ 的各个元素按如下方式定义：

$$\Omega_{ij} = \begin{cases} \frac{\mathbf{prox}_{\gamma g}(\lambda_i)-\mathbf{prox}_{\gamma g}(\lambda_j)}{\lambda_i-\lambda_j}, & \text{若 } \lambda_i \neq \lambda_j, \\ \in \partial(\mathbf{prox}_{\gamma g}(\lambda_i)), & \text{若 } \lambda_i = \lambda_j. \end{cases} \tag{18}$$

- 半正定锥的指示函数:

$$\Pi_{\mathbb{S}^n_+}(X) = Q\mathbf{diag}((\lambda_1)_+, ..., (\lambda_n)_+)Q^\top, \tag{19}$$

其中$X = Q\mathbf{diag}(\lambda(X))Q^\top$ 是实对称矩阵X 的谱分解。
定义$\alpha = \{i|\lambda_i > 0\}$ 和$\bar{\alpha} = \{i|\lambda_i \leq 0\}$，则我们有$\Omega \subset \partial_B \Pi_{\mathbb{S}^n_+}(X)$，
其中

$$\Omega = \begin{pmatrix} \Omega_{\alpha\alpha} & k_{\alpha\bar{\alpha}} \\ k_{\alpha\bar{\alpha}}^\top & 0 \end{pmatrix}, \tag{20}$$

其中$\Omega_{\alpha\alpha} \in \mathbb{R}^{|\alpha|\times|\alpha|}$ 的元素全为1，而$k_{\alpha\bar{\alpha}} \in \mathbb{R}^{|\alpha|\times|\bar{\alpha}|}$ 且其第i 行第j
列元素为

$$\frac{\lambda_i}{\lambda_i - \lambda_j}, \quad i \in \alpha, j \in \bar{\alpha}. \tag{21}$$

Outline

半光滑

- 设$F:\Omega\rightarrow\mathbb{R}^m$是局部李普希兹连续的，如果下面条件满足则称$F$在$x$上是半光滑的
  (a) F在x点具有方向导数;
  (b) 对于任意的d和$J\in\partial F(x+d)$,下面的关系成立

$$\|F(x+d)-F(x)-Jd\|_2=o(\|d\|_2)\quad \text{当 } d\rightarrow 0.$$

如果（b）被替换下面的关系

$$\|F(x+d)-F(x)-Jd\|_2=O(\|d\|_2^2)\quad \text{当 } d\rightarrow 0.$$

那么称F在x上是强半光滑的。

半光滑

- 值得强调的是，在一些文献中并半光滑的定义不需要定义(a),这对于我们设计后面的算法并没有本质的影响。
- 半光滑性和强半光滑性具有很好的运算性质。半光滑性和强半光滑性在数乘、求和和复合运算下都是封闭的。
- 光滑函数、所有的凸函数，分段连续可微的函数都是半光滑的。具有李普希兹连续梯度的可微函数，p范数$\|\cdot\|_p$和分段线性函数是强半光滑的。一个向量值函数是半光滑的（或强半光滑的）当且仅当每个元素函数是半光滑的(或强半光滑的)。
- 很多函数的邻近算子具有半光滑性和和强半光滑性
  - The proximal mapping of $\|x\|_1$ and $\|x\|_\infty$ is strongly semi-smooth.
  - The projection over a polyhedral set is strongly semi-smooth.
  - The projections over symmetric cones are strongly semi-smooth.
  - In many applications, the proximal mapping is shown to be piecewise C^1 and hence semi-smooth.

Outline

基追踪（BP）问题

考虑问题

$$\min_{x\in\mathbb{R}^n} \quad \|x\|_1 \quad \text{s.t.} \quad Ax=b.$$

其对偶问题：

$$\min_{y\in\mathbb{R}^m} \quad b^\mathrm{T}y, \quad \text{s.t.} \quad \|A^\mathrm{T}y\|_\infty \le 1.$$

通过引入变量s，上述问题可以等价地写成

$$\min_{y\in\mathbb{R}^m, s\in\mathbb{R}^n} \quad b^\mathrm{T}y, \quad \text{s.t.} \quad A^\mathrm{T}y-s=0,\ \|s\|_\infty \le 1. \tag{22}$$

引入拉格朗日乘子λ和罚因子σ，对偶问题的增广拉格朗日函数为

$$L_\sigma(y,s,\lambda)=b^\mathrm{T}y+\lambda^\mathrm{T}(A^\mathrm{T}y-s)+\frac{\sigma}{2}\|A^\mathrm{T}y-s\|_2^2, \quad \|s\|_\infty \le 1.$$

那么，增广拉格朗日函数法的迭代格式为：

$$\begin{cases} (y^{k+1},s^{k+1}) = \displaystyle\operatorname*{argmin}_{y,\|s\|_\infty\le 1} \left\{ b^\mathrm{T}y+\frac{\sigma}{2}\|A^\mathrm{T}y-s+\frac{\lambda}{\sigma_k}\|_2^2 \right\}, \\ \lambda^{k+1} = \lambda^k+\sigma(A^\mathrm{T}y^{k+1}-s^{k+1}) \end{cases}$$

固定y求解只关于s的最小化问题得到

$$s = \mathcal{P}_{\|s\|_\infty \le 1}\left(A^\mathrm{T} y + \frac{\lambda}{\sigma}\right). \tag{23}$$

将s的表达式代入增广拉格朗日函数中，我们得到

$$L_\sigma(y, \lambda) = b^\mathrm{T} y + \frac{\sigma}{2}\left\|\psi\left(A^\mathrm{T} y + \frac{\lambda}{\sigma}\right)\right\|_2^2 - \frac{\lambda^2}{2\sigma},$$

其中$\psi(x) = \mathrm{sign}(x)\max\{|x| - 1, 0\}$。消去$s$的增广拉格朗日函数法为：

$$\begin{cases} y^{k+1} = \operatorname*{argmin}_y \left\{b^\mathrm{T} y + \frac{\sigma}{2}\left\|\psi\left(A^\mathrm{T} y + \frac{\lambda}{\sigma}\right)\right\|_2^2\right\}, \\ \lambda^{k+1} = \sigma\psi\left(A^\mathrm{T} y^{k+1} + \frac{\lambda^k}{\sigma}\right) \end{cases} \tag{24}$$

半光滑牛顿法

- 函数$L_\sigma(y,\lambda^k)$ 关于y 是连续可微的，且其梯度为

$$\nabla_y L_{\sigma_k}(y,\lambda^k)=b+\sigma_k A\psi\left(A^{\mathrm{T}}y+\frac{\lambda^k}{\sigma_k}\right).$$

- 函数$L_{\sigma_k}(y,\lambda^k)$并不是二阶可微的，但是$\nabla_y L_{\sigma_k}(y,\lambda^k)$是广义可微且半光滑，其一个广义雅可比矩阵为

$$J_k=AD_kA^{\mathrm{T}},$$

其中D_k是对角矩阵，对角元为

$$(D_k)_{ii}=\begin{cases}1 & 若 |(A^{\mathrm{T}}y^{k+1}+\frac{\lambda^k}{\sigma_k})_i|>1,\\ 0 & 若 |(A^{\mathrm{T}}y^{k+1}+\frac{\lambda^k}{\sigma_k})_i|\le 1.\end{cases}$$

半光滑牛顿法

- 对每一个增广拉格朗日函数使用半光滑牛顿法进行迭代：

$$y^{k+1,l+1} = y^{k+1,l} + \alpha d^l$$

- 半光滑牛顿方向：

$$(J_k + \mu I)d^l = -\nabla_y L_{\sigma_k}(y^{k+1,l}, \lambda^k)$$

- 计算的有效性：利用D_k 的稀疏结构
- 收敛性质

SDP

A reference is: Zhao, Xin-Yuan, Defeng Sun, and Kim-Chuan Toh. “A Newton-CG augmented Lagrangian method for semidefinite programming." SIAM Journal on Optimization 20.4 (2010): 1737-1765.
`http://epubs.siam.org/doi/abs/10.1137/080718206`.

- Consider the semi-definite programming (P)

$$\begin{aligned} \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \mathcal{A}X = b, \\ & X \succeq 0 \end{aligned}$$

- The dual problem (D) is

$$\begin{aligned} \max \quad & b^\top y \\ \text{s.t.} \quad & \mathcal{A}^* y + S = C, \\ & S \succeq 0 \end{aligned}$$

- the augmented Lagrangian function:

$$L_\sigma(y,S,X^k) = -b^\top y + \langle X, S - \mathcal{A}^* y + C\rangle + \frac{\sigma}{2}\|S - \mathcal{A}^* y + C\|_F^2$$

- Starting from X^0, the augmented Lagrangian method solves the dual problem (D) by

$$(y^{k+1}, S^{k+1}) = \arg \min_{S \succeq 0, y \in \mathbb{R}^m} L_\sigma(y,S,X^k),$$
$$X^{k+1} = X^k + \sigma(S^{k+1} - \mathcal{A}^* y^{k+1} + C),$$

- The variable S is eliminated as $S^{k+1} = \Pi_{\mathcal{S}_+^n}(\mathcal{A}^* y^{k+1} - C - X^k/\sigma)$, where $\Pi_{\mathcal{S}_+^n}$ is the projection on semidefinite matrix cone. Consequently, SDPNAL solves an equivalent form

$$y^{k+1} = \arg\min \tilde{L}_{\sigma^k}(y, X^k) \quad (25)$$
$$X^{k+1} = \Pi_{\mathcal{S}_+^n}(X^k - \sigma(\mathcal{A}^* y^{k+1} - C)), \quad (26)$$

where $\tilde{L}_\sigma(y,X) = b^T y + \frac{1}{2\sigma}(||\Pi_{\mathcal{S}_+^n}(X - \sigma(\mathcal{A}^* y - C))||_F^2 - ||X||_F^2)$.

- Then the subproblem (25) is minimized by using a semismooth Newton method to certain accuracy. The gradient and an alternative element of the generalized Hessian of $\tilde{L}_\sigma(y,X)$ with respect to y is

$$\nabla_y \tilde{L}_\sigma(y,X) = b - \mathcal{A}\Pi_{\mathcal{S}^n_+}(X - \sigma(\mathcal{A}^* y - C)), \quad (27)$$

$$V \in \sigma \mathcal{A} \partial \Pi_{\mathcal{S}^n_+}(X - \sigma(\mathcal{A}^* y - C))\mathcal{A}^*. \quad (28)$$

- For fixed y and X, the corresponding semi-smooth Newton step is

$$(V + \epsilon I)d = \nabla_y L_\sigma(y,X), \quad (29)$$

where ϵ is a small constant.

Outline

Composite convex program

Consider the following composite convex program

$$\min_{x \in \mathbb{R}^n} \quad f(x) + h(x),$$

where f and h are convex, f is differentiable but h may not

Many applications:

- Sparse and low rank optimization: $h(x) = \|x\|_1$ or $\|X\|_*$ and many other forms.
- Regularized risk minimization: $f(x) = \sum_i f_i(x)$ is a loss function of some misfit and h is a regularization term.
- Constrained program: h is an indicator function of a convex set.

A General Recipe

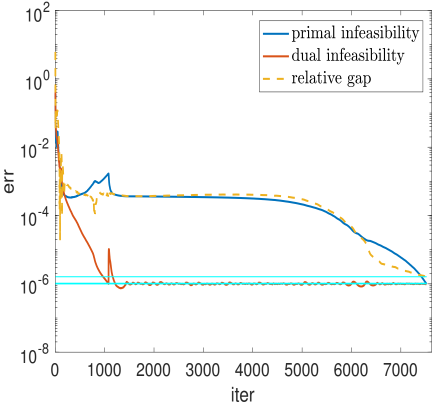
Goal: study approaches to bridge the gap between first-order and second-order type methods for composite convex programs.

key observations:

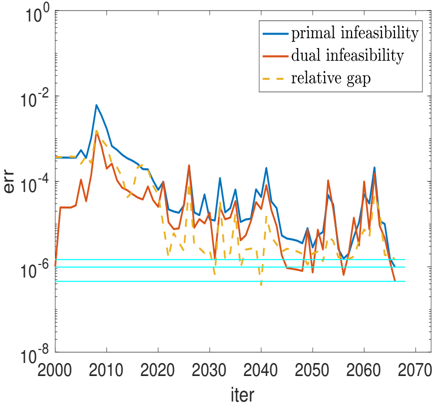
- Many popular first-order methods can be equivalent to some fixed-point iterations: $x^{k+1} = T(x^k)$;
  - **Advantages:** easy to implement; converge fast to a solution with moderate accuracy.
  - **Disadvantages:** slow tail convergence.
- The original problem is equivalent to the system $F(x) := (I - T)(x) = 0$.
- Newton-type method since $F(x)$ is semi-smooth in many cases
- Computational costs can be controlled reasonably well

An SDP From Electronic Structure Calculation

system: BeO



(a) ADMM, CPU: 2003s



(b) Semi-smooth Newton, CPU: 635s

Operator splitting and fixed-point algorithm

Examples:

- forward-backward splitting(FBS).
- Douglas-Rachford splitting(DRS).
- Peaceman-Rachford splitting(PRS).
- alternating direction method of multipliers(ADMM).

Advantages:

- easy to implement;
- converge fast to a solution with moderate accuracy.

Disadvantages:

- slow tail convergence.

Forward-backward splitting (FBS)

- Consider $\min_{x \in \mathbb{R}^n} \quad f(x) + h(x)$
- the *proximal mapping* of f is defined by

$$\text{prox}_{tf}(x) := \operatorname*{argmin}_{u \in \mathbb{R}^n} \{ f(u) + \frac{1}{2t} \|u - x\|_2^2 \}.$$

- Proximal gradient method or the FBS is the iteration

$$x^{k+1} = \text{prox}_{tf}(x^k - t\nabla h(x^k)), k = 0, 1, \cdots ,$$

- Equivalent to a fixed-point iteration

$$x^{k+1} = T_{\text{FBS}}(x^k).$$

where

$$T_{\text{FBS}} := \text{prox}_{tf} \circ (I - t\nabla h).$$

Douglas-Rachford splitting (DRS)

- DRS is the following update:

$$
\begin{aligned}
x^{k+1} &= \mathrm{prox}_{th}(z^k), \\
y^{k+1} &= \mathrm{prox}_{tf}(2x^{k+1} - z^k), \\
z^{k+1} &= z^k + y^{k+1} - x^{k+1}.
\end{aligned}
$$

- Equivalent to a fixed-point iteration

$$
z^{k+1} = T_{\mathrm{DRS}}(z^k),
$$

where

$$
T_{\mathrm{DRS}} := I + \mathrm{prox}_{tf} \circ (2\mathrm{prox}_{th} - I) - \mathrm{prox}_{th}.
$$

Semi-smooth Newton system

- Solve $F(z) = T(z) - z = 0$ and $T(z)$ is a fixed-point mapping.
- $J_k \in \partial_B F(z^k)$: positively semidefinite.
- regularized Newton's method

$$(J_k + \mu_k I)d = -F_k,$$

  where $F_k = F(z^k)$, $\mu_k = \lambda_k \|F_k\|$ and $\lambda_k > 0$ is a regularization parameter.
- solve the linear system inexactly.

$$r_k := (J_k + \mu_k I)d^k + F_k.$$

- seek to step d^k by solving the system approximately such that

$$\|r_k\| \leq \tau \min\{1, \lambda_k \|F_k\| \cdot \|d^k\|\},$$

  where $0 < \tau < 1$ is some positive constant.

Semi-smooth Newton method

- Select $0 < v < 1$, $0 < \eta_1 \le \eta_2 < 1$ and $1 < \gamma_1 \le \gamma_2$. $\underline{\lambda} > 0$
- A trial point $u^k = z^k + d^k$
- Define a ratio

$$\rho_k = \frac{-\left\langle F(u^k), d^k \right\rangle}{\|d^k\|_F^2}.$$

- Update the point

$$z^{k+1} = \begin{cases} u^k, \text{ if } \|F(u^k)\|_F \le \nu \max\limits_{\max(1,k-\zeta+1)\le j\le k} \|F(z^j)\|_F, & \text{[Newton]} \\ z^k, \text{otherwise.} & \text{[failed]} \end{cases}$$

- Update the regularization prameter

$$\lambda_{k+1} \in \begin{cases} (\underline{\lambda}, \lambda_k), & \text{if } \rho_k \ge \eta_2, \\ [\lambda_k, \gamma_1 \lambda_k], & \text{if } \eta_1 \le \rho_k < \eta_2, \\ (\gamma_1 \lambda_k, \gamma_2 \lambda_k], & \text{otherwise,.} \end{cases}$$

Ensuring global convergence I

- If the residual F is not reduced sufficiently or certain other conditions are not met, switching to first order methods. Note that F itself is a first order methods
- construct another point from the Newton step?
- X. Xiao, Y. Li, Z. Wen, L, Zhang, A Regularized Semi-Smooth Newton Method with Projection Steps for Composite Convex Programs, Journal of Scientfic Computing, 2018, Vol 76, No. 1, pp 364-389
- Y. Li, Z. Wen, C. Yang, Y. Yuan, A Semi-smooth Newton Method For semidefinite programs and its applications in electronic structure calculations, SIAM Journal on Scientific Computing, Vol 40, No. 6, 2018, A4131A4157

Ensuring global convergence II: projection step

- $d^k = 0$, then x_k is the optimal solution.
- A trial point
$$u^k = z^k + d^k.$$
- d_k is small enough,
$$\langle F(u^k), z^k - u^k \rangle = -\langle F(u^k), d^k \rangle > 0.$$
- By monotonicity of F, for any optimal solution z^*
$$\langle F(u^k), z^* - u^k \rangle \leq 0.$$
- Therefore the hyperplane
$$H_k := \{z \in \mathbb{R}^n | \langle F(u^k), z - u^k \rangle = 0\}$$
strictly separates z^k from the solution set Z^*.

Ensuring global convergence II: projection step

- Define a ratio
$$\rho_k = \frac{-\left\langle F(u^k), d^k \right\rangle}{\|d^k\|^2}.$$
- If ρ_k is big enough,
$$z^{k+1} = z^k - \frac{\left\langle F(u^k), z^k - u^k \right\rangle}{\|F(u^k)\|^2} F(u^k),$$
which is the projection onto the hyperplane H_k.
- If ρ_k is too small, $z^{k+1} = z^k$ and increase the parameter.

Ensuring global convergence II: projection step

- Select some parameters $0 < \eta_1 \leq \eta_2 < 1$ and $1 < \gamma_1 \leq \gamma_2$. $\underline{\lambda} > 0$ is a small positive constant.
- Update the point

$$z^{k+1} = \begin{cases} z^k - \frac{\langle F(u^k), z^k - u^k \rangle}{\|F(u^k)\|^2} F(u^k), & \text{if } \rho_k \geq \eta_1, \\ z^k, & \text{otherwise.} \end{cases}$$

- Update the regularization prameter

$$\lambda_{k+1} \in \begin{cases} (\underline{\lambda}, \lambda_k), & \text{if } \rho_k \geq \eta_2, \\ [\lambda_k, \gamma_1 \lambda_k], & \text{if } \eta_1 \leq \rho_k < \eta_2, \\ (\gamma_1 \lambda_k, \gamma_2 \lambda_k], & \text{otherwise,.} \end{cases}$$

- For any $z^* \in Z^*$ and any successful iteration

$$\|z^{k+1} - z^*\|^2 \leq \|z^k - z^*\|^2 - \|z^{k+1} - z^k\|^2.$$

Global convergence

Assumption:

- Assume that $F : \mathbb{R}^n \to \mathbb{R}^n$ is strongly semi-smooth and monotone.
- Suppose that there exists a constant $c_1 > 0$ such that $\|J_k\| \leq c_1$ for any $k \geq 0$ and any $J_k \in \partial_B F(z^k)$.

Global Convergence

The sequence $\{z^k\}$ generated by our algorithm converges to some point $\bar{z}$ such that $F(\bar{z}) = 0$ from any initial point.

Local Quadratic convergence

Assumption:

- The mapping F is BD-regular at z^*, that is, all elements in $\partial_B F(z^*)$ are nonsingular.

Local Quadratic convergence

For any Newton step and $z^k \in N(z^*, \varepsilon_1)$ with some $\varepsilon_1 > 0$, we have

$$\|z^{k+1} - z^*\|_2 \le c_2 \|z^k - z^*\|_2^2,$$

where c_2 is some positive constant.

- If z^k is close enough to z^*, the condition $\|F(u^k)\|_2 \le \nu \|F(z^k)\|_2$ is always satisfied.
- Our algorithm turns to a second-order Newton method in a neighborhood of z^*.

Applications to the FBS Method

- Consider the ℓ_1-regularized optimization problem of the form

$$\min \ \mu\|x\|_1 + h(x), \quad h(x) = \frac{1}{2}\|Ax - b\|_2^2$$

- Let $f(x) = \mu\|x\|_1$. The system of nonlinear equations is

$$F(x) = x - \mathrm{prox}_{tf}(x - t\nabla h(x)) = 0.$$

- The generalized Jacobian matrix of $F(x)$ is

$$J(x) = I - M(x)(I - t\partial^2 h(x)),$$

  where $M(x) \in \partial\mathrm{prox}_{tf}(x - t\nabla h(x))$ and $\partial^2 h(x)$ is the generalized Hessian matrix of $h(x)$.

- $M(z)$ is diagonal matrix whose diagonal entries are

$$(M(z))_{ii} = \begin{cases} 1, & \text{if } |z_i| > \mu t, \\ 0, & \text{otherwise.} \end{cases}$$

l1-regularized optimization problems

- introduce the index sets

$$\mathcal{I}(x) := \{i : |(x - t\nabla h(x))_i| > t\mu\} = \{i : (M(x))_{ii} = 1\},$$
$$\mathcal{O}(x) := \{i : |(x - t\nabla h(x))_i| \le t\mu\} = \{i : (M(x))_{ii} = 0\}.$$

- The Jacobian matrix can be represented by

$$J(x) = \begin{pmatrix} t(\partial^2 h(x))_{\mathcal{I}(x)\mathcal{I}(x)} & t(\partial^2 h(x))_{\mathcal{I}(x)\mathcal{O}(x)} \\ 0 & I \end{pmatrix}.$$

- Let $\mathcal{I} = \mathcal{I}(x^k)$ and $\mathcal{O} = \mathcal{O}(x^k)$. Then one can reduce the Newton system to a small system.

$$s^k_{\mathcal{O}} = -\frac{1}{1+\mu_k} F_{k,\mathcal{O}},$$
$$(t(\partial^2 h(x))_{\mathcal{I}\mathcal{I}} + \mu I) s^k_{\mathcal{I}} = -F_{k,\mathcal{I}} - t(\partial^2 h(x))_{\mathcal{I}\mathcal{O}} s^k_{\mathcal{O}}.$$

l1-regularized optimization problems

Table: Total number of A- and A^T- calls N_A and CPU time (in seconds) averaged over 10 independent runs with dynamic range 20 dB

method	$\epsilon : 10^{-0}$		$\epsilon : 10^{-2}$		$\epsilon : 10^{-4}$		$\epsilon : 10^{-6}$	
	time	N_A	time	N_A	time	N_A	time	N_A
SNF	1.12	84.6	3.19	254.2	3.87	307	4.5	351
SNF(aCG)	1.11	84.6	3.19	254.2	4.19	331.2	4.3	351.2
ASSN	1.15	89.8	2.2	173	3.15	246.4	3.76	298.2
SSNP	2.52	199	8.05	649.4	20.7	1679.8	29.2	2369.6
ASLB(2)	0.803	57	1.66	121	2.79	202.4	3.63	264.6
ASLB(1)	0.586	42.2	1.29	92	2.54	181.4	3.85	275
FPC-AS	1.45	109.8	7.08	510.4	10	719.8	10.3	743.6
SpaRSA	5.46	517.2	5.9	539.8	6.75	627	9.05	844.4

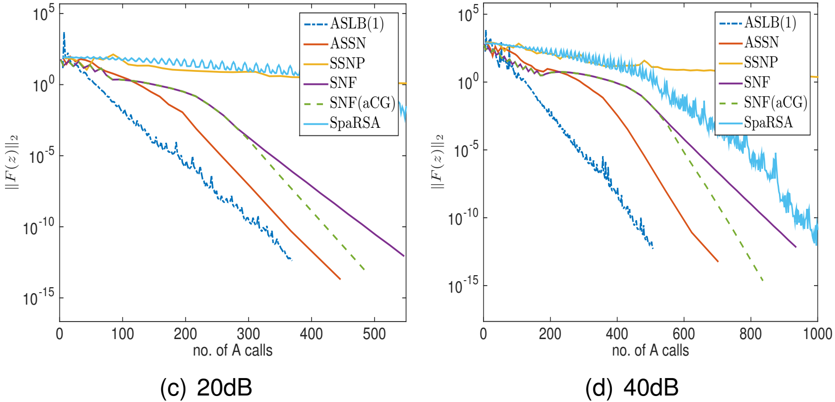
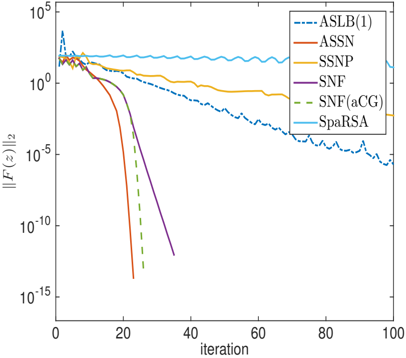
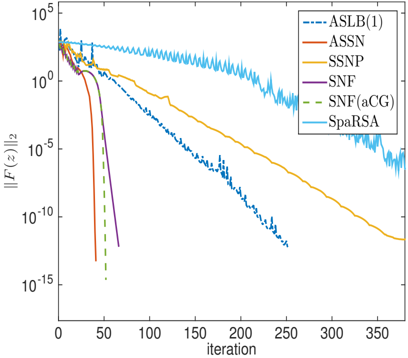


Figure: residual history with respect to total number of A- and A^T- calls N_A

l1-regularized optimization problems



(a) 20dB



(b) 40dB

Figure: residual history with respect to total number of iterations

Applications to the FBS Method

- The fixed-point mapping

$$F(x) = \text{prox}_{tf}(x - t\nabla h(x)) - x.$$

- The generalized Jacobian matrix of $F(x)$ is

$$J(x) = M(x)(I - t\partial^2 h(x)) - I,$$

where $M(x) \in \partial \text{prox}_{tf}(x - t\nabla h(x))$ and $\partial^2 h(x)$ is the generalized Hessian matrix of $h(x)$.

LASSO Regression

- The Lasso regression problem

$$\min \frac{1}{2}\|Ax - b\|_2^2 \text{ s.t. } \|x\|_1 \leq \lambda,$$

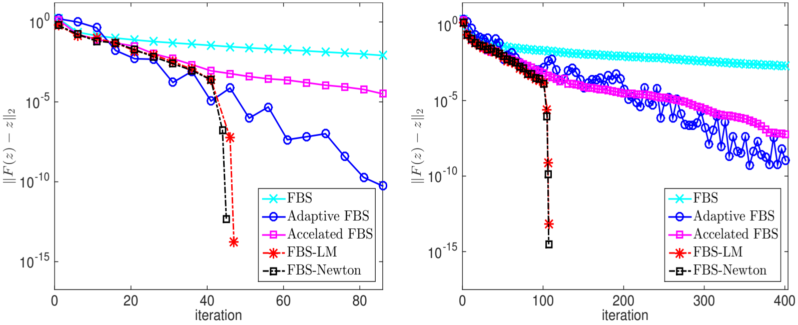
where $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$ and $\lambda \geq 0$ are given.

- $h(x) = \frac{1}{2}\|Ax - b\|_2^2$ and $f(x) = 1_\Omega(x)$, where $\Omega = \{x \mid \|x\|_1 \leq \lambda\}$.
- For a given $z \in \mathbb{R}^n$, let $|z_{[1]}| \geq |z_{[2]}| \geq \ldots \geq |z_{[n]}|$, the Jacobian matrix $M(z)$

$$M(z)_{ij} = \begin{cases} 1 & \text{if } \alpha < 0, j = i \\ 1 - \alpha \mathrm{sign}(z_i)\mathrm{sign}(z_j)/p, & \text{if } |z_i| \geq \alpha \text{ and } \alpha > 0, j = [1], \ldots, [p]. \end{cases}$$

where α be the largest value of $\left(\sum_{i=1}^k |z_{[i]}| - \lambda\right)/k$, $k = 1, \ldots, n$, and p be the corresponding k of α.

LASSO Regression



(a) $k = 50$ (b) $k = 150$

Figure: residual history of LASSO on $n = 1000$, $m = 500$ and $\mu = 0.9\|x\|_1$

Logistic Regression

- Sparse logistic regression problem

$$\min \ \mu\|x\|_1 + h(x),$$

where $\sum_{i=1}^m \log(e^{A_i x} + 1) - b_i^T A_i x$.

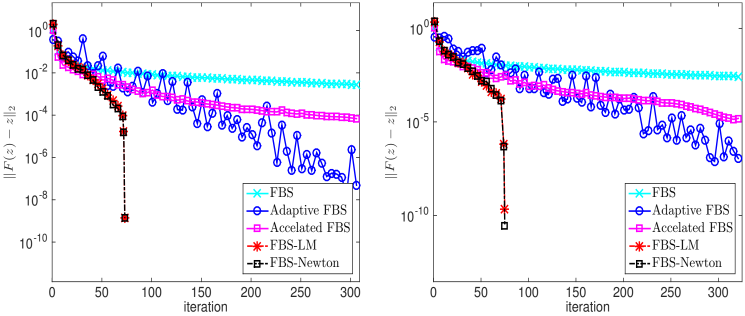
- The proximal mapping corresponding to $f(x) = \mu\|x\|_1$

$$\left(\mathrm{prox}_{tf}(z)\right)_i = \mathrm{sign}(z_i)\max(|z_i| - \mu t, 0).$$

- the Jacobian matrix $M(z)$ is diagonal matrix whose diagonal entries are

$$(M(z))_{ii} = \begin{cases} 1, & \text{if } |z_i| > \mu t, \\ 0, & \text{otherwise.} \end{cases}$$

Logistic Regression



(a) $k = 200$ (b) $k = 600$

Figure: residual history of the logistic regression problem on $n = 2000$, $m = 1000$ and $\mu = 1$

General Quadratic Programming

- The general quadratic programming

$$\min_{x\in\mathbb{R}^n} \frac{1}{2}x^TQx + c^Tx, \text{ s.t. } Ax \le b,$$

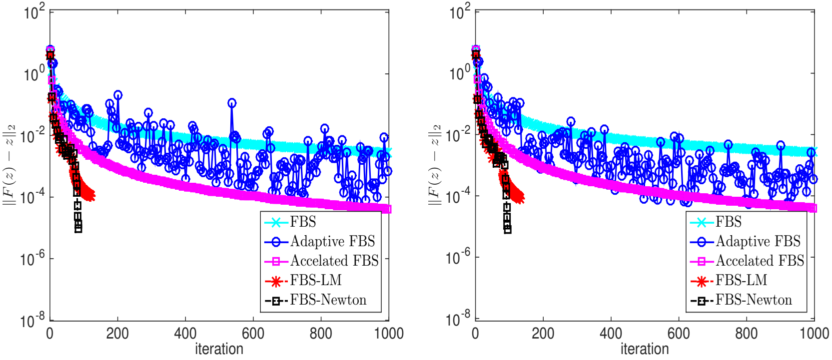
  where $Q \in R^{n\times n}$ is symmetric positive definite, $A \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m$.
- The dual problem is

$$\max_{y\ge 0}\min_{x\in\mathbb{R}^n} \frac{1}{2}x^TQx + c^Tx + y^T(Ax - b),$$

  which is equivalent to

$$\min_{y\ge 0} \frac{1}{2}y^T(AQ^{-1}A^T)y + (AQ^{-1}c + b)^Ty.$$

General Quadratic Programming



(a) LISWET1 (b) LISWET2

Figure: residual history of quadratic programming

Applications to the DRS Method

- Optimization problems

$$\min f(x), \text{ s.t. } Ax = b,$$

  where $A \in \mathbb{R}^{m \times n}$ is of full row rank and $b \in \mathbb{R}^m$.

- $h(x) = 1_\Omega(x)$, where $\Omega = \{x \mid Ax = b\}$.

- The proximal mapping with respect to $h(x)$ is

$$\text{prox}_{th}(x) = \mathcal{P}_\Omega(x) = (I - \mathcal{P}_{A^T})x + (A^T(AA^T)^{-1})b,$$

  where $\mathcal{P}_{A^T} = A^T(AA^T)^{-1}A$.

Applications to the DRS Method

- The DRS fixed-point mapping reduces to

$$F(z) = \mathrm{prox}_{tf}((2D - I)z + 2\beta) - Dz - \beta,$$

  where

$$D = I - \mathcal{P}_{A^T} \quad \text{and} \quad \beta = (A^T(AA^T)^{-1})b.$$

- The generalized Jacobian matrix of $F(z)$ is in the form of

$$J(z) = M(z)(2D - I) - D = \Psi(z) - \Phi(z)\mathcal{P}_{A^T},$$

  where $M(z) \in \partial\mathrm{prox}_{tf}((2D - I)z + 2\beta)$, $\Psi(z) = M(z) - I$ and $\Phi(z) = 2M(z) - I$.

Applications to the DRS Method

- The ℓ_1 minimization problem:

$$\min_{x \in \mathbb{R}^n} \quad \|x\|_1, \text{ s.t.} \quad Ax = b.$$

- Let $f(x) = 1_\Omega(Ax - b)$ and $h(x) = \|x\|_1$, where the set $\Omega = \{0\}$. The system of nonlinear equations is

$$F(z) = \text{prox}_{th}(z) - \text{prox}_{tf}(2\text{prox}_{th}(z) - z) = 0.$$

- Hence, a generalized Jacobian matrix of $F(z)$ is in the form of

$$J(z) = M(z) + D(I - 2M(z)).$$

- A generalized Jacobian matrix $M(z) \in \partial\text{prox}_{th}(z)$ is a diagonal matrix with diagonal entries

$$M_{ii}(z) = \begin{cases} 1, & |(z)_i| > t, \\ 0, & \text{otherwise.} \end{cases}$$

Basis Pursuit

- Make the assumption that $AA^\top = I$. Then we can obtain
$$\text{prox}_{tf}(z) = z - A^\top(Az - b).$$
A generalized Jacobian matrix $D \in \partial\text{prox}_{tf}((2\text{prox}_{th}(z) - z))$ is taken as follows
$$D = I - A^\top A.$$

- Let $W = (I - 2M(z))$ and $H = W + M(z) + \mu I$. The diagonal entries of matrix W and H are
$$W_{ii}(z) = \begin{cases} -1, & |(z)_i| > t, \\ 1, & \text{otherwise} \end{cases} \quad \text{and} \quad H_{ii}(z) = \begin{cases} \mu, & |(z)_i| > t, \\ 1 + \mu, & \text{otherwise.} \end{cases}$$

- Using the binomial inverse theorem, we obtain the inverse matrix
$$\begin{aligned} (J(z) + \mu I)^{-1} &= (H - A^\top AW)^{-1} \\ &= H^{-1} + H^{-1}A^\top(I - AWH^{-1}A^\top)^{-1}AWH^{-1}. \end{aligned}$$

Basis Pursuit

- Then $WH^{-1} = \frac{1}{1+\mu}I - S$, where S is a diagonal matrix with diagonal entries

$$S_{ii}(z) = \begin{cases} \frac{1}{\mu} + \frac{1}{1+\mu}, & |(z)_i| > t, \\ 0, & \text{otherwise.} \end{cases}$$

- Hence, $I - AWH^{-1}A^\top = (1 - \frac{1}{1+\mu})I + ASA^\top$.
- Define the index sets

$$\mathcal{I}(x) := \{i : |(z)_i| > t\} = \{i : M_{ii}(x) = 1\},$$
$$\mathcal{O}(x) := \{i : |(z)_i| \leq t\} = \{i : M_{ii}(x) = 0\}$$

- $A_{\mathcal{I}(x)}$ denote the matrix containing the column $\mathcal{I}(x)$ of A, then we have

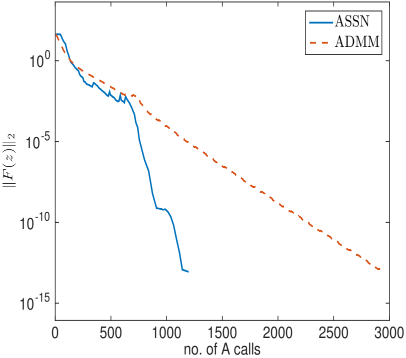
$$ASA^\top = (\frac{1}{\mu} + \frac{1}{1+\mu})A_{\mathcal{I}(x)}A_{\mathcal{I}(x)}^\top.$$

Basis Pursuit

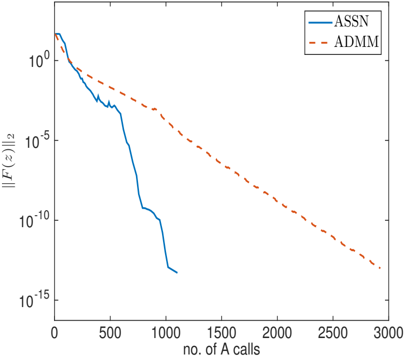
Table: Total number of A- and A^T- calls N_A, CPU time (in seconds) and relative error with dynamic ranges 60dB and 80dB

method	$\epsilon : 10^{-2}$			$\epsilon : 10^{-4}$			$\epsilon : 10^{-6}$		
	time	N_A	rerr	time	N_A	rerr	time	N_A	rerr
ADMM	7.44	599	1.90e-03	13.5	980	2.50e-06	18.7	1403	2.91e-08
ASSN	5.48	449	1.32e-03	9.17	740	1.92e-06	10.2	802	1.93e-08
SPGL1	55.3	2367	5.02e-03	70.7	2978	5.02e-03	89.4	3711	5.02e-03
method	$\epsilon : 10^{-2}$			$\epsilon : 10^{-4}$			$\epsilon : 10^{-6}$		
	time	N_A	rerr	time	N_A	rerr	time	N_A	rerr
ADMM	7.8	592	5.38e-04	13.8	1040	2.48e-06	17.7	1405	2.35e-08
ASSN	4.15	344	5.19e-04	7.92	618	1.21e-06	8.74	702	5.62e-09
SPGL1	32.2	1368	4.86e-04	56.1	2396	4.86e-04	67.4	2840	4.86e-04

Basis Pursuit

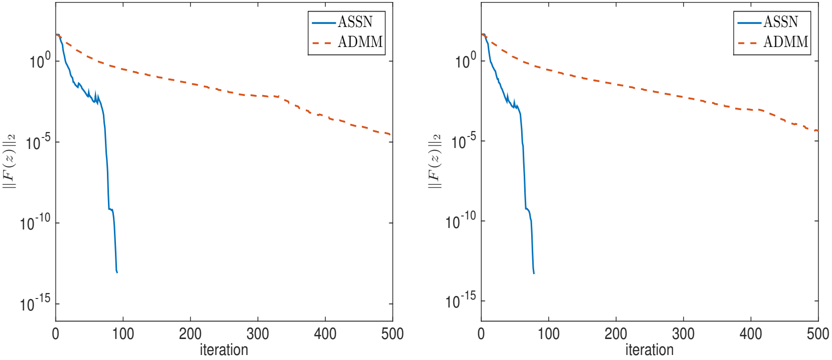


(a) 60dB



(b) 80dB

Figure: residual history with respect to the total number of A- and A^T- calls N_A



(a) 60dB (b) 80dB

Figure: residual history with respect to the total number of iterations

SDP

- Consider the semi-definite programming(SDP)

$$\begin{aligned} \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \mathcal{A}X = b, \\ & X \succeq 0 \end{aligned}$$

- $f(X) = \langle C, X \rangle + 1_{\{\mathcal{A}X=b\}}(X)$.
- $h(X) = 1_K(X)$, where $K = \{X : X \succeq 0\}$.
- Proximal Operator:

$$\text{prox}_{th}(Z) = \arg\min_X \frac{1}{2}\|X - Z\|_F^2 + th(X)$$

- Let $Z = Q\Sigma Q^T$ be the spectral decomposition

$$\begin{aligned} \text{prox}_{tf}(Y) &= (Y + tC) - \mathcal{A}^*(\mathcal{A}Y + t\mathcal{A}C - b), \\ \text{prox}_{th}(Z) &= Q_\alpha \Sigma_\alpha Q_\alpha^T, \end{aligned}$$

Semi-smooth Newton System

- assumption: $\mathcal{A}\mathcal{A}^* = I$
- The binomial inverse theorem yields the inverse matrix

$$
\begin{aligned}
(J_k + \mu_k I)^{-1} &= (H - A^T A W)^{-1} \\
&= H^{-1} + H^{-1} A^T (I - AWH^{-1}A^T)^{-1} AWH^{-1}.
\end{aligned}
$$

- computational cost $O(n^2 \min\{r, |n-r|\})$, where r is the rank of primal variable.
- computational cost $O(\sum_i n_i^2 \min\{r_i, |n_i - r_i|\})$, if there is a block diagonal structure.

Semi-smooth Newton method

- Define $T = \tilde{Q}L\tilde{Q}^T$, where L is a diagonal matrix with diagonal entries

$$L_{ii}(z) = \begin{cases} 1, & (\Lambda)_{ii} = 1, \\ \frac{\omega\mu}{\mu+1-\omega}, & (\Lambda)_{ii} = \omega, \\ 0, & (\Lambda)_{ii} = 0. \end{cases}$$

- Then $H^{-1} = \frac{1}{\mu+1}I + \frac{1}{\mu(\mu+1)}T$ and $WH^{-1} = \frac{1}{1+\mu}I - (\frac{1}{\mu} + \frac{1}{\mu+1})T$.
- Hence,

$$\begin{aligned} & (J(Z) + \mu I)^{-1} \\ = \quad & \frac{1}{\mu(\mu+1)}(\mu I + T)(I + A^\top(\frac{\mu^2}{2\mu+1}I + ATA^\top)^{-1}A(\frac{\mu}{2\mu+1}I - T)). \end{aligned}$$

- $ATA^\top d = \mathcal{A}Q(\Omega_0 \circ (Q^T(D)Q))Q^T$, where $D = \mathcal{A}^*d$,

$$\Omega_0 = \begin{bmatrix} E_{\alpha\alpha} & l_{\alpha\bar{\alpha}} \\ l_{\alpha\bar{\alpha}}^T & 0 \end{bmatrix},$$

  and $E_{\alpha\alpha}$ is a matrix of ones and $l_{ij} = \frac{\mu k_{ij}}{\mu+1-k_{ij}}$
- computational cost $O(|\alpha|n^2)$

Switching between the ADMM and Newton steps

the reduced ratios of primal and dual infeasibilities

$$\omega_{\eta_p}^k = \frac{\text{mean}_{k-5 \le j \le k} \eta_p^j}{\text{mean}_{k-25 \le j \le k-20} \eta_p^j} \text{ and } \omega_{\eta_q}^k = \frac{\text{mean}_{k-5 \le j \le k} \eta_q^j}{\text{mean}_{k-25 \le j \le k-20} \eta_q^j}.$$

Repeat:

- Semi-smooth Newton steps (doSSN == 1)
  Select $J_k \in \partial_B F(Z^k)$ and solve the Newton system approximately.
  Compute $U^k = Z^k + S^k$. Then update Z^{k+1} and λ_{k+1}.
  If Newton step is failed, set $N_f = N_f + 1$.
  If $N_f \ge \bar{N}_f$ or the Newton step performs bad
     Set doSSN = 0 and parameters for the ADMM steps

- ADMM steps (doSSN == 0)
  Perform an ADMM step. Equivalently, it defines
  $Z^{k+1} = Z^k - F(Z^k)$.
  If the ADMM step performs bad
     Set doSSN = 1, $N_f = 0$ and parameters of the Newton steps

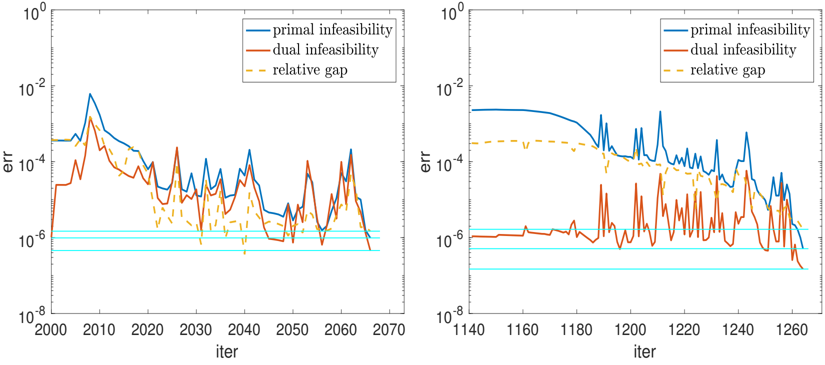
Comparison on electronic structure calculation

- The data set are used in the paper of Nakata, et al. Thanks Prof. Nakata Maho and Prof. Mituhiro Fukuta for sharing all data sets on 2RDM
- solver:
  - SDPNAL: Newton-CG Augmented Lagrangian Method proposed by Zhao, Sun and Toh
  - SDPNAL+: Enhanced version of SDPNAL by Yang, Sun and Toh
  - SSNSDP: the semi-smooth Newton method using stop rules $\eta_p < 3 \times 10^{-6}$ and $\eta_d < 3 \times 10^{-7}$.
- all experiments were performed on a computing cluster with an Intel Xeon 2.40GHz CPU that processes 28 cores and 256GB RAM.
- main criteria:

$$\eta_p = \frac{\|\mathcal{A}(X) - b\|_2}{\max(1, \|b\|_2)} \quad \eta_d = \frac{\|\mathcal{A}^* y - C - S\|_F}{\max(1, \|C\|_F)}$$

$$\eta_g = \frac{|b^T y - \mathrm{tr}(C^T X)|}{\max(1, \mathrm{tr}(C^T X))} \quad \mathrm{err} = b^T y - \mathrm{energy}_{\mathrm{fullCI}}$$

Comparison on electronic structure calculation



(a) BeO   (b) C2

Figure: SSNSDP: Relative gap, primal infeasibility and dual infeasibility

Comparison on electronic structure calculation

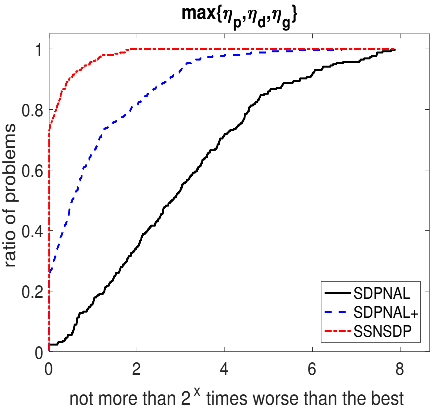
		ADMM						SSNSDP					
system	condition	err	η_p	η_d	η_g	it	t	err	η_p	η_d	η_g	it	t
BH_3O	PQGT1T2'	-1.4-3	9.9-7	8.8-7	2.5-6	2148	3954	-1.4-3	1.0-6	9.1-7	2.3-6	2138	3918
BeO	PQGT1T2	-1.9-3	8.8-7	1.1-6	4.4-7	10261	2003	-2.0-3	4.2-7	3.6-7	1.0-6	1487	635
BeO	PQGT1T2'	-2.0-3	1.0-6	1.0-6	1.6-6	7521	1492	-2.0-3	9.8-7	4.6-7	1.5-6	2066	593
C_2	PQGT1T2	1.7-2	9.5-3	1.9-6	1.6-3	20000	41694	-8.0-3	7.3-7	9.3-7	2.8-5	1165	14074
C_2	PQGT1T2'	-4.0-3	9.5-7	1.3-6	4.9-6	13363	28505	-3.7-3	7.0-7	2.2-7	2.3-6	1440	11849
CH	PQGT1T2	-2.0-3	9.9-7	1.1-6	3.9-6	12723	6292	-1.9-3	3.7-7	6.8-7	7.2-7	1625	1583
CH	PQGT1T2'	-7.5-4	1.0-6	1.1-6	5.1-6	3975	2140	-6.3-4	7.7-7	5.5-7	3.5-6	1597	1432

Figure: Comparison between ADMM and SSNSDP

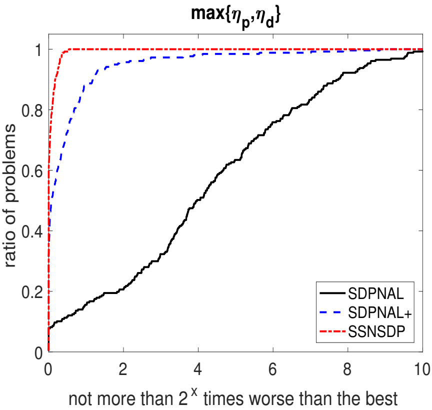
Comparison on electronic structure calculation

	SSNSDP						SDPNAL						SDPNAL+					
system	err	η_p	η_d	η_g	it	t	err	η_p	η_d	η_g	it	t	err	η_p	η_d	η_g	it	t
H_2O	-1.3-3	4.2-7	2.7-7	5.1-6	1605	3788	-1.9-3	7.4-5	4.9-7	1.1-4	266	5595	-2.0-3	7.4-7	8.9-7	1.1-5	3420	9253
H_3	-2.6-5	9.9-7	8.4-7	6.2-6	1511	42	-3.3-5	8.5-7	9.7-7	7.5-6	163	56	-1.6-5	1.1-6	9.4-7	1.9-6	1026	39
HF	-1.8-3	1.0-6	9.3-7	6.7-6	2589	1500	-2.3-3	5.6-5	6.9-7	7.5-5	236	1716	-2.3-3	8.4-7	9.6-7	1.2-5	3062	3208
HLi_2	-8.0-5	8.2-7	4.9-7	2.3-6	1624	791	-2.8-4	1.9-5	7.7-7	2.2-5	260	1105	-9.7-5	1.2-13	1.0-6	2.0-7	3820	1941
HN_2^+	-2.0-3	9.9-7	6.6-7	1.4-6	1742	645	-2.2-3	8.4-6	7.8-7	1.1-5	187	703	-1.9-3	9.1-7	8.3-7	1.2-6	1532	886
HNO	-1.2-3	4.7-7	3.8-7	8.2-7	2065	1984	-1.5-3	1.4-5	7.1-7	2.3-5	213	1530	-1.2-3	8.6-7	9.3-7	1.8-6	1286	1753
Li	-1.9-5	1.9-7	8.3-7	2.1-6	410	36	-1.7-5	2.1-7	6.8-7	1.8-6	145	23	-2.4-5	5.1-7	1.1-6	2.5-6	1123	14
Li_2	-7.3-5	4.3-7	4.4-7	2.2-6	1636	363	-2.0-4	2.5-5	6.9-7	2.5-5	262	497	-2.4-4	3.3-8	1.0-6	8.9-6	5826	1319
LiF	-5.9-4	7.4-7	1.0-6	2.0-6	2813	598	-6.6-4	9.6-6	6.2-7	1.1-5	217	547	-3.5-4	1.0-6	9.0-7	1.5-6	1830	833
LiH(1)	-3.0-5	4.6-7	2.4-7	1.8-6	1715	2273	-1.2-4	2.7-5	7.4-7	1.8-5	253	1765	-2.8-4	5.6-14	5.9-5	4.6-5	17840	10001
LiH(2)	-2.3-5	9.9-7	8.5-7	2.0-6	2154	42	-5.9-5	8.5-6	6.9-7	4.9-6	232	105	-7.1-5	4.3-7	9.8-7	4.5-6	1455	56
LiOH	-9.7-4	1.0-6	9.7-7	2.4-6	2340	809	-1.0-3	1.0-5	5.4-7	1.5-5	203	835	-6.7-4	7.9-7	7.0-7	7.0-7	2098	1499
N	-2.2-4	4.2-7	3.6-7	2.1-6	1608	385	-5.0-4	6.8-5	5.0-7	6.6-5	229	347	-1.1-3	3.8-7	1.4-6	1.1-5	20144	2663
N_2^+	-2.6-3	1.0-6	9.2-7	1.1-6	2434	328	-2.8-3	5.6-6	7.6-7	1.1-5	187	304	-2.8-3	7.6-7	1.0-6	2.0-7	3939	820
N_2	-1.6-3	8.0-7	5.7-7	2.4-6	1036	177	-1.5-3	8.6-6	4.4-7	8.2-6	180	287	-2.0-3	5.1-14	1.5-6	3.3-6	20058	2513
NH(1)	-9.0-4	7.4-7	6.1-7	4.0-6	1599	1468	-1.3-3	4.5-5	5.1-7	7.3-5	264	1998	-1.5-3	1.6-13	1.0-6	8.3-6	3434	3595
NH(2)	-5.1-4	2.9-7	2.2-7	3.0-6	1607	1614	-9.7-4	1.1-4	5.2-7	1.6-4	253	1726	-7.8-4	6.9-13	9.5-7	2.8-6	4046	3909
NH_2^-(1)	-1.3-3	8.0-7	3.1-7	6.1-6	1402	3283	-1.8-3	7.0-5	5.0-7	1.3-4	255	5370	-1.9-3	9.4-7	1.0-6	7.7-6	2602	8306
NH_2^-(2)	-1.9-4	4.9-7	9.2-7	1.3-6	906	44	-1.6-4	1.5-6	4.8-7	1.8-6	171	94	-1.9-4	2.0-7	9.8-7	1.1-6	817	46
NH_3^+	-3.5-4	6.6-7	5.0-7	1.0-6	1096	93	-3.7-4	1.3-6	5.6-7	1.7-6	195	177	-2.7-4	8.9-7	8.0-7	4.3-7	854	133
NH_3	-8.7-4	6.4-7	1.4-7	4.3-6	1307	11463	-1.6-3	9.6-6	5.8-7	1.7-5	259	13131	-2.1-3	9.3-6	4.2-6	1.3-6	298	10220
NH_4^+	-5.2-4	1.0-6	6.5-7	1.3-6	1603	173	-6.1-4	1.9-6	6.3-7	1.8-6	182	190	-6.8-4	4.6-7	9.8-7	2.4-6	1228	196
Na	-4.4-4	1.0-6	8.3-7	1.2-6	1575	127	-5.2-4	4.4-6	6.4-7	3.9-6	184	173	-4.2-4	1.2-7	9.5-7	1.1-6	724	105
NaH	-6.1-4	1.0-6	8.5-7	1.6-6	1782	371	-7.9-4	5.4-6	7.2-7	6.2-6	199	485	-3.9-4	6.3-7	8.4-7	2.8-7	1161	513
Ne	-2.1-3	1.0-6	8.4-7	8.6-6	1967	264	-2.5-3	2.0-5	7.7-7	3.4-5	208	319	-2.6-3	8.6-7	9.2-7	1.2-5	2370	495
O(1)	-1.5-3	9.7-7	1.7-7	2.0-6	1587	332	-2.0-3	2.1-5	4.5-7	2.9-5	216	332	-2.6-3	5.1-10	1.0-6	1.0-5	2651	736
O(2)	-9.1-4	9.5-7	9.8-7	4.6-6	2599	326	-1.2-3	7.4-5	5.6-7	9.1-5	217	328	-1.6-3	5.9-7	9.5-7	1.0-5	1661	542
O(3)	-1.9-3	8.8-7	1.4-7	2.0-6	1575	333	-2.5-3	1.8-5	5.3-7	2.0-5	235	347	-3.0-3	8.2-7	1.0-6	1.0-5	2696	707
O_2^+	-2.3-3	9.9-7	7.8-7	1.6-7	1729	232	-2.4-3	4.4-6	5.6-7	6.5-6	172	289	-2.5-3	3.6-7	9.7-7	1.6-6	939	246
P	-2.8-4	3.3-7	7.3-7	1.7-7	1675	1484	-1.1-3	7.0-6	6.3-7	7.0-6	208	1126	-6.3-4	3.5-13	1.0-6	7.2-7	640	2188
SiH_4	-1.1-3	1.0-6	7.3-7	2.1-6	1657	1471	-1.0-3	5.6-6	5.1-7	4.6-6	185	1715	-3.1-4	3.5-13	1.0-6	1.8-6	817	2322

Comparison on electronic structure calculation

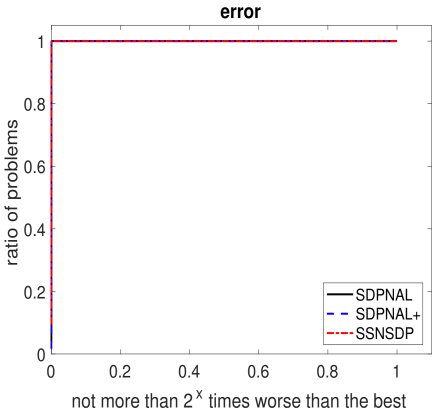


(a) $\max(\eta_p, \eta_d, \eta_g)$

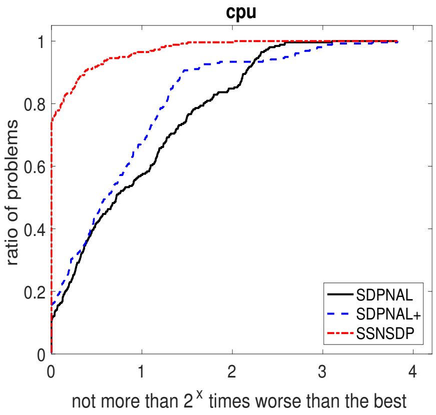


(b) η_d

Comparison on electronic structure calculation



(c) error



(d) cpu time

Comparison on electronic structure calculation

success: $\max\{\eta_p, \eta_d\} \leq 10^{-6}$

case	SSNSDP		SDPNAL		SDPNAL+	
	number	percentage	number	percentage	number	percentage
success	276	100%	53	19.2%	265	96%
fastest	205	74.3%	30	10.9%	41	14.9%
fastest under success	232	84.1%	3	1.09%	41	14.9%
not slower 1.2 times	236	85.5%	71	25.7%	87	31.5%
not slower 1.2 times under success	251	90.9%	5	1.81%	87	31.5%

Figure: Comparison between SDPNAL, SDPNAL+ and SSNSDP

Linear Programming

- The classic linear programming problem

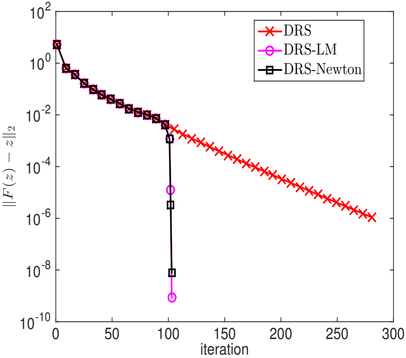
$$\min_{x\in\mathbb{R}^n} \quad c^T x, \text{ s.t.} \quad Ax = b,\ x \geq 0.$$

- Let $f(x) = c^T x + 1_K(x)$ where $K := \{x \mid x \geq 0\}$.
- Every element of the generalized Jacobian $\partial\mathcal{P}_K$ at $(2D-I)z+\beta$ is a diagonal matrix with diagonal entries

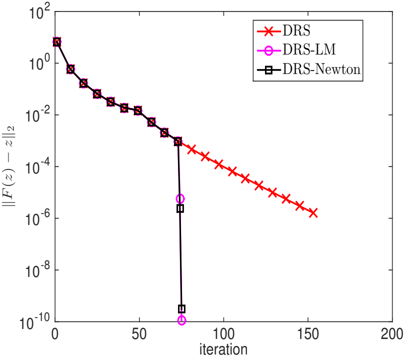
$$M_{ii}(z) \begin{cases} = 1, & ((2D-I)z+\beta)_i > 0, \\ = 0, & ((2D-I)z+\beta)_i < 0, \\ \in [0,1], & ((2D-I)z+\beta)_i = 0. \end{cases}$$

- Choose $M(z)$ such that $M_{ii}(z) = 1$ when $((2D-I)z+\beta)_i = 0$.
- we have

$$\begin{cases} \Psi_{ii}(z) = 0, \quad \Phi_{ii}(z) = 1, & ((2D-I)z+\beta)_i \geq 0, \\ \Psi_{ii}(z) = -1, \quad \Phi_{ii}(z) = -1, & ((2D-I)z+\beta)_i < 0. \end{cases}$$



(a) $m = 300$



(b) $m = 400$

Figure: residual history of the LP problem on $n = 1000$