

New Horizon of Mathematical Sciences
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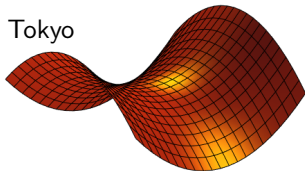
AUGMENTED LAGRANGIAN METHODS FOR CONVEX OPTIMIZATION

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Optimization Problems: Types and Algorithms¹

■ Types of Optimization

- Linear Programming
- Quadratic Programming
- Semidefinite Programming
- MPEC
- Nonlinear Least Squares
- Nonlinear Equations
- **Nondifferentiable Optimization**
- Global Optimization
- Derivative-Free Optimization
- Network Optimization

■ Algorithms

- Line Search
- Trust-Region
- (Nonlinear) Conjugate Gradient
- (Quasi-)Newton
- Truncated Newton
- Gauss Newton
- Levenberg-Marquardt
- Homotopy
- Gradient Projection
- Simplex Method
- Interior Point Methods
- Active Set Methods
- Primal-Dual Active Set Methods
- **Augmented Lagrangian Methods**
- Reduced Gradient
- Sequential Quadratic Programming

¹neos Optimization Guide: <http://www.neos-guide.org>

Problem and Objective

- Problem: A class of nonsmooth convex optimization

$$\min_x f(x) + \phi(Ex) \quad (1)$$

- X, H : real Hilbert spaces
- $f: X \rightarrow \mathbb{R}$: differentiable, $\nabla^2 f(x) \succeq mI$
- $\phi: H \rightarrow \mathbb{R}$: convex, nonsmooth(nondifferentiable)
- $E: X \rightarrow H$: linear

- ★ Optimality system

$$0 \in \nabla_x f(x) + E^\top \partial\phi(Ex) \quad (2)$$

- Objective: To develop Newton (-like) methods

- Applicable to a wide range of applications
- Fast and accurate
- Easy to implement

- Tool: **Augmented Lagrangian in the sense of Fortin.**

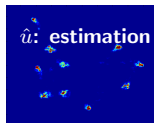
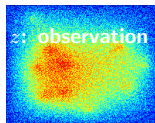
Motivating Examples (1/4)

■ Optimal control problem

$$\begin{aligned} \min \quad & \frac{1}{2} \int_0^T x(t)^\top Q x(t) + u(t)^\top R u(t) \, dt \\ \text{s.t.} \quad & \dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x_0 \\ & \|u(t)\| \leq 1. \end{aligned}$$

■ Inverse source problem

$$\begin{aligned} (\hat{y}, \hat{u}) = \arg \min_{(y,u) \in H_0^1(\Omega) \times L^2(\Omega)} \quad & (1/2)\|y - z\|_{L^2}^2 + (\alpha/2)\|u\|_{L^2}^2 + \beta\|u\|_{L^1} \\ \text{s.t.} \quad & -\Delta y = u \quad \text{on } \Omega, \\ & y = 0 \quad \text{on } \partial\Omega \end{aligned}$$



Motivating Examples (2)

- lasso (least absolute shrinkage and selection operator) [R.Tibshinari, 96]

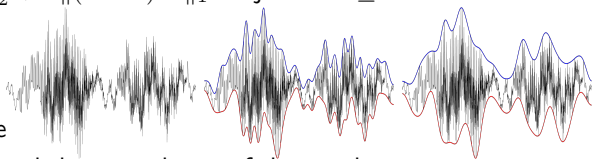
$$\min_{\beta \in \mathbb{R}^p} \|X\beta - y\|_2^2 \text{ subject to } \|\beta\|_1 \leq t. \quad \left(\min_{\beta \in \mathbb{R}^p} \|X\beta - y\|_2^2 + \lambda \|\beta\|_1 \right)$$

- $X = [\mathbf{x}^1, \dots, \mathbf{x}^N]^\top$
- $\mathbf{x}^i = (x_{i1}, \dots, x_{ip})^\top$: the predictor variables, $i = 1, 2, \dots, N$
- y_i : the responses, $i = 1, 2, \dots, N$

- envelope construction

$$\hat{x} = \arg \min_{x \in \mathbb{R}^n} \frac{1}{2} \|x - s\|_2^2 + \alpha \|(D^\top D)^2 x\|_1 \text{ subject to } s \leq x.$$

- s : noisy signal
- D : finite difference
- $\|(D^\top D)^2 x\|_1$: control the smoothness of the envelope x .



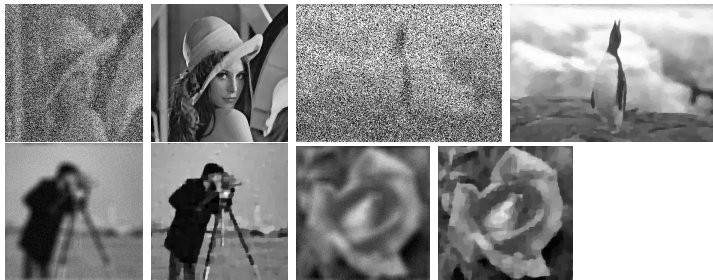
Motivating Examples (3/4)

■ total variation image reconstruction

$$\min \frac{1}{p} \|Kx - y\|_{L^p} + \alpha |x|_{TV} + \beta/2 \|x\|_{H^1}^2$$

for $p = 1$ or $p = 2$. K : blurring kernel.

$$|x|_{TV} = \sum_{i,j} \sqrt{([D_1x]_{i,j})^2 + ([D_2x]_{i,j})^2}$$



Motivating Examples (4/4)

- Quadratic programming

$$\min_x \frac{1}{2}(x, Ax) - (a, x) \quad \text{s.t.} \quad Ex = b, \quad Gx \geq g.$$

- Group LASSO

$$\min_{\beta} \frac{1}{2} \|X\beta - y\|^2 + \alpha \|\beta\|_G,$$

e.g. $G = \{\{1, 2\}, \{3, 4, 5\}\}$, $\|\beta\|_G = \sqrt{\beta_1^2 + \beta_2^2} + \sqrt{\beta_3^2 + \beta_4^2 + \beta_5^2}$.

- SVM
- ...

1. Augmented Lagrangian
2. Newton Methods
3. Numerical Test

Augmented Lagrangian

Method of multipliers for equality constraint

- equality constrained optimization problem

$$(P) \quad \min_x f(x) \text{ subject to } g(x) = 0$$

where $f: \mathbb{R}^n \rightarrow \mathbb{R}$ and $g: \mathbb{R}^n \rightarrow \mathbb{R}^m$ are differentiable.

- augmented Lagrangian (Hestenes, Powell 69), $c > 0$

$$\begin{aligned} L_c(x, \lambda) &= f(x) + \lambda^\top g(x) + (c/2) \|g(x)\|_{\mathbb{R}^m}^2 \\ &= f(x) + (c/2) \|g(x) + \lambda/c\|_{\mathbb{R}^m}^2 - 1/(2c) \|\lambda\|_{\mathbb{R}^m}^2. \end{aligned}$$

- method of multiplier¹

$$\lambda_{k+1} = \lambda_k + c[\nabla_\lambda d_c](\lambda_k).$$

- ★ method of multiplier is composed of two steps:

$$x^k = \arg \min_x L_c(x, \lambda^k)$$

$$\lambda_{k+1} = \lambda_k + c \nabla_\lambda L_c(x^k, \lambda^k) = \lambda_k + c g(x^k)$$

¹**def.:** $d_c(\lambda) := \min_x L_c(x, \lambda)$. **fact:** $\nabla d_c(\lambda) = [\nabla_\lambda L_c](x(\lambda), \lambda) = g(x(\lambda))$

A brief history of augmented Lagrangian methods (1/2)

■ equality constrained optimization

$$\begin{array}{ll}\min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & h(x) = 0\end{array}$$

- 1969 Hestenes[7], Powell[14]

■ inequality constrained optimization

$$\begin{array}{ll}\min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & g(x) \leq 0\end{array}$$

- 1973 Rockafellar[15, 16]

■ equality and inequality constrained optimization ■ nonsmooth convex optimization

$$\begin{array}{ll}\min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & h(x) = 0 \\ & g(x) \leq 0\end{array}$$

- 1982 Berstekas[2]

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

- 1975 Glowinski-Marroco[6]
- 1975 Fortin[4]
- 1976 Gabay-Mercier[5]
- 2000 Ito-Kunisch[9]
- 2009 Tomioka-Sugiyama[18]

A brief history of augmented Lagrangian methods (2/2)

■ Augmented Lagrangian Methods (Method of Multipliers)

year	authors	problem	algorithm
1969	Hestenes[7], Powell[14]	equality constraint	ALG1
1973	Rockafellar[15, 16]	inequality constraint	
1975	Glowinski-Marroco[6]	nonsmooth convex (FEM)	
1975	Fortin[4]	nonsmooth convex (FEM)	
1976	Gabay-Mercier[5]	nonsmooth convex (FEM)	ADMM ¹
1982	Berstekas[2]	equality and inequality constraints	
2000	Ito-Kunisch[9]	nonsmooth convex (PDE Opt.)	
2009	Tomioka-Sugiyama[18]	nonsmooth convex (Machine Learning)	DAL ²
2013	Patrinos-Bemporad [12]	convex composite	Proximal Newton FBN ³
2014	Patrinos-Stella -Bemporad[13]	(Optimal Control)	

¹Alternating Direction Method of Multipliers

²Dual-augmented Lagrangian method

³Forward-Backward-Newton

Augmented Lagrangian Methods [Glowinski+,75]

- nonsmooth convex optimization problem

$$\min_{x,v} f(x) + \phi(v), \quad \text{subject to} \quad v = Ex.$$

- augmented Lagrangian

$$L_c(x, v, \lambda) = f(x) + \phi(v) + (\lambda, Ex - v) + (c/2)\|Ex - v\|_{\mathbb{R}^m}^2$$

- dual function

$$d_c(\lambda) := \min_{x,v} L_c(x, v, \lambda)$$

- method of multipliers (ALG1)

$$\lambda_{k+1} = \lambda_k + c \nabla_{\lambda} d_c(\lambda_k).$$

- ★ method of multiplier is composed of two steps:

$$\begin{array}{ll} \text{step 1} & (x_{k+1}, v_{k+1}) = \arg \min_{x,v} L_c(x, v, \lambda_k) \\ \text{step 2} & \lambda_{k+1} = \lambda_k + c(Ex_{k+1} - v_{k+1}) \end{array}$$

Fact (gradient): $\nabla_{\lambda} d_c(\lambda) = [\nabla_{\lambda} L_c](x(\lambda), v(\lambda), \lambda)$

Augmented Lagrangian Methods [Gabay+,76]

- nonsmooth convex optimization problem

$$\min_{x,v} f(x) + \phi(v), \quad \text{subject to} \quad v = Ex.$$

- augmented Lagrangian

$$L_c(x, v, \lambda) = f(x) + \phi(v) + (\lambda, Ex - v) + (c/2)\|Ex - v\|_{\mathbb{R}^m}^2$$

- ADMM, alternating direction method of multiplier

$$\begin{aligned} \text{step 1} \quad x_{k+1} &= \arg \min_x L_c(x, v_k, \lambda_k) \\ \text{step 2} \quad v_{k+1} &= \arg \min_v L_c(x_{k+1}, v, \lambda_k) = \text{prox}_{\phi/c}(Ex_{k+1} + \lambda_k/c) \\ \text{step 3} \quad \lambda_{k+1} &= \lambda_k + c(Ex_{k+1} - v_{k+1}) \end{aligned}$$

Assumption: $\text{prox}_{\phi/c}(z) := \arg \min_v (\phi(v) + c/2\|v - z\|^2)$ has a closed-form representation (explicitly computable).

Augmented Lagrangian Methods [Fortin,75]

- nonsmooth convex optimization problem

$$\min_x f(x) + \phi(Ex)$$

- (Fortin's) augmented Lagrangian

$$L_c(x, \lambda) = \min_v L_c(x, v, \lambda) = f(x) + \phi_c(Ex + \lambda/c) - 1/(2c) \|\lambda\|_{\mathbb{R}^m}^2$$

where $\phi_c(z)$ is Moreau's envelope

- method of multiplier

$$\lambda_{k+1} = \lambda_k + c \nabla_{\lambda} d_c(\lambda_k)$$

def.(dual function):

$$d_c(\lambda) := \min_x L_c(x, \lambda).$$

- ★ method of multiplier is composed of two steps:

fact (gradient):

$$\nabla_{\lambda} d_c(\lambda) = [\nabla_{\lambda} L_c](x(\lambda), \lambda)$$

$$x_k = \arg \min_x L_c(x, \lambda_k)$$

$$\lambda_{k+1} = \lambda_k + c[Ex^k - \text{prox}_{\phi/c}(Ex^k + \lambda^k/c)]$$

Assumption: $\text{prox}_{\phi/c}(z) := \arg \min_v (\phi(v) + c/2 \|v - z\|^2)$ has a closed-form representation (explicitly computable).

- augmented Lagrangian for ALG1[Glowinski+,75], ADMM[Gabay+,76]

$$L_c(x, v, \lambda) = f(x) + \phi(v) + (\lambda, Ex - v) + (c/2)\|Ex - v\|_{\mathbb{R}^m}^2$$

- (Fortin's) augmented Lagrangian for ALM[Fortin,75]

$$\begin{aligned} L_c(x, \lambda) &= \min_v L_c(x, v, \lambda) \\ &= f(x) + \phi_c(Ex + \lambda/c) - 1/(2c)\|\lambda\|_{\mathbb{R}^m}^2 \end{aligned}$$

- Fortin's Augmented Lagrangian method has been ignored in the subsequent literature.
- The method was re-discovered by [Ito-Kunisch,2000] and by [Tomioka-Sugiyama,2009].

Moreau's envelope, proximal operator (1/3)

- Moreau's envelope (Moreau-Yosida regularization) of a closed proper convex function ϕ

$$\phi_c(z) := \min_v (\phi(v) + c/2 \|v - z\|^2)$$

- The proximal operator $\text{prox}_\phi(z)$ is defined by

$$\text{prox}_\phi(z) := \arg \min_v (\phi(v) + 1/2 \|v - z\|^2)$$

$$\begin{aligned} \text{prox}_{\phi/c}(z) &= \arg \min_v (\phi(v) + c/2 \|v - z\|^2) \\ &= \arg \min_v (\phi(v)/c + 1/2 \|v - z\|^2) \end{aligned}$$

- Moreau's envelope is expressed in terms of the proximal operator

$$\phi_c(z) = \phi(\text{prox}_{\phi/c}(z)) + c/2 \|\text{prox}_{\phi/c}(z) - z\|^2$$

Moreau's envelope, proximal operator (2/3)

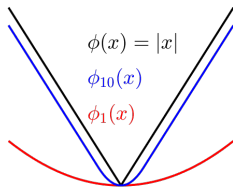
• ℓ_1 norm

$$\phi(x) = \|x\|_1, \quad x \in \mathbb{R}^n$$

$$\text{prox}_\phi(x)_i = \max(0, |x_i| - 1) \text{sign}(x_i),$$

$$G \in \partial_B(\text{prox}_\phi)(x)$$

$$G_{ii} = \begin{cases} 1 & |x_i| > 1, \\ 0 & |x_i| < 1, \\ \in \{0, 1\} & |x_i| = 1 \end{cases}$$



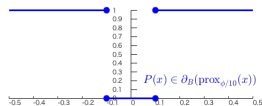
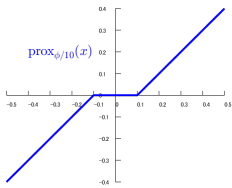
• Euclidean norm

$$\phi(x) = \|x\|, \quad x \in \mathbb{R}^n$$

$$\text{prox}_\phi(x) = \max(0, \|x\| - 1) \frac{x}{\|x\|},$$

$$\partial_B(\text{prox}_\phi)(x) =$$

$$\begin{cases} I - \frac{1}{\|x\|} (I - \frac{xx^\top}{\|x\|^2}) & \|x\| > 1, \\ 0 & \|x\| < 1, \\ \{0, I - \frac{1}{\|x\|} (I - \frac{xx^\top}{\|x\|^2})\} & \|x\| = 1 \end{cases}$$



Moreau's envelope, proximal operator (3/3)

■ Properties¹

- $\phi_c(z) \leq \phi(z)$, $\lim_{c \rightarrow \infty} \phi_c(z) = \phi(z)$

- $\phi_c(z) + (\phi^*)_{1/c}(cz) = (c/2)\|z\|^2$

def.(convex conjugate):

$$\phi^*(x^*) := \sup_x (\langle x^*, x \rangle - \phi(x)).$$

- $\nabla_z \phi_c(z) = c(z - \text{prox}_{\phi/c}(z))$

- $\|\text{prox}_{\phi/c}(z) - \text{prox}_{\phi/c}(w)\|^2 \leq (\text{prox}_{\phi/c}(z) - \text{prox}_{\phi/c}(w), z - w)$

- $\text{prox}_{\phi/c}(z) + (1/c)\text{prox}_{c\phi^*}(cz) = z$

- $\text{prox}_{\phi/c}$ is globally Lipschitz, almost everywhere differentiable

- $P \in \partial_B(\text{prox}_{\phi/c})(x)$ is a symmetric positive semidefinite that satisfies $\|P\| \leq 1$.

- $\partial_B(\text{prox}_{c\phi^*})(x) = \{I - P : P \in \partial_B(\text{prox}_{\phi/c})(x/c)\}$

¹[17, Bauschke+11],[13, Partrions+14]

Differentiability, Optimality condition

■ Fortin's augmented Lagrangian

$$L_c(x, \lambda) = f(x) + \phi_c(Ex + \lambda/c) - 1/(2c)\|\lambda\|_{\mathbb{R}^m}^2$$

■ Fortin's augmented Lagrangian L_c is convex and continuously differentiable with respect to x , and is concave and continuously differentiable with respect to λ .

$$\nabla_x L_c(x, \lambda) = \nabla_x f(x) + cE^\top (Ex + \lambda/c - \text{prox}_{\phi/c}(Ex + \lambda/c)),$$

$$\nabla_\lambda L_c(x, \lambda) = Ex - \text{prox}_{\phi/c}(Ex + \lambda/c).$$

■ The following conditions on a pair (x^*, λ^*) are equivalent.

- (a) $\nabla_x f(x^*) + E^\top \lambda^* = 0$ and $\lambda^* \in \partial\phi(Ex^*)$.
- (b) $\nabla_x f(x^*) + E^\top \lambda^* = 0$ and $Ex^* - \text{prox}_{\phi/c}(Ex^* + \lambda^*/c) = 0$.
- (c) $\nabla_x L_c(x^*, \lambda^*) = 0$ and $\nabla_\lambda L_c(x^*, \lambda^*) = 0$.
- (d) $L_c(x^*, \lambda) \leq L_c(x^*, \lambda^*) \leq L_c(x, \lambda^*), \quad \forall x \in X, \forall \lambda \in H$.

■ If there exists a pair (x^*, λ^*) that satisfies (d), then x^* is the minimizer of (1).

Newton Methods

Newton methods

■ Problem

$$\min_x f(x) + \phi(Ex)$$

■ Approaches

(1-1) Lagrange-Newton: Solve the optimality system by Newton method

$$\nabla_x L_c(x, \lambda) = 0 \quad \text{and} \quad \nabla_\lambda L_c(x, \lambda) = 0$$

(1-2) A special case ($E = I$). Solve the optimality system by Newton method

$$x = \text{prox}_{\phi/c}(x - \nabla_x f(x)/c)$$

(2) Apply Newton method to Fortin's augmented Lagrangian method

step 1 Solve for x_k : $\nabla_x L_c(x_k, \lambda_k) = 0$

step 2 $\lambda_{k+1} = \lambda_k + c(Ex_k - \text{prox}_{\phi/c_k}(Ex_k + \lambda_k/c))$.

★ For fixed λ_k

$$x_k = \arg \min_x L_c(x, \lambda_k) \quad \Longleftrightarrow \quad \nabla_x L_c(x_k, \lambda_k) = 0.$$

Lagrange-Newton method

- Lagrange-Newton method: Solve the optimality system by Newton method¹

$$\nabla_x L_c(x, \lambda) = 0 \quad \text{and} \quad \nabla_\lambda L_c(x, \lambda) = 0$$

- Newton system:

$$\left[\begin{array}{c|c} \nabla_x^2 f(x) + cE^\top(I - G)E & ((I - G)E)^\top \\ \hline (I - G)E & -c^{-1}G \end{array} \right] \begin{bmatrix} d_x \\ d_\lambda \end{bmatrix} = - \begin{bmatrix} \nabla_x L_c(x, \lambda) \\ \nabla_\lambda L_c(x, \lambda) \end{bmatrix}$$

where $G \in \partial(\text{prox}_{\phi/c})(Ex + \lambda/c)$

- or equivalently

$$\left[\begin{array}{c|c} \nabla_x^2 f(x) & E^\top \\ \hline (I - G)E & -c^{-1}G \end{array} \right] \begin{bmatrix} x^+ \\ \lambda^+ \end{bmatrix} = \begin{bmatrix} \nabla_x^2 f(x)x - \nabla_x f(x) \\ \text{prox}_{\phi/c}(z) - Gz \end{bmatrix}$$

where $z = Ex + \lambda/c$. $d_x = x^+ - x$, $d_\lambda = \lambda^+ - \lambda$.

¹When E is not surjective, the Newton system becomes inconsistent, i.e., there may be no solution to the Newton system. In this case, a proximal algorithm is employed to guarantee the solvability of the Newton system

Newton method for composite convex problem

■ Problem

$$\min_x f(x) + \phi(x)$$

■ Apply Newton method to the optimality condition

$$\begin{aligned}\nabla_x f(x) + \lambda &= 0, \quad x - \text{prox}_{\phi/c}(x + \lambda/c) = 0 \\ \iff x - \text{prox}_{\phi/c}(x - \nabla_x f(x)/c) &= 0\end{aligned}$$

■ Define $F_c(x) = L_c(x, -\nabla_x f(x))$.

■ Algorithm

step 1: $G \in \partial(\text{prox}_{\phi/c})(x - \nabla_x f(x)/c)$.

step 2: $(I - G(I - c^{-1}D^2 f(x)))d = -(x - \text{prox}_{\phi/c}(x - \nabla_x f(x)/c))$.

step 3: Armijo's rule: Find the smallest nonnegative integer j such that

$$\begin{aligned}F_c(x + 2^{-j}d) &\leq F_c(x) + \mu 2^{-j} \langle \nabla_x F_c(x), d \rangle \quad (0 < \mu < 1) \\ x^+ &= x + 2^{-j}d\end{aligned}$$

★ step 2: a variable metric gradient method on $F_c(x)$:

$$c(I - c^{-1}\nabla_x^2 f(x))(I - G(I - c^{-1}\nabla_x^2 f(x)))d = -\nabla_x F_c(x).$$

■ The algorithm is proposed in [12, Patrinos-Bemporad].

Newton method applied to the primal update

- Apply Newton method to solve the nonlinear equation arising from Fortin's augmented Lagrangian method

$$\text{step 1} \quad \nabla_x L_{c_k}(x, \lambda_k) = 0$$

$$\text{step 2} \quad \lambda_{k+1} = \lambda_k + c_k(Ex_k - \text{prox}_{\phi/c_k}(Ex_k + \lambda_k/c)).$$

- Newton system

$$(\nabla_x^2 f(x) + cE^\top(I - G)E)d_x = -\nabla_x L_{c_k}(x, \lambda)$$

Numerical Test

- ℓ^1 least square problems

$$\min_x \frac{1}{2} \|Ax - y\|^2 + \gamma \|x\|_1.$$

- The data set (A, y, x_0) : L1-Testset (mat files) available at <http://wwwopt.mathematik.tu-darmstadt.de/spear/>
- Used 200 datasets. (dimension of $x : 1,024 \sim 49,152$).
- Windows surface pro 3, Intel i5 / 8GB RAM.
- Comparison:
MOSEK (free academic license available at <https://mosek.com/>)
MOSEK is a software package for solving large scale sparse problems.
Algorithm: the interior-point method.
- $c = 0.99/\sigma_{\max}(A^T A)$.
- $\gamma = 0.01 \|A^T y\|_{\infty}$.
- Compute until $\sqrt{\|\nabla_x L_c(x^k, \lambda^k)\|^2 + \|\nabla_{\lambda} L_c(x^k, \lambda^k)\|^2} < 10^{-12}$ is met.

Newton method for ℓ^1 regularized L.S.

■ Newton system:

$$\begin{bmatrix} A^\top A & I \\ I - G & -cG \end{bmatrix} \begin{bmatrix} d_x \\ d_\lambda \end{bmatrix} = - \begin{bmatrix} A^\top (Ax - y) \\ x - \text{prox}_{\phi/c}(x + c\lambda) \end{bmatrix}$$

where $G = \partial(\text{prox}_{\phi/c})(x + c\lambda)$:

$$G_{ii} = 0 \quad \text{for } i \in \mathbf{o} := \{j \mid |x_j + c\lambda_j| \leq \gamma c, j = 1, 2, \dots, n\}$$

$$G_{ii} = 1 \quad \text{for } i \in \mathbf{o}^c = \{j \mid |x_j + c\lambda_j| > \gamma c, j = 1, 2, \dots, n\}$$

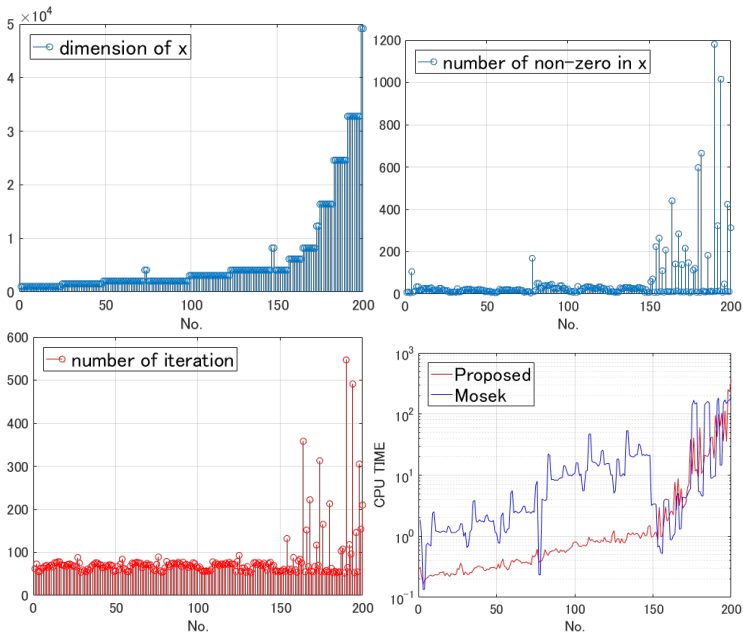
■ Simply the system.

$$d_x(\mathbf{o}) = -x(\mathbf{o})$$

$$\begin{aligned} A(:, \mathbf{o}^c)^\top A(:, \mathbf{o}^c) d_x(\mathbf{o}^c) = & - [\gamma \text{sign}(x(\mathbf{o}^c) + c\lambda(\mathbf{o}^c)) \\ & + A(:, \mathbf{o}^c)^\top (A(:, \mathbf{o}^c)x(\mathbf{o}^c) - y)] \end{aligned}$$

$$d_\lambda = -A^\top A(x + d_x) + A^\top y.$$

Results



QUESTIONS ?
COMMENTS ?
SUGGESTIONS ?

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