Convex–Composite Optimization

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Jim Burke

Collaborators

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Convex-Composite Optimization

$$\mathbf{P} \qquad \min_{x \in \mathbb{R}^n} f(x) := h(c(x)) + \ g(x)$$

$h : \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ is closed, proper, convex
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In general, these problems are **neither convex nor smooth**.

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Note that g can be absorbed into h.

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$$\tilde{h}(y,x) := h(y) + g(x) \quad \text{and} \quad \tilde{c}(x) \quad := (c(x), x),$$

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For simplicity, we usually take $g \equiv 0$.

But in the context of algorithmic implementations, it is often essential to treat g explicitly.

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1805 The Gauss-Newton method : $\min_x \frac{1}{2}\|c(x)\|_2^2$
Legendre 1805, Gauss 1809 (1795?)

Gauss, in 1809 at the age of 24, used the method to track the newly discovered asteroid Ceres. He also advanced Legendre's work by establishing connections to probability and statistics using the normal distribution.

Gauss also claimed to have been using the method for celestial computations since 1795 at the age of 10.

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70's
Anderson, Osborne, Watson: *Algorithms for nonlinear approximation*

80-90's
B., Conn, Ferris, **Fletcher**, Kawasaki, Masden, Poliquin, **Powell**, Osborne, Rockafellar, Womersley, Wright, Yuan

Recent (15-)
Aravkin, Bell, B., Chang, Cui, Duchi, Davis, Drusvyatskiy, Engle, Hoheisel, Hong, Lewis, Ioffe, Mohammadi, Mordukhovich, Pang, Paquette, Royset, Ruan, Sarabi, Zheng ...

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Non-linear least-squares: $f(x) = \|c(x)\|_2^2$

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where $C \subset \mathbb{R}^m$ is closed, convex (e.g., $C = \{0\}^p \times \mathbb{R}^q_-$), and $\operatorname{dist}(y \,|\, C) := \inf \{\|y - z\| \mid z \in C\}$.

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Non-linear programming (NLP): $\min \varphi(x) + \delta_C(\hat{c}(x))$.
Here $c(x) := (\varphi(x), \hat{c}(x))$ and $h(\mu, y) := \mu + \delta_C(y)$, where

$$\delta_C(y) = \begin{cases} 0, & y \in C, \\ +\infty, & \text{else.} \end{cases}$$

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Additive composite problems: $f(x) = \psi(x) + g(x)$ with $\psi \in \mathcal{C}^1$

Examples

Robust Phase Retrieval:

$$\min_x \frac{1}{m} \sum_{i=1}^{m} |\langle a_i, x \rangle^2 - b_i^2|$$

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Sparse Dictionary Learning:

$$\min_{D \in \mathbb{R}^{d \times n}, r_i \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \|x_i - D r_i\|_2 + \lambda \|r_i\|_1 \qquad \text{subject to} \quad \|D_i\| \leq 1$$

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Sparse/Robust Estimation and Kalman Smoothing:

$$\min_x V(k(x, z)) + W(q(x)),$$

where V and W are convex piecewise linear-quadratic penalties:

$$\rho(y) = \sup_{u \in U} \left\{ \langle u, b + By \rangle - \frac{1}{2} y^T M y \right\}.$$

ℓ_1, least-squares, elastic net, Vapnik Huber, ...

Rockafellar '88

Outline

1. First-Order Properties: directional derivatives and subgradient
2. The Convex-Composite Lagrangian
3. Second-Order Properties
4. Exact Penalization
5. Convexity of Convex-Composite Functions
6. Algorithms
   i. Sharpness
   ii. Newton's Method
   iii. Globalization
   iv. Complexity
   v. Stochastic Prox-Linear
7. Feature Selection for Mixed Effects Models

First-Order Properties

$$\mathbf{P} \qquad \min_{x\in\mathbb{R}^n} f(x) := h(c(x))$$

Standard first-order necessary conditions for optimality in **P** are

$$f'(x;d) \geq 0 \quad \forall\, d \in \mathbb{R}^n,$$

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Does the directional derivative exists?

We begin by assuming that h is finite valued.
Convexity implies that h is locally Lipschitz continuous, i.e.

$$\forall\, \bar{u} \quad \exists\, L > 0 \ : \ |h(u) - h(v)| \leq L\|u - v\| \quad \forall\, u, v \text{ near } \bar{u}.$$

The Directional Derivative $f'(x;d)$

$$|h(c(x)) - h(c(\overline{x}) + c'(\overline{x})(x - \overline{x}))| \le L|c(x) - [c(\overline{x}) + c'(\overline{x})(x - \overline{x})]| = o(\|x - \overline{x}\|)$$

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$$\begin{aligned} f'(x;d) = (h \circ c)'(x;d) &= \lim_{t \downarrow 0} \frac{h(c(x + td)) - h(c(x))}{t} \\ &= \lim_{t \downarrow 0} \frac{h(c(x) + tc'(x)d) - h(c(x))}{t} \\ &= h'(c(x); c'(x)d). \end{aligned}$$

The Subdifferential $\partial f(x)$

Recall that for a convex function φ, we have

$$\varphi'(y;v) = \sup\{\langle z, v\rangle \mid z \in \partial\varphi(y)\},$$

whenever $\partial\varphi(\overline{y}) \neq \emptyset$, where

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$$\nexists\, \tilde{x} \quad s.t. \quad c(\overline{x}) + c'(\overline{x})(\tilde{x} - \overline{x}) \in \mathrm{ri}\,(\mathrm{dom}\,(h))\,.$$

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A constraint qualification is employed to address this deficiency.

The Basic Constraint Qualification

Basic Constraint Qualification (BCQ) (Rockafellar '85):

$$\ker\left(c'(x)^T\right) \cap N\left(c(x)\,|\,\mathrm{dom}\,(h)\right) = \{0\}$$

where

$$N\left(\overline{y}\,|\,C\right) := \partial\delta_C(\overline{y}) = \{z \mid \langle z, y - \overline{y}\rangle \leq 0 \;\forall\, y \in C\}$$

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• If $f = h \circ c$ satisfies the BCQ at $x \in \mathrm{dom}\,(f)$, then f is *subdifferentially regular* at x with

$$\partial f(x) = c'(x)^T \partial h(c(x)) \quad \text{and}$$
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- $f = h \circ c$ satisfies the BCQ at $x \in \mathrm{dom}\,(f)$ if and only if

$$\left\{ y \in \partial h(c(x)) \;\middle|\; v = c'(x)^T y \right\} \text{ is compact } \forall\, v \in \partial f(x).$$

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$$N\left(\overline{y} \,|\, C\right) := \partial\delta_C(\overline{y}) = \{z \mid \langle z, y - \overline{y}\rangle \leq 0 \ \forall\, y \in C\}$$

is the normal cone to the convex set C at $\overline{y} \in C$.

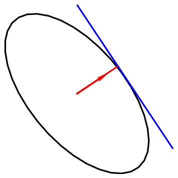
- $f = h \circ c$ satisfies the BCQ at $x \in \mathrm{dom}\,(f)$ if and only if

$$\left\{ y \in \partial h(c(x)) \,\middle|\, v = c'(x)^T y \right\} \text{ is compact } \forall\, v \in \partial f(x).$$

In the case of NLP, the BCQ is precisely the Mangasarian-Fromovitz constraint qualification (MFCQ).

Interlude: Support Functions and Conjugacy

$\sigma_S(z) := \sup_{x \in S} \langle z, x \rangle$



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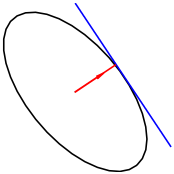

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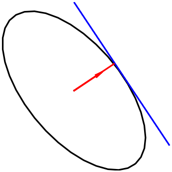

$$\sigma_S = \sigma_{\overline{\text{conv}}(S)}$$

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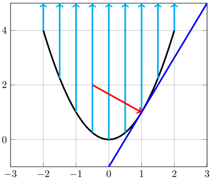

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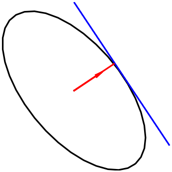

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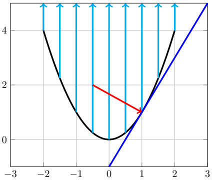

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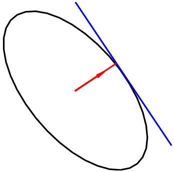

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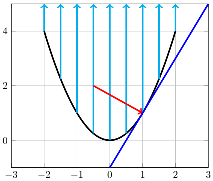

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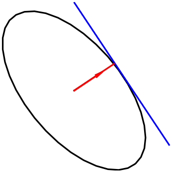

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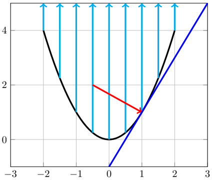

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Bi-conjugacy: If there exists x such that $-\infty < \varphi(x) < +\infty$, then

$$\mathrm{epi}\left(\varphi^{**}\right) = \overline{\mathrm{conv}}\,(\mathrm{epi}\,(\varphi)) \quad \text{so} \quad \varphi(x) \geq \varphi^{**}(x)\ \forall\, x.$$

If, in addition, $\mathrm{epi}\,(\varphi)$ is closed and convex, then $\varphi(x) = \varphi^{**}(x)$.

The Convex-Composite Lagrangian

$$\mathbf{P} \qquad \min_{x\in\mathbb{R}^n} h(c(x))$$

- The Lagrangian for $\mathbf{P}$:

$$L(x, y \quad) := \langle y, c(x)\rangle - h^*(y)$$

The Convex-Composite Lagrangian

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- First-Order Optimality Conditions:

$$\overline{x} \in \operatorname{argmin}_x f \;\implies\; 0 \in \partial f(\overline{x}) \iff \begin{pmatrix} 0 \\ 0 \end{pmatrix} \in \begin{pmatrix} \partial_x L(\overline{x},\overline{y}) \\ \partial_y(-L)(\overline{x},\overline{y}) \end{pmatrix}$$

In the case of NLP, the Lagrangian optimality conditions are precisely the KKT conditions.

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Rockafellar ('23) has recently introduced a notion of augmented Lagrangians for convex-composite functions and proposed an associated AL method.

Second-Order Optimality Conditions

Theorem: (B.-Poliquin '92) (Necessity) *If* $\overline{x}$ *is a local solution to* $\min_x f(x)$ *at which the BCQ is satisfied, then*

$$h''(c(\overline{x});\, c'(\overline{x})d) + \max_{y \in M(\overline{x})} d^T \nabla^2_{xx} L(\overline{x}, y) d \ \geq \ 0$$

for all $d \in \mathbb{R}^n$ *such that* $df(\overline{x})(d) \leq 0$ *where*

$$h''(c(\overline{x});\, c'(\overline{x})d) := \liminf_{u \to d,\, t \downarrow 0} \frac{h(c(\overline{x}) + tc'(\overline{x})u) - f(\overline{x}) - tdf(\overline{x})(d)}{\frac{1}{2}t^2}$$

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Example:

$$h \in \mathcal{C}^2 \implies \nabla^2 f(x) = c'(x)^T \nabla^2 h(c(x)) c'(x) \;+\; \sum_{i=1}^{m} y_i \nabla^2 c_i(x),$$

where $y = \nabla h(c(x))$.

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Mohammadi and Sarabi '20 use Rockafellar's notion of *parabolic regularity* '85 and metric subregularity to give a new approach to the necessity theorem and extend the sufficiency theorem.

"Exactness" and the Pasch-Hausdorff Envelope

Pasch-Hausdorff Envelope:

$$h_\alpha(y) := \inf_w [h(w) + \alpha \|y - w\|]$$

h_α is finite-valued and globally α-Lipschitz.

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Example:

$h(y) := \delta_\Omega(y) \implies h_\alpha(y) := \alpha \inf_{w\in\Omega} \|y - w\| = \alpha \mathrm{dist}\,(y\,|\Omega\,)$.

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Exactness: Does $\operatorname{argmin} f \ = \ \operatorname{argmin} f_\alpha$?

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If $\overline{x}$ is a local solution to $\min_x f(x)$ at which c is locally Lipschitz and the BCQ is satisfied, then there is an $\bar{\alpha} > 0$ such that $\overline{x}$ is a local solution to $\min_x f_\alpha(x)$ with $f(\overline{x}) = f_\alpha(\overline{x})$ for all $\alpha > \bar{\alpha}$.

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NLP exact penalization as well as other exact penalization results for this class follow from this theorem since $(\delta_\Omega)_\alpha(x) = \alpha \mathrm{dist}\,(y \,|\Omega\,)$.

When is a convex-composite function convex?

Observe that

$$f(x) = h(c(x)) = h^{**}(c(x)) = \sup_y [\langle y, c(x) \rangle - h^*(y)].$$

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where $\mathrm{hzn}\,(h) := \{ z \mid h(x + \lambda z) \leq h(x)\ \forall x \in \mathrm{dom}\,(h),\ \lambda > 0 \}$.

Convex convex-composite functions

Theorem:(B.-Hoheisel-Nguyen '21)
If $c : \Omega \to \mathbb{R}^m$ *is convex wrt* $(-\mathrm{hzn}\,(h))$, *then* $f = h \circ c$ *is convex.*

If, in addition,

$$c(\mathrm{ri}\,(\Omega) \cap \mathrm{ri}\,(\mathrm{dom}\,(h)) \neq \emptyset,$$

then

$$(h \circ c)^*(p) = \min_{v \in \mathbb{R}^m} h^*(v) + \langle v, c(\cdot)\rangle^*(p)$$

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$$\partial(h \circ c)(\bar{x}) = \bigcup_{v \in \partial h(c(\bar{x}))} \partial\langle v, c(\cdot)\rangle(\bar{x}) \quad (\bar{x} \in \mathrm{dom}\,(h \circ c)).$$

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Borwein '74, Bot-Wanka-Grad-Hodrea '06-'10,
Combari-Lagdhir-Thibault '94, Pennanen '99

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Applications: conic programming, Kiefer-Gaffe-Krafft inequalities, matrix-fractional functions, variational Gram functions, spectral functions, generalized Farkas theorems, ...

Algorithms

$$\mathbf{P}_k \qquad \min_{\left\|x-x^k\right\|\leq\eta_k} h\left(c(x^k)+\nabla c(x^k)[x-x^k]\right)+\frac{1}{2}(x-x^k)^\top H_k(x-x^k),$$

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Algorithms

$$\mathbf{P}_k \qquad \min_{\left\| x - x^k \right\| \le \eta_k} h\left(c(x^k) + \nabla c(x^k)[x - x^k] \right) + \frac{1}{2}(x - x^k)^\top H_k (x - x^k),$$

- Newton-like method: $H_k \approx \nabla^2_{xx} L(x^k, y^k)$
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- $\mathbf{P}_k$ may or may not be convex depending on whether $H_k \succeq 0$.

Algorithm for NLP

NLP minimize $\phi(x)$

subject to $f_i(x) = 0,\ i = 1, \ldots, s,\ f_i(x) \leq 0,\ i = s+1, \ldots, m.$

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- Convex-Composite Framework

$$h(\mu, y) = \mu + \delta_K(y), \qquad K := \{0\}^s \times \mathbb{R}_-^{m-s}$$

$$c(x) = (\phi(x), \hat{c}(x))$$

$$L(x, y) = \phi(x) + \sum_{k=1}^{m} y_i \hat{c}_i(x) \; - \delta_{K^\circ}(y), \quad K^\circ = \mathbb{R}^s \times \mathbb{R}_+^{m-s}$$

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- Subproblems: Sequential quadratic programming (SQP)

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The Sharp Case

The set $C := \operatorname{argmin} h$ is said to be a set of *sharp minima* for h if

$$\exists\, \alpha > 0 \quad s.t. \quad h(c) \geq h_{\min} + \alpha \operatorname{dist}(c \,|\, C) \;\; \forall\, c \in \mathbb{R}^m.$$

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Li-Wang '02 use the same proof technique but slightly weaken the sharpness hypothsis.

Newton's Method in General: Hypotheses

Assume h is convex piecewise linear-quadratic (PLQ), i.e.,

$\mathrm{dom}\,(h) = \bigcup_{i=1}^{N} C_i$ with each C_i convex polyhedral, and

$h(z) = \frac{1}{2}\langle z, Q_k z\rangle + \langle b_k, z\rangle + \beta_k$ on C_i with $Q_k \in \mathbb{S}^m$.

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- second-order sufficiency.

In the case of NLP, these assumptions reduce the usual NLP assumptions.

Convergence of Newton's Method

Theorem: (B.-Engle '19) If (x^0, y^0) is sufficiently close to $(\overline{x}, \overline{y})$, then the Newton sequence $\{(x^k, y^k)\}$ satisfies

(i) $c(x^{k-1}) + \nabla c(x^{k-1})(x^k - x^{k-1}) \in$ active manifold (active constr. ID),

(ii) $y^k \in \mathrm{ri}\left(\partial h(c(x^{k-1}) + \nabla c(x^{k-1})(x^k - x^{k-1}))\right)$ (str. compl.),

(iii) $$\begin{array}{rl} y^k & \in \partial h(c(x^k) + c'(x^k)(x^k - x^{k-1}) \\ 0 & = \nabla c(x^{k-1})^\top y^k + \nabla^2_{xx} L(x^k, y^k)(x^k - x^{k-1}) \end{array}$$ (1st-order opt.),

(iv) x^{k+1} is a strong local minimizer of $\mathbf{P_k}$ (2nd order suff.),

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Proof uses Robinson's *generalized equations*, Rockafellar's PLQ 2^{nd}-order theory, metric subregularity, and Lewis' *partial smoothness* techniques.

Globalization and descent

$$\mathbf{P} \qquad \min_{x\in\mathbb{R}^n} f(x) := h(c(x)) + g(x),$$

where $h : \mathbb{R}^m \to \mathbb{R}$ convex, $g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ proper, convex, loc. Lipschitz relative to $\mathrm{dom}\,(g)$, and $c : \mathbb{R}^n \to \mathbb{R}^m$ is $\mathcal{C}^1$.

$$\mathbf{P}_k \qquad \min_{\|d\|\leq\eta_k} h(c(x^k) + \nabla c(x^k)d) + \frac{1}{2}d^T H_k d + g(x^k + d)$$

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Define

$$\Delta f(x; d) := h(c(x) + \nabla c(x)d) + \frac{1}{2}d^T H_k d + g(x + d) - f(x).$$

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Recall that

$$f'(x; d) = \lim_{t\downarrow 0} \tfrac{\Delta f(x;td)}{t} = \inf_{t>0} \tfrac{\Delta f(x;td)}{t}.$$

Backtracking, Weak Wolfe, Trust Regions

(B. –Engle '19)

Assume $f'(x;d) \leq \Delta f(x;d) \leq \tau \min_{\|d\| \leq \eta} \Delta f(x;d) < 0$ for $\tau \in (0,1)$.

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Weak Wolfe: With $0<\sigma_1<\sigma_2<1$ choose $t>0$ to satisfy

$$\begin{array}{ll} \mathrm{WW1} & f(x+td) \le f(x) + \sigma_1 t \Delta f(x;d), \text{ and} \\ \mathrm{WW2} & \sigma_2 \Delta f(x;d) \le \Delta f(x+td;d)\ . \end{array}$$

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Trust Region: With $\|d\| \le \delta$ and
$0 < \gamma_1 \le \gamma_2 < 1 \le \gamma_3, 0 < \beta_1 \le \beta_2 < \beta_3 < 1$ update δ as follows:

$$r = [f(x+d) - f(x)]/[\Delta f(x;d)]$$

$$\delta \in \begin{cases} [\delta,\ \gamma_3\delta] & \text{, if } r > \beta_3, \\ \{\delta\} & \text{, if } \beta_2 \le r \le \beta_3, \\ [\gamma_1\delta,\ \gamma_2\delta] & \text{, if } r < \beta_2. \end{cases}$$

Global Convergence: $x^{k+1} := x^k + \tau_k d^k$

- **Backtracking**: $\sum_{k=0}^{\infty} \frac{\Delta f(x^k; d^k)^2}{\left\|d^k\right\|_2^2} < \infty$, in particular, $\Delta f(x^k; d^k) \to 0$.

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In all cases, cluster points $\overline{x}$ satisfy $0 \in \partial f(\overline{x})$.

Complexity: Drusvyatskiy-Paquette '18

Inexact Prox-Linear Algorithms:

- Additional Assumptions:

(i) h is L-Lipschitz: $\|h(u) - h(v)\| \leq L\|u - v\| \quad \forall\, u, v \in \mathbb{R}^m$.

(ii) c is β-Lipschitz. $\|c(x) - h(z)\| \leq \beta\|x - z\| \quad \forall\, x, z \in \mathbb{R}^n$.

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Inexact Prox-Linear Algorithms:

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  - **(i)** h is L-Lipschitz:
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- Prox-Linear ingredients:

$$S_t(x) := \operatorname*{argmin}_z f_t(z;x) := h(c(x) + \nabla c(x)(z-x)) + g(z) + \frac{1}{2t}\|z-x\|_2^2$$

$$\mathcal{G}_t(x) := t^{-1}(x - S_t(x))$$

optimality $\implies \mathcal{G}_t(\overline{x}) = 0 \quad \forall\, t > 0$

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- Algorithm: $x^{k+1} \approx S_t(x^k)$ (or an ϵ_k-approx. min of $f_t(z;x^k)$)
- Convergence: If $t < (L\beta)^{-1}$, then

$$\min_{j=1,\ldots,N} \left\|\mathcal{G}_t(x^j)\right\|_2^2 \leq \frac{2(f(x^0) - \hat{f} + \sum_{j=1}^N \epsilon_j)}{tN}$$

where $\hat{f} := \liminf_k f(x^k)$.

Stochastic Prox Linear

Duchi-Ruan '17, Davis-Drusvyatskiy '19

$$f(x) = \mathbb{E}_{\xi \sim P}[h(c(x, \xi), \xi)] + g(x),$$

Stochastic Prox Linear

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$$f(x) = \mathbb{E}_{\xi \sim P}[h(c(x,\xi),\xi)] + g(x),$$

Input: $x^0 \in \mathbb{R}^n$, $\bar{\rho} > \rho$ where $h \circ c + g$ is ρ-weakly convex, $\gamma > 0$, an iteration count T.

Step: $t = 1, 2, \ldots, T$

$$\left\{ \begin{array}{l} \text{Sample } \xi_t \sim P \\ \\ \beta_t = \bar{\rho} + \gamma^{-1}\sqrt{T+1} \\ \\ \text{Set} \\ x^{t+1} = \operatorname{argmin}_x \left\{ r(x) + h(c(x^t,\xi_t) + c'(x^t,\xi_t)(x - x^t), \xi_t) + \frac{\beta_t}{2}\left\|x - x^t\right\|_2^2 \right\} \end{array} \right\}$$

Sample: $t^* \in \{0, 1, \ldots, T\}$ according to $\mathbb{P}(t^* = t) \propto \frac{\bar{\rho} - \rho}{\beta_t - \rho}$.

Return: x^{t^*}

Convergence

$$\mathrm{E}\left[\left\|\nabla f_{1/\bar{\rho}}(x^{t^*})\right\|_2^2\right] \leq \frac{2(\bar{\rho}(f_{1/\bar{\rho}}(x^0) - \min_x f) + 2\bar{\rho}^2 L^2 \gamma^2}{\bar{\rho} - \rho} \cdot \left(\frac{\bar{\rho} - \rho}{T+1} + \frac{1}{\gamma\sqrt{T+1}}\right) ,$$

where

$$f_{1/\bar{\rho}}(x) := \min_z [f(z) + \frac{\rho}{2}\|z - x\|_2^2]$$

$$L = \sqrt{\mathbb{E}_\xi[\ell(\xi)]^2]}\sqrt{\mathbb{E}_\xi[M(\xi)]^2]}.$$

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$$\mathrm{E}\left[\left\|\nabla f_{1/\bar\rho}(x^{t^*})\right\|_2^2\right] \le \frac{2(\bar\rho(f_{1/\bar\rho}(x^0)-\min_x f)+2\bar\rho^2L^2\gamma^2}{\bar\rho-\rho}\cdot\left(\frac{\bar\rho-\rho}{T+1}+\frac{1}{\gamma\sqrt{T+1}}\right),$$

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SIAM Prize Session: 2023 SIAG/OPT Best Paper Prize Lecture:
Stochastic Model-Based Minimization of Weakly Convex Functions

Damek Davis, Cornell University, U.S.

Dmitriy Drusvyatskiy, University of Washington, U.S.

Friday, June 2, 9:15 AM - 10:45 AM Room: Grand Ballroom B/C/D, 2nd floor

Feature Selection in Mixed Effects Models

Linear mixed-effects (LME) models are often used for analyzing nested or combined data across a range of groups or clusters.

Covariates are used to separate the total population variability (the fixed effects) from the group variability (the random effects).

Due to strength across groups, LMEs can estimate key statistics when the within group data is limited or highly variable.

Feature selection in mixed effects models finds a sparse set of covariates that explain
(i) the mean behavior across groups, and
(ii) the variability between groups.

Linear Mixed-Effects (LME) Model

$$\mathbf{y}_i = X_i\beta + Z_i u_i + \varepsilon_i, \quad i = 1 \dots m$$
$$u_i \sim N(0, \Gamma), \quad \Gamma \in \mathbb{S}^q_+$$
$$\varepsilon_i \sim N(0, \Lambda_i), \quad \Lambda_i \in \mathbb{S}^{n_i}_{++}$$

where

- y_i are known observations,
- $\beta \in \mathbb{R}^p$ is an unknown vector of fixed (mean) covariates,
- $u_i \in \mathbb{R}^q$ are unobserved random effects distributed $N(0, \Gamma)$,
- Λ_i known observation error covariance matrices,
- $\Gamma := \operatorname{Diag}\gamma,\ \gamma \in \mathbb{R}^s_+$ unknown random effects covariance matrix,
- $\Omega_i(\Gamma) := Z_i \Gamma Z_i^T + \Lambda_i$ the marginalized covariance.

Linear Mixed-Effects (LME) Model

$$\begin{aligned} \mathbf{y}_i &= X_i\beta + Z_i u_i + \varepsilon_i, \quad i = 1 \ldots m \\ u_i &\sim N(0, \Gamma), \quad \Gamma \in \mathbb{S}^q_+ \\ \varepsilon_i &\sim N(0, \Lambda_i), \quad \Lambda_i \in \mathbb{S}^{n_i}_{++} \end{aligned}$$

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- Λ_i known observation error covariance matrices,
- $\Gamma := \operatorname{Diag}\gamma,\ \gamma \in \mathbb{R}^s_+$ unknown random effects covariance matrix,
- $\Omega_i(\Gamma) := Z_i \Gamma Z_i^T + \Lambda_i$ the marginalized covariance.

The marginalized negative log-likelihood function

$$\mathcal{L}(\beta, \gamma) := \sum_{i=1}^{m} \frac{1}{2}(y_i - X_i\beta)^T \Omega_i(\Gamma)^{-1}(y_i - X_i\beta) + \frac{1}{2}\ln\det\Omega_i(\Gamma).$$

Maximum likelihood estimates for β and γ solve

$$\min_{\beta, \gamma \in \mathbb{R}^q_+} \ \mathcal{L}(\beta, \gamma)$$

Convex-Composite Structure

$\frac{1}{2}(y_i - X_i\beta)^T \Omega_i(\Gamma)^{-1}(y_i - X_i\beta)$ is convex-composite.

Matrix Fractional Functions
(B.-Gao-Hoheisel '15,'18)

Given the graph of the mapping $Y \mapsto -\frac{1}{2}YY^T$,

$$\mathcal{G} := \left\{ \left(Y, -\frac{1}{2}YY^T \right) \,\middle|\, Y \in \mathbb{R}^{n\times m} \right\},$$

we have

$$\sigma_{\mathcal{G}}(X,V) = \begin{cases} \frac{1}{2}\mathrm{tr}\left(X^T V^\dagger X\right) & \text{if } \mathrm{rge}\, X \subset \mathrm{rge}\, V,\ V \in \mathbb{S}^n, \\ +\infty & \text{else,} \end{cases}$$

where $V^\dagger$ is the Moore-Penrose pseudo inverse of V.

Feature Selection for Linear Mixed Effects

$$\min_{\beta \in \mathbb{R}^p, \gamma \in \mathbb{R}^q_+} \mathcal{L}(\beta, \gamma) + R(\beta, \gamma)$$

$$\mathcal{L}(\beta, \gamma) := \sum_{i=1}^{m} \frac{1}{2}(y_i - X_i\beta)^T \Omega_i(\Gamma)^{-1}(y_i - X_i\beta) + \frac{1}{2}\ln\det\Omega_i(\Gamma)$$

$\mathcal{L}$ is smooth on its domain.

R is closed, proper, convex with easily computed *prox operator*.

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$\mathcal{L}$ is weakly convex since

$$\nabla^2\mathcal{L}(\beta, \gamma) = H(\beta, \gamma) - \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{2}(Z_i^T \Omega_i(\gamma)^{-1} Z_i)^{\circ 2} \end{bmatrix},$$

where $H(\beta, \gamma)$ is always positive semi-definite.

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Apply PGD!

Feature Selection

$$\min_{\beta\in\mathbb{R}^p,\gamma\in\mathbb{R}^q_+} \mathcal{L}(\beta,\gamma) + R(\beta,\gamma)$$

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$$\mathcal{L}(\beta,\gamma) := \tfrac{1}{2}(y - X\beta)^T \Omega(\Gamma(\gamma))^{-1}(y - X\beta) + \tfrac{1}{2}\ln\det\Omega(\Gamma(\gamma)).$$

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The relaxed model problem (Decouple and smooth)

$$\min_{(\beta,\gamma),(\tilde{\beta},\tilde{\gamma}),\tilde{\gamma}\geq 0} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \frac{\eta}{2}\left\| \begin{array}{c} \beta - \tilde{\beta} \\ \gamma - \tilde{\gamma} \end{array} \right\|_2^2 + R(\tilde{\beta},\tilde{\gamma}),$$

where

$$\varphi(\gamma,\mu) := \begin{cases} -\mu\sum_{i=1}^q \ln(\gamma_i/\mu) & ,\ \mu > 0, \\ \delta_{\mathbb{R}^q_+}(\gamma) & ,\ \mu = 0, \\ +\infty & ,\ \mu < 0. \end{cases}$$

Optimal value function reformulation

$$\min_{(\beta,\gamma),(\tilde{\beta},\tilde{\gamma}),\tilde{\gamma}\geq 0} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \frac{\eta}{2}\left\| \begin{array}{c} \beta - \tilde{\beta} \\ \gamma - \tilde{\gamma} \end{array} \right\|_2^2 + R(\tilde{\beta},\tilde{\gamma}),$$

Optimal value function reformulation:

$$\mathcal{P}_{\eta,\mu} \quad \min_{(\tilde{\beta},\tilde{\gamma})} u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) + R(\tilde{\beta},\tilde{\gamma}) + \delta_{\mathbb{R}^q_+}(\tilde{\gamma})$$

where

$$u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) := \min_{(\beta,\gamma)} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \frac{\eta}{2}\left\| \begin{array}{c} \beta - \tilde{\beta} \\ \gamma - \tilde{\gamma} \end{array} \right\|_2^2.$$

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$$u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) := \min_{(\beta,\gamma)} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \frac{\eta}{2}\left\| \begin{array}{c} \beta - \tilde{\beta} \\ \gamma - \tilde{\gamma} \end{array} \right\|_2^2.$$

Apply the PGD algorithm to $\mathcal{P}_{\eta,\mu}$ with

$$\nabla u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) = \begin{pmatrix} \tilde{\beta} - \bar{\beta} \\ \tilde{\gamma} - \bar{\gamma} \end{pmatrix}, \quad \text{(locally Lipschitz)}$$

with $\begin{pmatrix} \bar{\beta} \\ \bar{\gamma} \end{pmatrix} = \operatorname{argmin}_{(\beta,\gamma)} \mathcal{L}_{\eta,\mu}((\beta,\gamma),(\tilde{\beta},\tilde{\gamma})).$

Performance

Regilarizer	Model Metric	PGD	MSR3	MSR3-fast
L0	Accuracy	0.89	**0.92**	**0.92**
	Time	41.68	88.54	**0.13**
L1	Accuracy	0.73	**0.88**	**0.88**
	Time	38.39	9.13	**0.13**
ALASSO	Accuracy	0.88	**0.92**	0.91
	Time	34.55	65.19	**0.12**
SCAD	Accuracy	0.71	**0.93**	0.92
	Time	77.62	84.67	**0.17**

The Experiment. The number of fixed effects p and random effects q is 20. $\beta = \gamma = [\frac{1}{2}, \frac{2}{2}, \frac{3}{2}, \dots, \frac{10}{2}, 0, 0, 0, \dots, 0]$

$$\begin{aligned} y_i &= X_i\beta + Z_i u_i + \varepsilon_i, \quad \varepsilon_i \sim N(0, 0.3^2 I) \\ X_i &\sim N(0, I)^p, \quad Z_i = X_i \\ u_i &\sim N(0, \operatorname{Diag}\gamma) \end{aligned}$$

9 groups sizes $[10, 15, 4, 8, 3, 5, 18, 9, 6]$

Each experiment is repeated 100 times.

More Details

MS219: Modeling and Optimization in Global Health II
Aleksei Sholokhov, Friday, June 2, 12:15pm
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Thank You!