

First-Order Methods in Convex Optimization: From Discrete to Continuous and Vice-versa

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The 8-th Chinese–German Workshop on Computational
and Applied Mathematics
School of Mathematics, Sichuan University
23th-27th Sept., 2024

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Outline

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Problem setting

- ▶ Composite convex optimization (CCO) problem

$$\inf_{x \in \mathbb{X}} F(x) := f(x) + g(Ax) \quad (\text{CCO})$$

Assumptions:

- * \mathbb{X}, \mathbb{Y} : Hilbert spaces with inner product $\langle \cdot, \cdot \rangle$ ¹
 - * $A : \mathbb{X} \rightarrow \mathbb{Y}$: bounded linear operator
 - * $f, g : \mathbb{X}(\mathbb{Y}) \rightarrow (-\infty, +\infty]$: CCP² with constants $\mu_f(\mu_g) \geq 0$
 - * Consistent condition: $A \text{dom } f \cap \text{dom } g \neq \emptyset$
- ▶ Linearly constrained optimization (LCO) problem

$$\inf_{x \in \mathbb{X}} f(x) \quad \text{s.t. } Ax = b \quad (\text{LCO})$$

- ▶ Bilinear saddle-point (BSP) problem

$$\inf_{x \in \mathbb{X}} \sup_{y \in \mathbb{Y}} \mathcal{L}(x, y) := f(x) + \langle y, Ax \rangle - g(y) \quad (\text{BSP})$$

- ▶ Many applications in:

- TV model (Image processing), Machine learning ...
- p -Laplacian (Numerical PDEs), Optimal transport, ...

¹When no confusion arises, we use the same bracket $\langle \cdot, \cdot \rangle$ for the inner products on \mathbb{X} and \mathbb{Y} .

²CCP means closed, convex and proper.

Optimality condition and Algorithm class

- First-order optimality conditions:

$$\text{For (CCO)} \quad 0 \in \partial f(x^*) + A^* \partial g(Ax^*)$$

$$\text{For (LCO)} \quad 0 \in \begin{bmatrix} \partial f(x^*) + A^* y^* \\ b - Ax^* \end{bmatrix}$$

$$\text{For (BSP)} \quad 0 \in \begin{bmatrix} \partial f(x^*) + A^* y^* \\ \partial g^*(y^*) - Ax^* \end{bmatrix}$$

- A unified abstract presentation: Finding a zero point $0 \in M(\mathbf{x}^*)$ of a maximal monotone operator $M : \mathcal{X} \rightarrow 2^{\mathcal{X}}$.
- We are mainly interested in First-Order Methods (FOM) that produce the iteration sequence $\{x_k\}$ with the access **only** to³

$$\nabla f / \mathbf{prox}_f, \quad \nabla g / \mathbf{prox}_g$$

or (for $f = f_1 + f_2$, $g = g_1 + g_2$)

$$\nabla f_1 / \mathbf{prox}_{f_2}, \quad \nabla g_1 / \mathbf{prox}_{g_2}$$

³Here and in what follows, \mathbf{prox}_f denotes the **proximal mapping** of f :

$$\mathbf{prox}_f(x) = \operatorname{argmin} \{f(y) + 1/2 \|x - y\|^2\}$$

Proximal-gradient methods for (CCO) with $A = I$

- ▶ Gradient descent (GD) and Proximal point algorithm (PPA):

$$x_{k+1} = x_k - s \nabla F(x_k), \quad x_{k+1} = x_k - s \nabla F(x_{k+1})^4$$

- ▶ Proximal-gradient method (PGM): $x_{k+1} = x_k - s(\nabla f(x_k) + \nabla g(x_{k+1}))$

- * Also known as Forward-Backward Splitting
- * $O(1/k)$ for convex and $(1 - 1/\kappa_f)$ for strongly convex

- ▶ Heavy ball (HB)⁵: $x_{k+1} = x_k - s \nabla F(x_k) + \beta_k \overbrace{(x_k - x_{k-1})}^{\text{Momentum}}$

- * Better than GD with $\beta_k \in (0, 1)$
- * Optimal choice of strongly convex case

- ▶ Nesterov accelerated gradient (NAG-1983, NAG-2004):

$$x_{k+1} = \bar{x}_k - s \nabla F(\bar{x}_k), \quad \bar{x}_{k+1} = x_{k+1} + \beta(x_{k+1} - x_k)$$

- * $O(1/k^2)$ with $\beta_k = k/(k+3)$
- * $O(1 - 1/\sqrt{\kappa_f})^k$ with $\beta_k = (\sqrt{\kappa_f} - 1)/(\sqrt{\kappa_f} + 1)$
- * **Optimal rate**
- * Proximal gradient version = FISTA

- ▶ Güler's PPA (**SIOPT**, 1994)

$$x_{k+1} = \bar{x}_k - s \nabla F(x_{k+1}), \quad \bar{x}_{k+1} = x_{k+1} + \beta(x_{k+1} - x_k)$$

⁴ This presentation is equivalent to $x_{k+1} = \text{prox}_{sF}(x_k)$

⁵ Polyak, 1964

Augmented Lagrangian methods for (LCO)

- ▶ Augmented Lagrangian method (ALM)

$$x_{k+1} = \underset{x \in \mathbb{X}}{\operatorname{argmin}} \left\{ \mathcal{L}(x, \lambda_k) + \frac{\sigma}{2} \|Ax - b\|^2 \right\}, \quad \lambda_{k+1} = \lambda_k + \sigma(Ax_{k+1} - b)$$

- ▶ Equivalent to Bregman method and dual PPA

- ▶ Linearization (L-ALM) and relaxation (ADMM)

- ▶ $O(1/k^2)$ acceleration with **momentum** for the dual variable ⁶

- ▶ Acceleration with **momentum** for the primal variable ⁷

- * $O(\frac{1}{k})$ for convex and $O(\frac{1}{k^2})$ for strongly convex (**Optimal**) ⁸

- * Extension to two block case (Acc-ADMM) ⁹

⁶He and Yuan, 2013; Kang et al. **JSC**, 2013

⁷Xu, **SIOPT**, 2017

⁸Ouyang and Xu, **SIOPT**, 2021

⁹Sabach and Teboulle, **SIOPT**, 2022; Zhang et al. arXiv:2206.05088, 2022

Primal-dual methods for (BSP)

- ▶ Extensions of GD and PPA:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - sM(\mathbf{x}_k), \quad \mathbf{x}_{k+1} = \mathbf{x}_k - sM(\mathbf{x}_{k+1})$$

Diverge Full coupling

- ▶ Extra-gradient method (EGM, with ergodic rate $O(1/k)$)¹⁰

$$\mathbf{x}_k = \mathbf{x}_k - sM(\mathbf{x}_k), \quad \mathbf{x}_{k+1} = \mathbf{x}_k - sM(\mathbf{x}_k)$$

- ▶ Primal-dual hybrid gradient method (PDHG) (Preconditioned PPA)

$$\mathbf{x}_{k+1} = \mathbf{x}_k - sQ^{-1}M(\mathbf{x}_{k+1}), \quad Q = \begin{bmatrix} I & -sA^* \\ O & I \end{bmatrix}$$

- ▶ Also known as the primal-dual proximal splitting (PDPS)

$$\begin{cases} x_{k+1} = \mathbf{prox}_{sf}(x_k - sA^*y_k) \\ y_{k+1} = \mathbf{prox}_{sg}(y_k + sAx_{k+1}) \end{cases}$$

- ▶ Diverge even for LP (He et al. **JMIV**, 2017)

¹⁰ Ergodic means for the average $\bar{\mathbf{x}}_N = \sum_{i=0}^N a_i \mathbf{x}_i / \sum_{i=0}^N a_i$

- A symmetrized precondition remedy

$$\mathbf{x}_{k+1} = \mathbf{x}_k - sQ^{-1}M(\mathbf{x}_{k+1}), \quad Q = \begin{bmatrix} I & -sA^* \\ -sA & I \end{bmatrix}$$

- This is the Chambolle–Pock (CP) ¹¹

$$\begin{cases} x_{k+1} = \mathbf{prox}_{sf}(x_k - sA^*y_k) \\ y_{k+1} = \mathbf{prox}_{sg}(y_k + sA(2x_{k+1} - x_k)) \end{cases}$$

- **Optimal ergodic rate:** $O(1/k)$ for convex, $O(1/k^2)$ for partially strongly convex and ρ^k for strongly convex
- Inertial corrected PDPS ¹² (IC-PDPS, with **momentum** and **correction**)

$$\begin{cases} \mathbf{x}_{k+1} = \bar{\mathbf{x}}_k - Q_{k+1}^{-1}M(\mathbf{x}_{k+1}) + \underbrace{\hat{Q}_{k+1}(\mathbf{x}_{k+1} - \mathbf{x}_k)}_{\text{Correction}}, \\ \bar{\mathbf{x}}_{k+1} = \mathbf{x}_{k+1} + \Lambda_{k+1}(\mathbf{x}_{k+1} - \mathbf{x}_k), \end{cases}$$

- **Optimal nonergodic rate**

¹¹Chambolle and Pock, **JMIV**, 2013

¹²Valkonen, **SIOPT**, 2020

Motivation

- ▶ Almost all FOMs (**without momentum**) in the form

$$X^+ = \Gamma(s, X)$$

- ▶ This is very close to **Numerical Discretization**
- ▶ Can we have a unified continuous perspective on FOMs?
- ▶ How about the numerical analysis approach for FOMs?

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$O(s^r)$ -resolution framework

Definition 1 (Lu, MAPR, 2022)

Given a FOM $X^+ = \Gamma(s, X)$ **with** $\Gamma(0, X) = X$, if there is an ODE system

$$X' = \Gamma_0(X) + s\Gamma_1(X) + \cdots + s^r\Gamma(X) \quad (1)$$

that satisfies $\|X(s) - X^+\| = o(s^{r+1})$ with $r \geq 0$, where $X(s)$ is the solution of (1) with $X(0) = X$, then we call (1) the $O(s^r)$ -resolution ODE of the FOM $X^+ = \Gamma(s, X)$

Theorem 1 (Lu, MAPR, 2022)

Given a FOM $X^+ = \Gamma(s, X)$ **with** $\Gamma(0, X) = X$ and sufficiently smooth $\Gamma(s, X)$ in both s and X Then its $O(s^r)$ -resolution ODE **exists uniquely**.

$O(s^r)$ -resolution without momentum

Look at $E(s) = X(s) - X^+ = X - \Gamma(s, X) + \int_0^s X'(t, s) dt$ and the Taylor expansion at $s = 0$

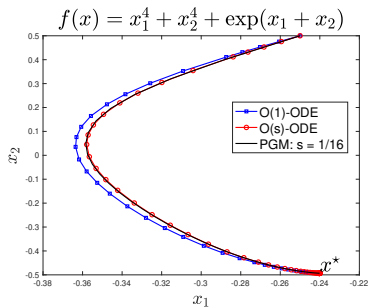
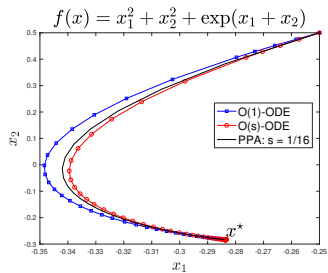
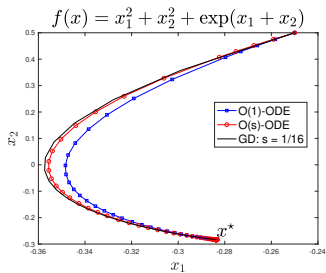
$$E(s) = E(0) + E'(0)s + \cdots + \frac{E^{(r+1)}(0)}{(r+1)!} s^{r+1} + o(s^{r+1})$$

Essentially, we have $E(0) = E'(0) = \cdots = E^{(j)}(0) = 0$. This gives Γ_j

Corollary 1 (Lu, MAPR, 2022)

- (i) The $O(1)$ -resolution ODE of GD, PPA and PGM: $X' = -\nabla F(X)$
- (ii) The $O(s)$ -resolution ODE of GD is $X' = -\nabla F(X) - \frac{s}{2} \nabla^2 F(X) \cdot \nabla F(X)$
- (iii) The $O(s)$ -resolution ODE of PPA is $X' = -\nabla F(X) + \frac{s}{2} \nabla^2 F(X) \cdot \nabla F(X)$
- (iv) The $O(s)$ -resolution ODE of PGM is

$$X' = -\nabla F(X) + \frac{s}{2} (\nabla^2 g(X) - \nabla^2 f(X)) \cdot \nabla F(X)$$



Corollary 2 (Lu, **MAPR**, 2022)

(i) *The $O(1)$ -resolution ODE of GD, PPA, PDHG, CP and EGM are*

$$X' = -M(X)$$

(ii) *The $O(s)$ -resolution ODE of GD is*

$$X' = -M(X) - \frac{s}{2} \nabla M(X) \cdot M(X)$$

(iii) *The $O(s)$ -resolution ODE of PPA and EGM are the same*

$$X' = -M(X) + \frac{s}{2} \nabla M(X) \cdot M(X)$$

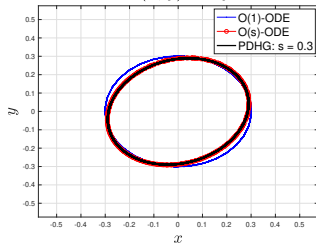
(iv) *The $O(s)$ -resolution ODE of PDHG is*

$$X' = -M(X) + \frac{s}{2} \left[\nabla M(X) + \begin{bmatrix} O & O \\ 2A & O \end{bmatrix} \right] \cdot M(X)$$

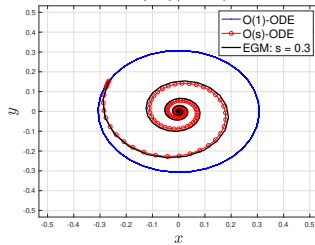
(iv) *The $O(s)$ -resolution ODE of CP is*

$$X' = -M(X) + \frac{s}{2} \left[\nabla M(X) + \begin{bmatrix} O & 2A^* \\ 2A & O \end{bmatrix} \right] \cdot M(X)$$

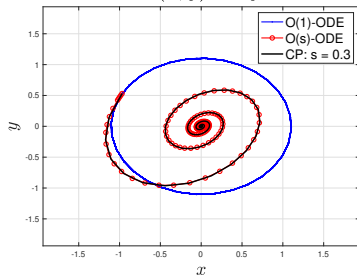
$$\mathcal{L}(x, y) = xy$$



$$\mathcal{L}(x, y) = xy$$



$$\mathcal{L}(x, y) = xy$$



$O(s^r)$ -resolution with momentum

- For a general momentum method

$$x_{k+1} = x_k - s \nabla F(x_k) + \underbrace{\beta(s)(x_k - x_{k-1})}_{\text{Momentum}} - \beta(s)s [\nabla F(x_k) - \nabla F(x_{k-1})]$$

there is **No such condition** $\Gamma(0, X) = 0$.

- Key observation: **A hybrid gradient descent transformation**

$$\frac{x_{k+1} - x_k + s \nabla F(x_k)}{\sqrt{s}\beta(s)} = \beta(s) \cdot \frac{x_k - x_{k-1} + s \nabla F(x_{k-1})}{\sqrt{s}\beta(s)} - \sqrt{s} \nabla F(x_k)$$

which leads to

$$\begin{cases} x_{k+1} = x_k + \sqrt{s}\beta(s)v_{k+1} - s \nabla F(x) \\ v_{k+1} = v_k + (\beta(s) - 1)v_k - \sqrt{s} \nabla F(x) \end{cases}$$

with $\lim_{s \rightarrow 0} (\beta(s) - 1)/\sqrt{s} = 0$

- This gives a new system of $X = (x, v)$ that satisfies $X^+ = \Gamma(\sqrt{s}, X)$ with $\Gamma(0, X) = 0$
- The same idea works for other momentum methods with **dynamically changing parameters** and **primal-dual methods**

Theorem 2

- (i) *The $O(1)$ -resolution ODE of HB and NAG with optimal β for strongly convex objective are the same ¹³:*

$$\begin{bmatrix} x \\ v \end{bmatrix}' = \begin{bmatrix} v \\ -2\sqrt{\mu}v - \nabla F(x) \end{bmatrix} \iff x'' + 2\sqrt{\mu}x' + \nabla F(x) = 0$$

- (ii) *The $O(1)$ -resolution ODE of NAG-1983/FISTA for convex objective is*

$$\begin{bmatrix} x \\ v \\ \gamma \end{bmatrix}' = \begin{bmatrix} v \\ -\frac{3}{2\sqrt{\gamma}}v - \nabla F(x) \\ \sqrt{\gamma} \end{bmatrix} \iff x'' + \frac{3}{2\sqrt{\gamma}}x' + \nabla F(x) = 0$$

Since $\gamma = t^2/4$, this gives the Su-Boyd-Candès (JMLR, 2016)

$$x'' + \frac{3}{t}x' + \nabla F(x) = 0$$

¹³Polyak. 1964; Siegel. 2019; Wilson et al. *JMLR*, 2021; Shi et al., *Math. Program.*, 2022;

(iii) The $O(1)$ -resolution ODE of NAG-2004 is ¹⁴

$$\begin{bmatrix} x \\ v \\ \gamma \end{bmatrix}' = \begin{bmatrix} v \\ -\frac{3+\mu\gamma}{2\sqrt{\gamma}}v - \nabla F(x) \\ \sqrt{\gamma}(1 - \mu\gamma) \end{bmatrix} \iff x'' + \frac{3+\mu\gamma}{2\sqrt{\gamma}}x' + \nabla F(x) = 0$$

(iv) The $O(1)$ -resolution ODE of IC-PDPS is ¹⁵

$$\begin{bmatrix} \mathbf{x} \\ \mathbf{v} \\ \Upsilon \\ \theta \end{bmatrix}' = \begin{bmatrix} \mathbf{v} - \mathbf{x} \\ -\theta\Upsilon^{-1}[S(\mathbf{v} - \mathbf{x}) + M(\mathbf{x})] \\ 2\text{diag}(S)\Upsilon \\ \theta \end{bmatrix}$$

In second-order form

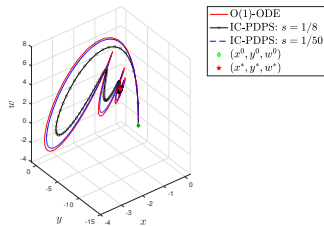
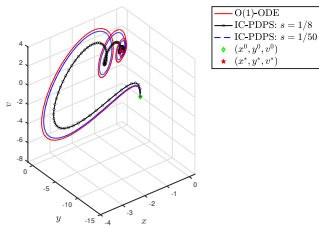
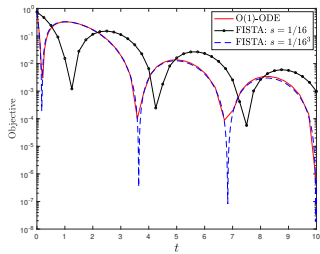
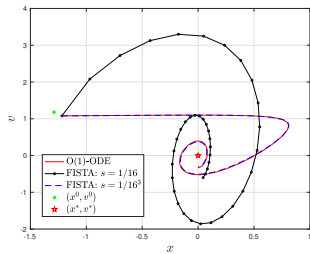
$$\Upsilon \mathbf{x}'' + [\theta S + \Upsilon] \mathbf{x}' + \theta M(\mathbf{x}) = 0, \quad S = \begin{bmatrix} \mu_f I & A^* \\ A & \mu_g I \end{bmatrix}$$

In component wise

$$\begin{cases} \gamma x'' + (\gamma + \mu_f \theta) x' + \theta \nabla_x \mathcal{L}(x, y + y') = 0 \\ \beta y'' + (\beta + \mu_g \theta) y' + \theta \nabla_y \mathcal{L}(x + x', y) = 0 \end{cases}$$

¹⁴L., and Long Chen. *Math. Program.*, 2022.

¹⁵L. *arXiv:2405.14098v1*, 2024.



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Semi-implicit AGD

For unconstrained minimization problem, we present a compact form of the $O(1)$ -resolution ODE of NAG-2004 with time scaling:

$$\begin{aligned}\gamma x'' + (\mu + \gamma)x' + \nabla F(x) &= 0 \\ \gamma' - \mu + \gamma &= 0\end{aligned}\quad (\text{NAG flow})$$

- ▶ Semi-implicit scheme for Accelerated Gradient Descent (AGD) ¹⁶

$$\gamma_k \cdot \frac{\frac{x_{k+1} - x_k}{\alpha_k} - \frac{x_k - x_{k-1}}{\alpha_{k-1}}}{\alpha_k} + (\mu + \gamma_k) \cdot \frac{x_{k+1} - x_k}{\alpha_k} + \nabla F(\bar{x}_k) = 0$$

- ▶ Composite case $F = f + g$

$$\gamma_k \cdot \frac{\frac{x_{k+1} - x_k}{\alpha_k} - \frac{x_k - x_{k-1}}{\alpha_{k-1}}}{\alpha_k} + (\mu + \gamma_k) \cdot \frac{x_{k+1} - x_k}{\alpha_k} + \nabla f(\bar{x}_k) + \nabla g(x_{k+1}) = 0$$

- ▶ Lyapunov analysis (optimal rate)

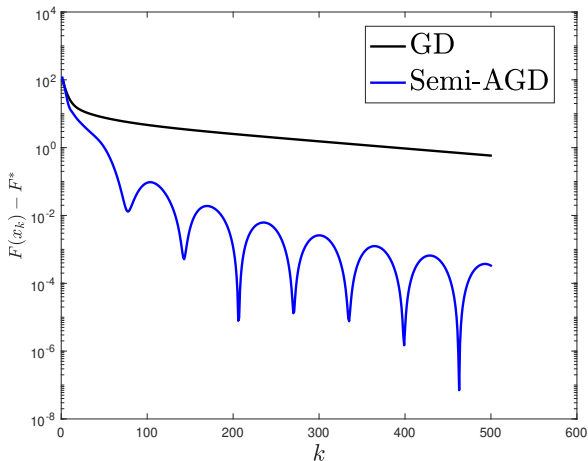
$$\mathcal{E}_k := F(x_k) - F(x^*) + \frac{\gamma_k}{2} \|v_k - x^*\|^2 \leq \min \left\{ \frac{L}{k^2}, \left(1 + \sqrt{\frac{\mu_f}{L_f}} \right)^{-k} \right\}$$

¹⁶L., and Long Chen. *Math. Program.*, 2022/*arXiv:1912.09276*, 2019; L. *Optimization*, 2023.

Find $u \in H_0^1(\Omega)$ such that

$$-\Delta u = f \quad \text{in } \Omega = (0, 1)^2$$

Use $P1$ Lagrange element with uniform mesh size $h = 2^{-5}$. The DoF is $N = \dim V_h = (1/h + 1)^2 = 1089$.



Restarting

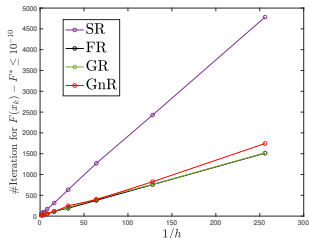
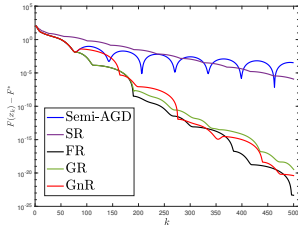
► Restarting scheme

Function restart (FR) : $\frac{dF(x(t))}{dt} > 0$ O'Donoghue and Candès (FoCM, 2015)

Gradient restart (GR) : $\langle \nabla F(x(t)), x'(t) \rangle > 0$ O'Donoghue and Candès, (FoCM, 2015)

Speed restart (SR) : $\frac{d \|x'(t)\|^2}{dt} < 0$ Su-Boyd-Candès (JMLR, 2016)

Gradient norm restart (GnR) : $\frac{d \|\nabla F(x(t))\|^2}{dt} > 0$



Restart works very well with the iteration complexity $\sim \sqrt{\kappa}$

This yield the linear rate $\exp(-k/\sqrt{\kappa})$

Implicit-explicit AALM

For (LCO), we propose a simplified form of the $O(1)$ -resolution ODE of IC-PDPS:

$$\begin{aligned}\gamma x'' + (\mu + \gamma)x' + \nabla f(x) + A^\top y &= 0 \\ \beta y' + b - A(x + x') &= 0 \\ \gamma' - \mu + \gamma &= 0 \\ \beta' + \beta &= 0\end{aligned}\quad (\text{APD flow})$$

- Implicit-explicit scheme for Accelerated Augmented Lagrangian Method (AALM) ¹⁷

$$\begin{aligned}\gamma_k \cdot \frac{\frac{x_{k+1} - x_k}{\alpha_k} - \frac{x_k - x_{k-1}}{\alpha_{k-1}}}{\alpha_k} + (\mu + \gamma_k) \cdot \frac{x_{k+1} - x_k}{\alpha_k} + \nabla f(\bar{x}_k) + A^\top \bar{y}_k &= 0 \\ \beta_k \frac{y_{k+1} - y_k}{\alpha_k} + b - A(x_{k+1} + (x_{k+1} - x_k)/\alpha_k) &= 0\end{aligned}$$

- Lyapunov analysis (optimal nonergodic rate)

$$\mathcal{E}_k := \mathcal{L}(x_k, y^*) - \mathcal{L}(x^*, y_k) + \frac{\gamma_k}{2} \|v_k - x^*\|^2 + \frac{\beta_k}{2} \|y_k - y^*\|^2 \leq \begin{cases} Ck^{-1}, & \mu = 0, \\ Ck^{-2}, & \mu > 0. \end{cases}$$

- ▶ For extension to the Hölder case $\nabla f \in C^{0,\nu}$ and application to optimal transport (ODE+AMG+SsN), see Hu et al. (JSC,2023) and L. (JOTA, 2024).
- ▶ For the separable case $f(x) = f_1(x_1) + f_2(x_2)$, we have implicit-explicit schemes for accelerated ADMM; see L. and Zhang (arXiv:2109.13467v2, 2023).

Semi-implicit APDGS

For (BSP), we have a simplified form of the $O(1)$ -resolution ODE of IC-PDPS:

$$\begin{aligned}\Upsilon \mathbf{x}'' + [S + \Upsilon] \mathbf{x}' + M(\mathbf{x}) &= 0 \\ \Upsilon' - \Sigma + \Upsilon &= 0\end{aligned}\quad (\text{APDG flow})$$

- Implicit-explicit scheme for Accelerated Primal-Dual Gradient Splitting (APDGS)¹⁸

$$\begin{aligned}\gamma_k \cdot \frac{\frac{x_{k+1} - x_k}{\alpha_k} - \frac{x_k - x_{k-1}}{\alpha_{k-1}}}{\alpha_k} + (\mu_f + \gamma_k) \cdot \frac{x_{k+1} - x_k}{\alpha_k} + \nabla f(\bar{x}_k) + A^\top \bar{y}_k &= 0 \\ \beta_k \cdot \frac{\frac{y_{k+1} - y_k}{\eta_k \alpha_k} - \frac{y_k - y_{k-1}}{\eta_{k-1} \alpha_{k-1}}}{\alpha_k} + (\mu_g / \eta_k + \beta_k) \cdot \frac{y_{k+1} - y_k}{\alpha_k} + \eta_k (\nabla g(\bar{y}_k) - A \bar{x}_{k+1}) &= 0\end{aligned}$$

- Lyapunov analysis (optimal nonergodic rate)

$$\mathcal{E}_k = \mathcal{L}(x_k, y^*) - \mathcal{L}(x^*, y_k) + \frac{\gamma_k}{2} \|v_k - x^*\|^2 + \frac{\beta_k}{2} \|w_k - y^*\|^2 \leq \begin{cases} \frac{C}{k}, & \mu_f = \mu_g = 0, \\ \frac{C}{k^2}, & \mu_f + \mu_g > 0, \\ \rho^k, & \mu_f \mu_g > 0, \end{cases}$$

¹⁸L. arXiv:2407.20195, 2024.

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► Conclusion:

- * A unified $O(s^r)$ -resolution framework for FOMs
- * A time discretization approach to construct FOMs
- * A Lyapunov function analysis for optimal convergence rate
- * Some numerical illustration with restarting

► Future topics:

- * Extension to nonlinear saddle-point problems (General convex optimization with **nonlinear but convex** constraint)
- * Restarting with **uniform convergence rate** independent on the condition number (Multilevel + restarting)
- * Restart analysis for the primal-dual dynamics (**No descent**)
- * Application to nonlinear variational problems (**Nonconvex but with special structure**) and optimal transport
- * Accelerated multiobjective gradient methods

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Thanks for your listening!

Any questions?