Chapter 2
Optimization Algorithms

Convex Optimization for Machine Learning & Computer Vision
WS 2019/20

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Gradient Methods
Proximal Algorithms
Convergence Theory
Acceleration
Summary

Gradient-based Methods

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Overview of this section

Unconstrained, differentiable, possibly nonconvex optimization

Problem setting:

$$\text{minimize } J(u) \quad \text{over } u \in \mathbb{E}.$$

Assume:

1. $J : \mathbb{E} \to \mathbb{R}$ is continuously differentiable.
2. There exists a global minimizer u^*. (Typically, an optim algorithm seeks for a local minimizer s.t. $\nabla J(u^*) = 0$.)

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Methods under consideration:

1. (Scaled) gradient descent.
2. Line search method.
3. Majorize-minimize method.

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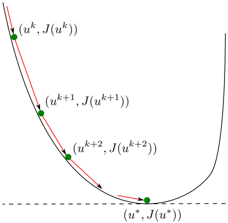
Analytical questions:

1. Convergence (or not); global vs. local convergence.
2. Convergence rate (in special cases).

Descent method



Descent method

Initialize $u^0 \in \mathbb{E}$. Iterate with $k = 0, 1, 2, ...$

1. If the stopping criteria $\|\nabla J(u^k)\| \leq \epsilon$ is *not* satisfied, then continue; otherwise return u^k and stop.
2. Choose a **descent direction** $d^k \in \mathbb{E}$ s.t.
$$\left\langle \nabla J(u^k), d^k \right\rangle < 0.$$
3. Choose an "appropriate" step size $\tau^k > 0$, and update
$$u^{k+1} = u^k + \tau^k d^k.$$

Descent direction

Theorem

If $\langle \nabla J(u^k), d^k \rangle < 0$, then $J(u^k + \tau d^k) < J(u^k)$ for all sufficiently small $\tau > 0$.

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Proof: Use the Taylor expansion:

$$
\begin{aligned}
J(u^k + \tau d^k) &= J(u^k) + \tau \left\langle \nabla J(u^k), d^k \right\rangle + o(\tau) \\
&= J(u^k) + \tau \left(\left\langle \nabla J(u^k), d^k \right\rangle + o(1) \right) < J(u^k) \quad \text{as } \tau \to 0^+.
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Choices of descent direction

1. Gradient/Steepest descent:
   $d^k = -\nabla J(u^k) = \arg\min_{d \in \mathbb{E},\, \|d\| \le 1} \left\langle \nabla J(u^k), d \right\rangle$.
2. Scaled gradient: $d^k = -(H^k)^{-1} \nabla J(u^k)$.
3. Newton: $H^k = \nabla^2 J(u^k)$, assuming J is twice continuously differentiable and $\nabla^2 J(u^k)$ is spd.
4. Quasi-Newton: $H^k \approx \nabla^2 J(u^k)$, H^k is spd.

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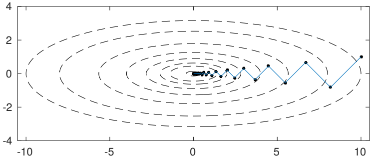
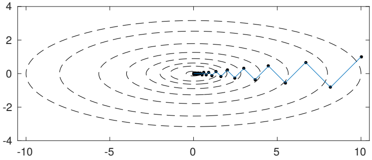
Gradient descent with exact line search



- Gradient descent with *exact* line search:

$$u^{k+1} = u^k - \tau^k \nabla J(u^k),$$
$$\tau^k = \arg\min_{\tau \geq 0} J(u^k - \tau \nabla J(u^k)).$$

Gradient descent with exact line search



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- Case study: $J(u) = \frac{1}{2}\langle u, Qu\rangle - \langle b, u\rangle$, matrix Q is spd.
  - $\nabla J(u) = Qu - b, \quad \|\cdot\|_Q^2 \equiv \langle \cdot, Q\cdot\rangle.$

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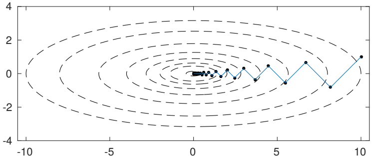

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  - $\nabla J(u) = Qu - b, \quad \|\cdot\|_Q^2 \equiv \langle \cdot, Q\, \cdot \rangle.$
  - $\tau^k = \arg\min_{\tau\geq 0} J(u^k - \tau\nabla J(u^k)) = \dfrac{\|\nabla J(u^k)\|^2}{\|\nabla J(u^k)\|_Q^2} \quad \Rightarrow$

$$\|u^{k+1} - u^*\|_Q^2 = \left(1 - \frac{\|\nabla J(u^k)\|^4}{\|\nabla J(u^k)\|_Q^2 \|\nabla J(u^k)\|_{Q^{-1}}^2}\right) \|u^k - u^*\|_Q^2$$
$$\leq \left(\frac{\lambda_{\max}(Q) - \lambda_{\min}(Q)}{\lambda_{\max}(Q) + \lambda_{\min}(Q)}\right)^2 \|u^k - u^*\|_Q^2.$$

Inexact line search

Backtracking line search

- Sufficient decrease condition (let $c_1 \in (0, 1)$):

$$J(u^k + \tau d^k) \leq J(u^k) + c_1 \tau \left\langle \nabla J(u^k), d^k \right\rangle. \qquad \text{(A)}$$

- Curvature condition (let $c_2 \in (c_1, 1)$):

$$\left\langle \nabla J(u^k + \tau d^k), d^k \right\rangle \geq c_2 \left\langle \nabla J(u^k), d^k \right\rangle. \qquad \text{(C)}$$

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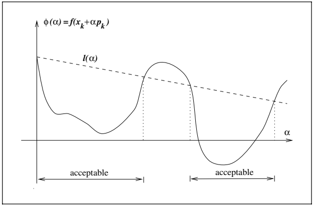
- (A) $\rightsquigarrow$ **Armijo** line search; (A) & (C) $\rightsquigarrow$ **Wolfe-Powell** l.s.

Armijo l.s.



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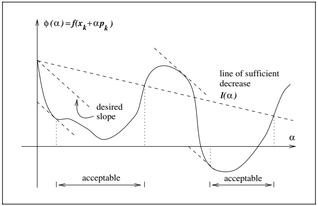

Convergence of backtracking line search

Lemma (feasibility of line search)

Assume that $J : \mathbb{E} \to \mathbb{R}$ is continuously differentiable, $\left\langle \nabla J(u^k), d^k \right\rangle < 0 \ \forall k$, and $0 < c_1 < c_2 < 1$. Then there exists an open interval in which the step size τ satisfies (A) and (C).

Proof: on board.

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<u>Proof</u>: on board.

Theorem (Zoutendijk)

Assume that $J : \mathbb{E} \to \mathbb{R}$ is cont'ly differentiable, and (A) and (C) are both satisfied with $0 < c_1 < c_2 < 1$ for each k. In addition, J is μ-Lipschitz differentiable on $\{u \in \mathbb{E} : J(u) \leq J(u^0)\}$. Then

$$\sum_{k=0}^{\infty} \frac{\left| \langle \nabla J(u^k), d^k \rangle \right|^2}{\|d^k\|^2} < \infty.$$

<u>Proof</u>: on board.

Remark

If $\dfrac{\left| \langle \nabla J(u^k), d^k \rangle \right|}{\|\nabla J(u^k)\| \|d^k\|} \geq \text{constant} > 0$, then $\lim_{k \to \infty} \|\nabla J(u^k)\| = 0$.

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Majorize-minimize method

Majorizing function

A function $\widehat{J}(\cdot\,; u)$ is a **majorant** of J at $u \in \mathbb{E}$ if

$$\begin{cases} \widehat{J}(u; u) = J(u), \\ \widehat{J}(\cdot\,; u) \geq J(\cdot). \end{cases}$$

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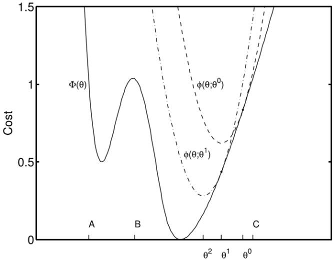
Majorize-minimize (MM) algorithm

Let $\widehat{J}(\cdot; u)$ majorize J $\forall u \in \mathbb{E}$. Then the MM iteration reads:

$$u^{k+1} \in \arg\min_u \widehat{J}(u; u^k).$$



Gradient descent as MM

Remark

1. Monotonic decrease of objectives:

$$J(u^{k+1}) \leq \widehat{J}(u^{k+1}; u^k) \leq \widehat{J}(u^k; u^k) = J(u^k).$$

2. Efficiency of MM relies on the choice of the majorant $\widehat{J}(\cdot; u)$, i.e., $\widehat{J}(\cdot; u)$ is easy to minimize.
3. Common choices of $\widehat{J}(\cdot; u)$ are quadratics.

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Gradient descent as MM

- Observe that $u^{k+1} = u^k - \tau \nabla J(u^k)$ iff

$$u^{k+1} = \arg\min_u J(u^k) + \left\langle \nabla J(u^k), u - u^k \right\rangle + \frac{1}{2\tau}\|u - u^k\|^2.$$

- When $J(u^k) + \langle \nabla J(u^k), \cdot - u^k \rangle + \frac{1}{2\tau}\| \cdot - u^k\|^2 \ge J(\cdot)$ holds?

Gradient descent as MM

Lemma

Assume that $J : \mathbb{E} \to \mathbb{R}$ is μ-Lipschitz differentiable. Then $\forall u, v \in \mathbb{E}$:

$$|J(v) - J(u) - \langle \nabla J(u), v - u \rangle| \leq \frac{\mu}{2} \|v - u\|^2.$$

Proof: on board.

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with $\tau \in (0, 1/\mu]$ yields $\lim_{k\to\infty} \nabla J(u^k) = 0$.

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<u>Proof</u>: on board.

Recipe of convergence

By solving the surrogate problem in MM, we achieve: (1) sufficient decrease in the objective; (2) inexact optimality condition which matches the exact OC in the limit.

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Agenda for the rest of the chapter

- Four proximal algorithms in convex optimization:
  - Forward-backward splitting (FBS) ($=$ proximal gradient method).
  - Alternating direction method of multipliers (ADMM).
  - Primal-dual hybrid gradient (PDHG).
  - Douglas-Rachford splitting (DRS), Peaceman-Rachford splitting (PRS).
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- A common theme: "operator splitting" & extensively use prox operations.
- We'll cover: (1) Derivation of algorithms; (2) Connections between algorithms; (3) Demo in Python; and ...
- Unified convergence analysis.
- Acceleration techniques.

Forward-backward splitting

- Consider the convex optimization problem:

$$\min_u F(u) + G(u),$$

with G differentiable and F possibly non-differentiable.

- Its minimizer is characterized by

$$0 \in \partial F(u) + \nabla G(u).$$

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- **Forward-backward splitting** (FBS):

$$\begin{aligned} u^{k+1} &= \mathrm{prox}_{\tau F}(u^k - \tau \nabla G(u^k)) \\ &= (I + \tau \partial F)^{-1} \circ (I - \tau \nabla G)(u^k). \end{aligned}$$

- FBS as *semi-implicit Euler scheme*:

$$\frac{u^{k+1} - u^k}{\tau} \in -\partial F(u^{k+1}) - \nabla G(u^k).$$

Example: Split feasibility problem

Split feasibility problem

Given nonempty, closed, convex sets $C_1 \subset \mathbb{E}_1$, $C_2 \subset \mathbb{E}_2$, and linear operator $K : \mathbb{E}_1 \to \mathbb{E}_2$, find $u \in \mathbb{E}_1$ s.t. $u \in C_1,\ Ku \in C_2$.

- Variational model:

$$\min_{u \in \mathbb{E}_1} \delta_{C_1}(u) + \frac{1}{2}\|Ku - \mathrm{proj}_{C_2}(Ku)\|^2.$$

Note that $\frac{1}{2}\|v - \mathrm{proj}_{C_2}(v)\|^2 = \mathrm{env}_1\, \delta_{C_2}(v)$.

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- Optimality condition:

$$0 \in \partial \delta_{C_1}(u) + K^\top (I - \mathrm{proj}_{C_2})(Ku).$$

  Recall that $\nabla \mathrm{env}_1\, \delta_{C_2}(v) = (I - \mathrm{prox}_{\delta_{C_2}})(v)$.

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- Apply FBS $\Rightarrow$

$$\begin{aligned} u^{k+1} &= (I + \tau \partial \delta_{C_1})^{-1}(u^k - \tau K^\top (I - \mathrm{proj}_{C_2})(Ku^k)) \\ &= \mathrm{proj}_{C_1}(u^k - \tau K^\top (I - \mathrm{proj}_{C_2})(Ku^k)). \end{aligned}$$

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Alternating direction method of multipliers

- Consider

$$\min_{u,v} \; J(u,v) = F(v) + G(u) + \delta\{Ku - v = 0\},$$

given proper, convex, lsc functions F, G and matrix K.

Alternating direction method of multipliers

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given proper, convex, lsc functions F, G and matrix K.

- *Augmented Lagrangian* ($\tau > 0$):

$$\mathcal{L}_\tau(u,v;p) = F(v) + G(u) + \langle p, Ku - v\rangle + \frac{\tau}{2}\|Ku - v\|^2,$$

such that

$$\min_{u,v} J(u,v) = \inf_{u,v}\sup_{p} \mathcal{L}_\tau(u,v;p).$$

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- **Alternating direction method of multipliers** (ADMM):

$$\begin{cases} u^{k+1} \in \arg\min_u G(u) + \left\langle p^k, Ku \right\rangle + \frac{\tau}{2}\|Ku - v^k\|^2, \\ v^{k+1} \in \arg\min_v F(v) - \left\langle p^k, v \right\rangle + \frac{\tau}{2}\|Ku^{k+1} - v\|^2, \\ p^{k+1} = p^k + \tau(Ku^{k+1} - v^{k+1}). \end{cases}$$

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Example: Consensus ADMM

- **Empirical risk minimization** (ERM):

$$\min_u \; F(u) + \frac{1}{n}\sum_{i=1}^{n} G_i(u),$$

where G_i represents the training error on sample (x_i, y_i):

$$G_i(u) = \text{loss}(h(x_i; u), y_i),$$

and F represents the model prior.

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- **Consensus optimization**:

$$\min_{u,\{v_i\}} \; F(u) + \frac{1}{n}\sum_{i=1}^{n} G_i(v_i)$$
$$\text{s.t.} \;\; v_i = u \quad \forall i \in \{1, ..., n\}.$$

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- Augmented Lagrangian:

$$\mathcal{L}_\tau(u, \{v_i\}, \{p_i\}) = F(u) + \frac{1}{n}\sum_{i=1}^{n}\left(G_i(v_i) + \langle p_i, v_i - u\rangle + \frac{\tau}{2}\|v_i - u\|^2 \right).$$

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- **Consensus ADMM**:

$$u^{k+1} = \mathrm{prox}_{F/\tau}\left(\frac{1}{n}\sum_{i=1}^{n}\left(v_i^k + \frac{1}{\tau}p_i^k\right)\right),$$
$$\forall i: \; v_i^{k+1} = \mathrm{prox}_{G_i/\tau}\left(u^{k+1} - \frac{1}{\tau}p_i^k\right),$$
$$\forall i: \; p_i^{k+1} = p_i^k + \tau(v_i^{k+1} - u^{k+1}).$$

Primal-dual hybrid gradient

- By Fenchel-Rockafellar duality theorem, we reformulate

$$\min_u \; F(Ku) + G(u)$$

as the saddle-point problem:

$$\sup_p \inf_u \langle p, Ku \rangle + G(u) - F^*(p).$$

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Primal-dual hybrid gradient

- By Fenchel-Rockafellar duality theorem, we reformulate

$$\min_{u} \; F(Ku) + G(u)$$

as the saddle-point problem:

$$\sup_{p} \inf_{u} \langle p, Ku \rangle + G(u) - F^*(p).$$

- **Primal-dual hybrid gradient** (PDHG) ($st > \|K\|^2$):

$$u^{k+1} = \arg\min_{u} \left\langle u, K^\top p^k \right\rangle + G(u) + \frac{s}{2}\|u - u^k\|^2,$$
$$p^{k+1} = \arg\min_{p} -\left\langle K(2u^{k+1} - u^k), p \right\rangle + F^*(p) + \frac{t}{2}\|p - p^k\|^2.$$

- Optimality conditions for the updates:

$$0 \in \partial G(u^{k+1}) + K^\top p^k + s(u^{k+1} - u^k),$$
$$0 \in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + t(p^{k+1} - p^k).$$

Scaled primal-dual hybrid gradient

- Recall PDGH:

$$
\begin{aligned}
0 &\in \partial G(u^{k+1}) + K^\top p^k + s(u^{k+1} - u^k), \\
0 &\in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + t(p^{k+1} - p^k).
\end{aligned}
$$

- Replace s, t by spd matrices $S, T \rightsquigarrow$ Scaled PDHG:

$$
\begin{aligned}
0 &\in \partial G(u^{k+1}) + K^\top p^k + S(u^{k+1} - u^k), \\
0 &\in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + T(p^{k+1} - p^k).
\end{aligned}
$$

- Scaled PDHG in compact form:

$$
0 \in \begin{bmatrix} S & -K^\top \\ -K & T \end{bmatrix} \left(\begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix} - \begin{bmatrix} u^k \\ p^k \end{bmatrix} \right) + \begin{bmatrix} \partial G & K^\top \\ -K & \partial F^* \end{bmatrix} \begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix}.
$$

Scaled primal-dual hybrid gradient

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- Scaled PDHG is a **customized proximal iteration**:

$$\boxed{0 \in M(\xi^{k+1} - \xi^k) + R(\xi^{k+1})} \;\Leftrightarrow\; \boxed{\xi^{k+1} = (M + R)^{-1} M \xi^k}$$

- Sufficient conditions to ensure convergence:
(1) M is spd matrix; (2) R is maximal monotone operator.

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Interpret ADMM as customized proximal iteration

- Recall ADMM (with reordered updates):

$$v^{k+1} \in \arg\min_{v} F(v) - \left\langle p^k, v \right\rangle + \frac{\tau}{2}\|Ku^k - v\|^2, \tag{1}$$

$$p^{k+1} = p^k + \tau(Ku^k - v^{k+1}), \tag{2}$$

$$u^{k+1} \in \arg\min_{u} G(u) + \left\langle p^{k+1}, Ku \right\rangle + \frac{\tau}{2}\|Ku - v^{k+1}\|^2. \tag{3}$$

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Interpret ADMM as customized proximal iteration

- Recall ADMM (with reordered updates):

$$v^{k+1} \in \arg\min_v F(v) - \left\langle p^k, v \right\rangle + \frac{\tau}{2}\|Ku^k - v\|^2, \tag{1}$$

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$$u^{k+1} \in \arg\min_u G(u) + \left\langle p^{k+1}, Ku \right\rangle + \frac{\tau}{2}\|Ku - v^{k+1}\|^2. \tag{3}$$

- ADMM as customized proximal iteration:

$$(1) \;\Rightarrow\; 0 \in \partial F(v^{k+1}) - p^k + \tau(v^{k+1} - Ku^k), \tag{4}$$

$$(3) \;\Rightarrow\; 0 \in \partial G(u^{k+1}) + K^\top p^{k+1} + \tau K^\top (Ku^{k+1} - v^{k+1}), \tag{5}$$

$$(2),(4) \;\Rightarrow\; p^{k+1} \in \partial F(v^{k+1}) \;\Leftrightarrow\; v^{k+1} \in \partial F^*(p^{k+1}), \tag{6}$$

$$(2),(5) \;\Rightarrow\; 0 \in \partial G(u^{k+1}) + K^\top(2p^{k+1} - p^k) + \tau K^\top K(u^{k+1} - u^k), \tag{7}$$

$$(2),(6) \;\Rightarrow\; 0 \in -Ku^k + \frac{1}{\tau}(p^{k+1} - p^k) + \partial F^*(p^{k+1}), \tag{8}$$

$$(7),(8) \;\Rightarrow\; 0 \in \begin{bmatrix} \tau K^\top K & K^\top \\ K & \frac{1}{\tau} I \end{bmatrix} \begin{bmatrix} u^{k+1} - u^k \\ p^{k+1} - p^k \end{bmatrix} + \begin{bmatrix} \partial G & K^\top \\ -K & \partial F^* \end{bmatrix} \begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix}.$$

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Reflection operator

- Given a proper, convex, lsc function $J : \mathbb{E} \to \overline{\mathbb{R}}$ and $\tau > 0$, we call

$$\mathrm{refl}_{\tau J} = 2\,\mathrm{prox}_{\tau J} - I = 2(I + \tau\partial J)^{-1} - I$$

the **reflection operator** on ∂J.

- In a more general definition for "refl", ∂J is replaced by a *maximal monotone operator*.
  - We don't formally introduce maximal monotone operator.
  - Fact: For any proper, convex, lsc function J, ∂J is indeed a maximal monotone operator.

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  - We don't formally introduce maximal monotone operator.
  - Fact: For any proper, convex, lsc function J, ∂J is indeed a maximal monotone operator.

- Fixed points of $\mathrm{refl}_{\tau J}$:

$$\begin{aligned} & u = \mathrm{refl}_{\tau J}(u) \\ \Leftrightarrow\ & u = 2\,\mathrm{prox}_{\tau J}(u) - u \\ \Leftrightarrow\ & u = \mathrm{prox}_{\tau J}(u) \\ \Leftrightarrow\ & 0 \in \partial J(u). \end{aligned}$$

Douglas-Rachford- & Peaceman-Rachford splitting

- Consider the *monotone inclusion* problem:

$$0 \in \partial F(u) + \partial G(u).$$

Douglas-Rachford- & Peaceman-Rachford splitting

- Consider the *monotone inclusion* problem:

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- **Douglas-Rachford splitting** (DRS):

$$\begin{cases} u^{k+1} = \operatorname{prox}_{\tau G}(v^k), \\ v^{k+1} = v^k - u^{k+1} + \operatorname{prox}_{\tau F}(2u^{k+1} - v^k). \end{cases} \tag{DRS}$$

- **Peaceman-Rachford splitting** (PRS):

$$\begin{cases} u^{k+1} = \operatorname{prox}_{\tau G}(v^k), \\ v^{k+1} = v^k - 2u^{k+1} + 2\operatorname{prox}_{\tau F}(2u^{k+1} - v^k). \end{cases} \tag{PRS}$$

- DRS & PRS in compact forms:

$$v^{k+1} = \left(\frac{1}{2}I + \frac{1}{2}\operatorname{refl}_{\tau F} \circ \operatorname{refl}_{\tau G}\right)(v^k), \tag{DRS'}$$

$$v^{k+1} = (\operatorname{refl}_{\tau F} \circ \operatorname{refl}_{\tau G})(v^k). \tag{PRS'}$$

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Douglas-Rachford- & Peaceman-Rachford splitting

Fixed points of DRS & PRS:

$$
\begin{aligned}
& v = \mathrm{refl}_{\tau F}(\mathrm{refl}_{\tau G}(v)) = 2\,\mathrm{prox}_{\tau F}(\mathrm{refl}_{\tau G}(v)) - \mathrm{refl}_{\tau G}(v) \\
\Leftrightarrow\ & \mathrm{prox}_{\tau F}(\mathrm{refl}_{\tau G}(v)) = \mathrm{prox}_{\tau G}(v) \\
\Leftrightarrow\ & \mathrm{refl}_{\tau G}(v) \in (I + \tau\partial F)(\mathrm{prox}_{\tau G}(v)) \\
\Leftrightarrow\ & 2\,\mathrm{prox}_{\tau G}(v) - v \in \mathrm{prox}_{\tau G}(v) + \tau\partial F(\mathrm{prox}_{\tau G}(v)) \\
\Leftrightarrow\ & \mathrm{prox}_{\tau G}(v) - v \in \tau\partial F(\mathrm{prox}_{\tau G}(v)) \\
\Leftrightarrow\ & u = \mathrm{prox}_{\tau G}(v), \quad u - v \in \tau\partial F(u) \\
\Leftrightarrow\ & v \in u + \tau\partial G(u), \quad u - v \in \tau\partial F(u) \\
\Leftrightarrow\ & 0 \in \partial F(u) + \partial G(u).
\end{aligned}
$$

Interpret DRS as customized proximal iteration

- Apply DRS to: $\min_u F(u) + G(u)$. $\Rightarrow$

$$u^{k+1} = \mathrm{prox}_{\tau G}(v^k), \tag{1}$$
$$v^{k+1} = v^k - u^{k+1} + \mathrm{prox}_{\tau F}(2u^{k+1} - v^k). \tag{2}$$

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- DRS as customized proximal iteration ($p^k := (u^k - v^k)/\tau$):

$$\begin{aligned}
(1) \;&\Leftrightarrow\; u^{k+1} = \mathrm{prox}_{\tau G}(u^k - \tau p^k) \;\Leftrightarrow\; u^k - \tau p^k \in (I + \tau\partial G)u^{k+1} \\
&\Leftrightarrow\; 0 \in (u^{k+1} - u^k)/\tau + p^k + \partial G(u^{k+1}), \qquad (3) \\
(2) \;&\Leftrightarrow\; 2u^{k+1} - u^k + \tau p^k = \tau p^{k+1} + \mathrm{prox}_{\tau F}(2u^{k+1} - u^k + \tau p^k) \\
&\Rightarrow\; \tau p^{k+1} = (I - \mathrm{prox}_{\tau F})(2u^{k+1} - u^k + \tau p^k) \\
&\Leftrightarrow\; p^{k+1} = \mathrm{prox}_{\frac{1}{\tau}F^*}((2u^{k+1} - u^k)/\tau + p^k) \quad \text{by Moreau's identity} \\
&\Leftrightarrow\; (2u^{k+1} - u^k)/\tau + p^k \in \left(I + \frac{1}{\tau}\partial F^*\right)(p^{k+1}) \\
&\Leftrightarrow\; 0 \in \tau(p^{k+1} - p^k) + \partial F^*(p^{k+1}) - (2u^{k+1} - u^k), \qquad (4)
\end{aligned}$$

$$(3), (4) \;\Rightarrow\; 0 \in \begin{bmatrix} \frac{1}{\tau}I & -I \\ -I & \tau I \end{bmatrix} \begin{bmatrix} u^{k+1} - u^k \\ p^{k+1} - p^k \end{bmatrix} + \begin{bmatrix} \partial G & I \\ -I & \partial F^* \end{bmatrix} \begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix}.$$

Demo: Image segmentation

- Variational model:

$$\min_{u:\Omega\to\Delta^L} \sum_{j\in\Omega} \Big(\delta\{u_j \in \Delta^L\} + \langle u_j, f_j\rangle\Big) + \alpha \sum_{l=1}^{L} \|\nabla u^l\|_1,$$

where Δ^L is the probability simplex in $\mathbb{R}^L$.

- Segmentation results:

image

segmentation ($L = 4$)

- Demo code in PyTorch (possibly accelerated by GPU) is provided on the course webpage.

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Convergence Theory

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Fixed-point iteration

Fixed-point iteration

Proximal algorithm as *fixed-point iteration*:

$$u^{k+1} = \Phi(u^k).$$

Its convergence depends on the property of Φ.

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Fixed-point iteration

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Proximal algorithm as *fixed-point iteration*:

$$u^{k+1} = \Phi(u^k).$$

Its convergence depends on the property of Φ.

Definition

Let C be a nonempty, closed, convex subset of $\mathbb{E}$ (equipped with $\|\cdot\| = \sqrt{\langle \cdot, \cdot \rangle}$), and $\Phi : C \to \mathbb{E}$. Then Φ is:

1. μ-Lipschitz with modulus $\mu \geq 0$ if

$$\forall u, v \in C : \|\Phi(u) - \Phi(v)\| \leq \mu \|u - v\|.$$

2. **contractive** if Φ is μ-Lipschitz with modulus $\mu \in [0, 1)$.
3. **nonexpansive** if Φ is 1-Lipschitz.

Tao Wu
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Fixed-point iteration

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Remark

1. If Φ is contractive (mod. $\mu \in [0, 1)$), then by **Banach fixed point theorem** the iteration $u^{k+1} = \Phi(u^k)$ converges to the unique fixed point u^* linearly: $\|u^k - u^*\| \leq \mu^k \|u^0 - u^*\|$.

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2. Unfortunately, Banach fixed point theorem does not apply here. Most proximal algorithms consist of nonexpansive operators Φ (including proj, prox, and refl), which are not contractive but "averaged' operators".

Averaged operator

Definition

Let C be a nonempty, closed, convex subset of $\mathbb{E}$. Then a map $\Phi : C \to \mathbb{E}$ is α-**averaged**, with $\alpha \in (0, 1)$, if there exists a nonexpansive operator $\Psi : C \to \mathbb{E}$ such that

$$\Phi = (1 - \alpha)I + \alpha\Psi.$$

In particular, "$\frac{1}{2}$-averaged" is also called **firmly nonexpansive**.

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Proposition

Let C be a nonempty, closed, convex subset of $\mathbb{E}$, $\Phi : C \to \mathbb{E}$, and $\alpha \in (0,1)$. Then the following statements are equivalent:

1. Φ is α-averaged.
2. $(1-\frac{1}{\alpha})I + \frac{1}{\alpha}\Phi$ is nonexpansive.
3. $\forall u, v \in C : \|\Phi(u) - \Phi(v)\|^2 \leq \|u-v\|^2 - \frac{1-\alpha}{\alpha}\|(I-\Phi)(u) - (I-\Phi)(v)\|^2$.
4. $\forall u, v \in C : \|\Phi(u) - \Phi(v)\|^2 + (1-2\alpha)\|u-v\|^2 \leq$
   $2(1-\alpha)\langle u-v, \Phi(u)-\Phi(v)\rangle$.

Proof: on board.

Averaged operator in proximal algorithms

- Recall the customized proximal iteration:

$$u^{k+1} = \Phi^{(\text{cpi})}(u^k), \quad \Phi^{(\text{cpi})} = (M + R)^{-1} M,$$

  for given spd matrix M and monotone operator R.
  - One can verify that $\Phi^{(\text{cpi})}$ is firmly nonexpansive under the scaled norm $\|\cdot\|_M = \sqrt{\langle \cdot, M \cdot \rangle}$.

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- Recall Douglas-Rachford splitting (in compact form):

$$v^{k+1} = \Phi^{(\text{drs})}(v^k), \ \ \Phi^{(\text{drs})} = \frac{1}{2} I + \frac{1}{2} \operatorname{refl}_{\tau F} \circ \operatorname{refl}_{\tau G},$$

for some proper, convex, lsc functions $F, G : \mathbb{E} \to \overline{\mathbb{R}}$.

  - Since $\operatorname{refl}_{\tau F} = 2 \operatorname{prox}_{\tau F} - I$ is nonexpansive and so is $\operatorname{refl}_{\tau G}$, $\Phi^{(\text{drs})}$ is firmly nonexpansive.

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  for some proper, convex, lsc functions $F, G : \mathbb{E} \to \overline{\mathbb{R}}$.
  - Since $\mathrm{refl}_{\tau F} = 2\,\mathrm{prox}_{\tau F} - I$ is nonexpansive and so is $\mathrm{refl}_{\tau G}$, $\Phi^{(\mathrm{drs})}$ is firmly nonexpansive.

- Recall forward-backward splitting:

$$u^{k+1} = \Phi^{(\mathrm{fbs})}(u^k), \quad \Phi^{(\mathrm{fbs})} = \mathrm{prox}_{\tau F} \circ (I - \tau \nabla G),$$

  where G is μ-Lipschitz differentiable and $\tau \in (0, 2/\mu)$.
  - As a consequence of the Baillon-Haddad Theorem (next slide), $I - \tau\nabla G$ is an averaged operator. Hence, $\Phi^{(\mathrm{fbs})}$ is a composition of two averaged operators (again averaged).

Averaged operator in gradient descent

Theorem (Baillon-Haddad)

Let $J : \mathbb{E} \to \mathbb{R}$ be a convex, continuously differentiable function. Then ∇J is a nonexpansive operator iff ∇J is firmly nonexpansive.

Proof: on board.

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Averaged operator in gradient descent

Theorem (Baillon-Haddad)

Let $J : \mathbb{E} \to \mathbb{R}$ be a convex, continuously differentiable function. Then ∇J is a nonexpansive operator iff ∇J is firmly nonexpansive.

Proof: on board.

Corollary

Assume $G : \mathbb{E} \to \mathbb{R}$ is convex and μ-Lipschitz differentiable, and $\tau = 2\alpha/\mu$ with $\alpha \in (0, 1)$. Then $I - \tau\nabla G$ is α-averaged.

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Averaged operator in gradient descent

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Let $J : \mathbb{E} \to \mathbb{R}$ be a convex, continuously differentiable function. Then ∇J is a nonexpansive operator iff ∇J is firmly nonexpansive.

Proof: on board.

Corollary

Assume $G : \mathbb{E} \to \mathbb{R}$ is convex and μ-Lipschitz differentiable, and $\tau = 2\alpha/\mu$ with $\alpha \in (0, 1)$. Then $I - \tau\nabla G$ is α-averaged.

Proof: Since $\frac{1}{\mu}\nabla G$ is nonexpansive, by the Baillon-Haddad theorem, $\frac{1}{\mu}\nabla G$ is firmly nonexpansive, i.e., $\exists\Psi : \mathbb{E} \to \mathbb{E}$ nonexpansive s.t. $\frac{1}{\mu}\nabla G = \frac{1}{2}I + \frac{1}{2}\Psi$. Hence,

$$I - \tau\nabla G = (1 - \frac{\tau\mu}{2})I - \frac{\tau\mu}{2}\Psi = (1 - \alpha)I + \alpha(-\Psi),$$

i.e. $I - \tau\nabla G$ is α-averaged.

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Composition of averaged operators

In forward-backward splitting,

$$\Phi^{(\text{fbs})} = \text{prox}_{\tau F} \circ \left(I - \frac{2\alpha}{\mu} \nabla G \right)$$

appears as the composition of a $\frac{1}{2}$-averaged operator $\text{prox}_{\tau F}$ and an α-averaged operator $I - \frac{2\alpha}{\mu} \nabla G$ with $\alpha \in (0, 1)$.

Composition of averaged operators

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Theorem (composition of averaged operators)

Let C be a nonempty, closed, convex subset of $\mathbb{E}$. For each $i \in \{1, \ldots, m\}$, let $\alpha_i \in (0, 1)$ and $\Phi_i : C \to C$ be an α_i-averaged operator. Then

$$\Phi = \Phi_m \circ \ldots \circ \Phi_1$$

is α-averaged with

$$\alpha = \frac{m}{m - 1 + \frac{1}{\max_{1 \le i \le m} \alpha_i}}.$$

<u>Proof</u>: on board.

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Convex combination of averaged operators

Theorem (convex combination of averaged operators)

Let C be a nonempty, closed, convex subset of $\mathbb{E}$. For each $i \in \{1, ..., m\}$, let $\alpha_i \in (0, 1)$, $\omega_i \in (0, 1)$ and $\Phi_i : C \to \mathbb{E}$ be an α_i-averaged operator. If $\sum_{i=1}^{m} \omega_i = 1$ and $\alpha = \max_{1 \le i \le m} \alpha_i$, then

$$\Phi = \sum_{i=1}^{m} \omega_i \Phi_i$$

is α-averaged.

Proof: as exercise.

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Convergence of averaged-operator iterations

Theorem (Krasnoselskii)

Let C be a nonempty, closed, convex subset of $\mathbb{E}$, and $u^{k+1} = \Phi(u^k)$ for $k = 0, 1, 2, \ldots$ where $\Phi : C \to C$ satisfies:

1. Φ is α-averaged for some $\alpha \in (0, 1)$.
2. Φ has at least one fixed point.

Then $\{u^k\}$ converges to a fixed point of Φ.

<u>Proof</u>: on board.

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Extension of Krasnoselskii Theorem

> **Theorem (Krasnoselskii-Mann)**
>
> Let C be a nonempty, closed, convex subset of $\mathbb{E}$, and $u^{k+1} = (1-\tau^k)u^k + \tau^k \Psi(u^k)$ for $k = 0, 1, 2, \ldots$ where $\{\tau^k\} \subset [0, 1]$ s.t.
>
> $$\sum_{k=0}^{\infty} \tau^k (1-\tau^k) = \infty,$$
>
> and $\Psi : C \to C$ satisfies:
>
> 1. Ψ is nonexpansive.
> 2. Ψ has at least one fixed point.
>
> Then the sequence $\{u^k\}$ converges to a fixed point of Ψ.
>
> Proof: on board.

Extension of Krasnoselskii Theorem

Theorem (Krasnoselskii-Mann)

Let C be a nonempty, closed, convex subset of $\mathbb{E}$, and $u^{k+1} = (1 - \tau^k)u^k + \tau^k \Psi(u^k)$ for $k = 0, 1, 2, \ldots$ where $\{\tau^k\} \subset [0, 1]$ s.t.

$$\sum_{k=0}^{\infty} \tau^k (1 - \tau^k) = \infty,$$

and $\Psi : C \to C$ satisfies:

1. Ψ is nonexpansive.
2. Ψ has at least one fixed point.

Then the sequence $\{u^k\}$ converges to a fixed point of Ψ.

Proof: on board.

Remarks

1. Condition $\sum_{k=0}^{\infty} \tau^k(1 - \tau^k) = \infty$ is fulfilled if $\{\tau^k\} \subset [\epsilon, 1 - \epsilon]$ for some $\epsilon \in (0, 1/2]$.
2. Decay rate of fixed-point residual: $\|u^{k+1} - u^k\| = o(1/\sqrt{k})$.

Convergence in infinite dimensional space

Theorem (Krasnoselskii in Hilbert space)

Let C be a nonempty, closed, convex subset of a (real) Hilbert space $\mathbb{H}$, and $u^{k+1} = \Phi(u^k)$ for $k = 0, 1, 2, \ldots$ where $\Phi : C \to C$ satisfies:

1. Φ is α-averaged for some $\alpha \in (0, 1)$.
2. Φ has at least one fixed point.

Then $\{u^k\}$ converges *weakly* to a fixed point of Φ.

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Convergence in infinite dimensional space

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1. Φ is α-averaged for some $\alpha \in (0, 1)$.
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Then $\{u^k\}$ converges *weakly* to a fixed point of Φ.

Proof: ... $\Rightarrow \|u^{k+1} - \bar{u}\|^2 \leq \|u^0 - \bar{u}\|^2 - \frac{1-\alpha}{\alpha} \sum_{l=0}^{k} \|(I - \Phi)(u^l)\|^2$
$\Rightarrow$ (i) $\|u^k - \bar{u}\| \searrow c \geq 0$; (ii) $\sum_{k=0}^{\infty} \|(I - \Phi)(u^k)\|^2 < \infty$.
(i) $\Rightarrow \{u^k\}$ converges weakly to $u^* \in C$ along a subsequence;
(ii) & "demiclosedness principle" $\Rightarrow u^* - \Phi(u^*) = 0$. $\Rightarrow$ ... $\square$

Lemma (demiclosedness principle)

Let C be a nonempty, closed, convex subset of a (real) Hilbert space $\mathbb{H}$, and $\Phi : C \to \mathbb{H}$ be nonexpansive. For any sequence $\{u^k\} \subset C$ s.t. $\{u^k\}$ weakly converges to $u \in C$ and $u^k - \Phi(u^k)$ strongly converges to $v \in \mathbb{H}$, we have $u - \Phi(u) = v$.

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Linear convergence under strong monotonicity

- Recall the customized proximal iteration:

$$0 \in M(u^{k+1} - u^k) + R(u^{k+1}),$$

where M is spd matrix, R is (maximal) monotone operator.

Linear convergence under strong monotonicity

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- Let $u^* = \lim_{k\to\infty} u^k$, $0 \in R(u^*)$, and $\xi^{k+1} \in R(u^{k+1})$ s.t.

$$\begin{aligned} 0 &= \left\langle u^{k+1} - u^*, u^{k+1} - u^k \right\rangle_M + \left\langle u^{k+1} - u^*, \xi^{k+1} - 0 \right\rangle \\ &= \frac{1}{2}\|u^{k+1} - u^*\|_M^2 - \frac{1}{2}\|u^k - u^*\|_M^2 + \frac{1}{2}\|u^{k+1} - u^k\|_M^2 \\ &\quad + \left\langle u^{k+1} - u^*, \xi^{k+1} - 0 \right\rangle . \end{aligned}$$

Linear convergence under strong monotonicity

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- Previously, we only assume R is monotone

$$\begin{aligned} &\Rightarrow \left\langle u^{k+1} - u^*, \xi^{k+1} - 0 \right\rangle \geq 0 \\ &\Rightarrow \frac{1}{2}\|u^{k+1} - u^*\|_M^2 \leq \frac{1}{2}\|u^k - u^*\|_M^2 - \frac{1}{2}\|u^{k+1} - u^k\|_M^2. \end{aligned}$$

- Next we shall assume R is “strongly monotone”.

Linear convergence under strong monotonicity

Strongly monotone operator

- R is said μ-**strongly monotone** if $R - \mu I$ is monotone.
- For proper, convex, lsc function J, ∂J is μ-strongly monotone iff J is μ-strongly convex, i.e., $J - \frac{\mu}{2}\|\cdot\|^2$ is convex.

Linear convergence under strong monotonicity

Strongly monotone operator

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- R is μ-strongly monotone

$$
\begin{aligned}
&\Rightarrow \left\langle u^{k+1} - u^*, \xi^{k+1} - 0 \right\rangle \geq \mu \|u^{k+1} - u^*\|^2 \\
&\Rightarrow \left(\frac{1}{2} + \frac{\mu}{\lambda_{\max}(M)} \right) \|u^{k+1} - u^*\|_M^2 \\
&\qquad \leq \frac{1}{2}\|u^{k+1} - u^*\|_M^2 + \mu\|u^{k+1} - u^*\|^2 \leq \frac{1}{2}\|u^k - u^*\|_M^2 \\
&\Rightarrow \|u^{k+1} - u^*\|_M \leq \sqrt{\frac{1}{1 + 2\mu/\lambda_{\max}(M)}} \|u^k - u^*\|_M.
\end{aligned}
$$

Linear convergence under strong monotonicity

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- R is μ-strongly monotone

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&\Rightarrow \|u^{k+1} - u^*\|_M \leq \sqrt{\frac{1}{1 + 2\mu/\lambda_{\max}(M)}}\|u^k - u^*\|_M.
\end{aligned}
$$

- Recall in PDHG:

$$
R = \begin{bmatrix} \partial G & K^\top \\ -K & \partial F^* \end{bmatrix}.
$$

R is μ-strongly monotone $\Leftrightarrow$ G, F^* are μ-strongly convex;
F^* is μ-strongly convex $\Leftrightarrow$ F is $\frac{1}{\mu}$-Lipschitz differentiable.

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Acceleration Techniques

Tao Wu
Zhenzhang Ye

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Outline of the section

1. Accelerating gradient step:
   - Second-order methods (Newton).
   - Multistep methods:
     - Heavy-ball method (Polyak).
     - Accelerated gradient method (Nesterov).
   - Embedding acceleration into proximal algorithms.
2. Preconditioning proximal algorithms:
   - Preconditioned PDHG algorithm.
   - Diagonal preconditioners (Pock/Chambolle).
   - Application to problems on weighted graphs.

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Newton's method

- Consider minimizing $J : \mathbb{E} \to \mathbb{R}$. J is convex and twice continuously differentiable.
- Classical Newton method:

$$d^k = -[\nabla^2 J(u^k)]^{-1} \nabla J(u^k), \quad u^{k+1} = u^k + d^k.$$

- ..., which minimizes the local quadratic model:

$$d^k = \arg\min_d J(u^k) + \left\langle \nabla J(u^k), d \right\rangle + \frac{1}{2} \left\langle d, \nabla^2 J(u^k) d \right\rangle.$$

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- Local quadratic convergence near u^*, where $\nabla J(u^*) = 0$ and $\nabla^2 J(u^*)$ is spd:

$$\begin{aligned}
&\|u^{k+1} - u^*\| = \|u^k - u^* - [\nabla^2 J(u^k)]^{-1} \nabla J(u^k)\| \\
&\leq \|[\nabla^2 J(u^k)]^{-1}\| \|\nabla^2 J(u^k)(u^k - u^*) - (\nabla J(u^k) - \nabla J(u^*))\| \\
&= O(\|u^k - u^*\|^2).
\end{aligned}$$

- Can we use Newton step in proximal gradient method?

Proximal Newton method

$$\min_{u \in \mathbb{E}} F(u) + G(u),$$

where F is convex (possibly non-differentiable), G is convex and twice continuously differentiable.

Proximal Newton method

Initialize $u^0 \in \mathbb{E}$. Iterate with $k = 0, 1, 2, ...$

1. $d^k = \arg\min_d F(u^k + d) + \langle \nabla G(u^k), d \rangle + \frac{1}{2} \langle d, \nabla^2 G(u^k) d \rangle$.
2. $u^{k+1} = u^k + d^k$.

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Theorem (local quadratic convergence of proximal Newton)

The proximal Newton method converges locally quadratically to the (global) minimizer u^* if $\nabla^2 G(u^*)$ is spd.

Proof: on board.

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Proximal Newton method

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Proximal Newton method

Initialize $u^0 \in \mathbb{E}$. Iterate with $k = 0, 1, 2, \dots$

1. $d^k = \arg\min_d F(u^k + d) + \langle \nabla G(u^k), d \rangle + \frac{1}{2} \langle d, \nabla^2 G(u^k) d \rangle$.
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The proximal Newton method converges locally quadratically to the (global) minimizer u^* if $\nabla^2 G(u^*)$ is spd.

Proof: on board.

Remark

1. Ensure global convergence via backtracking line search.
2. Computation of d^k can be involved even if prox_F is easy.

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Heavy-ball (momentum) acceleration

Heavy-ball method

Assume J is convex and differentiable. Initialize $u^0 \in \mathbb{E}$ and $u^{-1} = u^0$. Iterate with step sizes $\tau, \theta > 0$:

$$u^{k+1} = u^k - \tau \nabla J(u^k) + \theta(u^k - u^{k-1}).$$

Heavy-ball (momentum) acceleration

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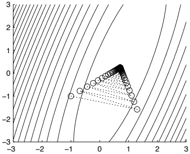
$$u^{k+1} = u^k - \tau \nabla J(u^k) + \theta(u^k - u^{k-1}).$$

- Invented by [Polyak, 1964]; $u^k - u^{k-1}$ is the *momentum*.
- Discretization of the 2nd-order ODE:

$$\theta \ddot{u} + (1-\theta)\dot{u} + \tau \nabla J(u) = 0.$$

- Alternative form implemented in machine learning:

$$v^{k+1} = \theta v^k - \tau \nabla J(u^k),$$
$$u^{k+1} = u^k + v^{k+1}.$$



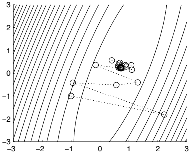


Figure: gradient descent (left) vs. heavy ball (right).

Heavy-ball method

- Quantitative analysis of heavy-ball method:

$$u^{k+1} = u^k - \tau \nabla J(u^k) + \theta(u^k - u^{k-1}).$$

$$\begin{bmatrix} u^{k+1} - u^* \\ u^k - u^* \end{bmatrix} = \begin{bmatrix} u^k + \theta(u^k - u^{k-1}) - u^* - \tau(\nabla J(u^k) - \nabla J(u^*)) \\ u^k - u^* \end{bmatrix}$$

$$= \begin{bmatrix} u^k + \theta(u^k - u^{k-1}) - u^* - \tau \nabla^2 J(\widetilde{u}^k)(u^k - u^*) \\ u^k - u^* \end{bmatrix} \quad (\widetilde{u}^k \in [u^k, u^*])$$

$$= \begin{bmatrix} (1+\theta)I - \tau \nabla^2 J(\widetilde{u}^k) & -\theta I \\ I & 0 \end{bmatrix} \begin{bmatrix} u^k - u^* \\ u^{k-1} - u^* \end{bmatrix} =: A^k \begin{bmatrix} u^k - u^* \\ u^{k-1} - u^* \end{bmatrix}.$$

Heavy-ball method

- Quantitative analysis of heavy-ball method:

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$$= \begin{bmatrix} (1+\theta)I - \tau \nabla^2 J(\widetilde{u}^k) & -\theta I \\ I & 0 \end{bmatrix} \begin{bmatrix} u^k - u^* \\ u^{k-1} - u^* \end{bmatrix} =: A^k \begin{bmatrix} u^k - u^* \\ u^{k-1} - u^* \end{bmatrix}.$$

- <u>Lemma</u>: Assume $\forall k : \mathrm{sr}(A^k) \le \rho$, then $\exists \epsilon_k \to 0^+$ s.t. $\|A^k A^{k-1} \cdots A^0\| \le (\rho + \epsilon_k)^k \ \forall k$. (sr = spectral radius)

Theorem

Assume $\forall k : \mu I \preceq \nabla^2 J(\widetilde{u}^k) \preceq LI$ for some constants $\mu, L > 0$. If $\theta \ge \max\{|1 - \sqrt{\tau\mu}|, |1 - \sqrt{\tau L}|\}^2$, then $\mathrm{sr}(A^k) = \sqrt{\theta} \ \ \forall k$.

<u>Proof</u>: on board.

- Apply the theorem with $\tau = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2}$, $\theta = \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^2$

$\Rightarrow$ asymptotic rate $\rho = \frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}$.

Nesterov's Accelerated gradient method

Minimize J that is convex and continuously differentiable.
Assume ∇J is L-Lipschitz continuous.

Accelerated gradient method

Initialize $u^0 \in \mathbb{E}$, and $u^{-1} = u^0,\ \beta^0 = 1$. Iterate with step size $0 < \tau \leq 1/L$:

1. $\beta^{k+1} = (1 + \sqrt{1 + 4(\beta^k)^2})/2,\ \theta^k = (\beta^k - 1)/\beta^{k+1}$.
2. $v^k = u^k + \theta^k(u^k - u^{k-1})$.
3. $u^{k+1} = v^k - \tau \nabla J(v^k)$.

- Originated from [Nesterov, 1983].
- The gradient is evaluated at the *extrapolated* point v^k.
- The analysis of this scheme is somewhat technical.

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Multistep proximal gradient method

We embed multistep acceleration into proximal gradient for:

$$\min_{u \in \mathbb{E}} F(u) + G(u),$$

where F is convex (possibly non-differentiable), G is convex and twice continuously differentiable, and $\mu I \preceq \nabla^2 G(\cdot) \preceq LI$.

Proximal heavy-ball method

Initialize $u^0 \in \mathbb{E}$, and set $u^{-1} = u^0,\ \tau = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2},\ \theta = \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$.
Iterate with $k = 0, 1, 2, ...$

$$u^{k+1} = \mathrm{prox}_{\tau F}(u^k - \tau \nabla G(u^k) + \theta(u^k - u^{k-1})).$$

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Initialize $u^0 \in \mathbb{E}$, and set $u^{-1} = u^0,\ \tau = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2},\ \theta = \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$.
Iterate with $k = 0, 1, 2, ...$

$$u^{k+1} = \text{prox}_{\tau F}(u^k - \tau \nabla G(u^k) + \theta(u^k - u^{k-1})).$$

Proximal accelerated gradient method

Initialize $u^0 \in \mathbb{E}$, and set $u^{-1} = u^0,\ \beta^0 = 1,\ 0 < \tau \leq 1/L$.
Iterate with $k = 0, 1, 2, ...$

1. $\beta^{k+1} = (1 + \sqrt{1 + 4(\beta^k)^2})/2,\ \theta^k = (\beta^k - 1)/\beta^{k+1}$.
2. $v^k = u^k + \theta^k(u^k - u^{k-1})$.
3. $u^{k+1} = \text{prox}_{\tau F}(v^k - \tau \nabla G(v^k))$.

Preconditioning iterative linear solvers

- Consider solving the linear system

$$Qu = b \quad \Leftrightarrow \quad \min_u \frac{1}{2} \langle u, Qu \rangle - \langle b, u \rangle ,$$

where $b \in \mathbb{R}^n$, $Q \in \mathbb{R}^{n \times n}$ is spd.

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  where $b \in \mathbb{R}^n,\ Q \in \mathbb{R}^{n \times n}$ is spd.
- Define the *condition number* $\kappa_Q = \dfrac{\lambda_{\max}(Q)}{\lambda_{\min}(Q)}$, then
  - Convergence rate for steepest descent: $\dfrac{\kappa_Q - 1}{\kappa_Q + 1}$.
  - Convergence rate for conjugate gradient: $\dfrac{\sqrt{\kappa_Q} - 1}{\sqrt{\kappa_Q} + 1}$.

Preconditioning iterative linear solvers

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  - Convergence rate for steepest descent: $\dfrac{\kappa_Q - 1}{\kappa_Q + 1}$.
  - Convergence rate for conjugate gradient: $\dfrac{\sqrt{\kappa_Q} - 1}{\sqrt{\kappa_Q} + 1}$.
  - Preconditioning (or rescaling) with spd $M \in \mathbb{R}^{n\times n}$:

$$\begin{cases} \widehat{Q} = M^{-1/2}QM^{-1/2},\ \widehat{u} = M^{1/2}u,\ \widehat{b} = M^{-1/2}b, \\ \text{Solve: } \min_{\widehat{u}} \frac{1}{2}\langle \widehat{u}, \widehat{Q}\widehat{u}\rangle - \langle \widehat{b}, \widehat{u}\rangle, \quad \text{ideally with } \kappa_{\widehat{Q}} \ll \kappa_Q. \end{cases}$$

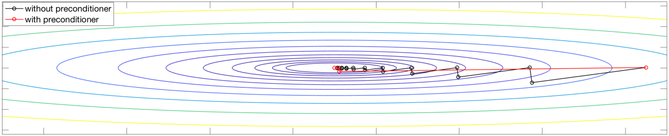

Figure: Steepest descent: without precond. vs. with precond.

Preconditioning PDHG

- Recall the saddle-point problem:

$$\max_{p} \min_{u} \langle p, Ku \rangle + G(u) - F^*(p).$$

- Recall the scaled PDHG:

$$0 \in \partial G(u^{k+1}) + K^\top p^k + S(u^{k+1} - u^k), \quad \{\text{primal update}\}$$
$$0 \in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + T(p^{k+1} - p^k). \quad \{\text{dual update}\}$$

- Compact-form PDHG:

$$0 \in \begin{bmatrix} S & -K^\top \\ -K & T \end{bmatrix} \left(\begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix} - \begin{bmatrix} u^k \\ p^k \end{bmatrix} \right) + \begin{bmatrix} \partial G & K^\top \\ -K & \partial F^* \end{bmatrix} \begin{bmatrix} u^{k+1} \\ p^{k+1} \end{bmatrix}.$$

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- Here S is primal preconditioner, T is dual preconditioner:

$$\begin{cases} \widehat{u} = S^{1/2}u, \ \widehat{p} = T^{1/2}p, \ \widehat{K} = T^{-1/2}KS^{-1/2}, \\ \widehat{G} = G \circ S^{-1/2}, \ \widehat{F} = F \circ T^{1/2}. \\ \text{Solve: } \max_{\widehat{p}} \min_{\widehat{u}} \langle \widehat{p}, \widehat{K}\widehat{u} \rangle + \widehat{G}(\widehat{u}) - \widehat{F}^*(\widehat{p}). \end{cases}$$

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Preconditioning PDHG

- Here $\color{red}{S}$ is primal preconditioner, $\color{blue}{T}$ is dual preconditioner:

$$\begin{cases} \widehat{u} = \color{red}{S}^{1/2}u, \ \widehat{p} = \color{blue}{T}^{1/2}p, \ \widehat{K} = \color{blue}{T}^{-1/2}K\color{red}{S}^{-1/2}, \\ \widehat{G} = G \circ \color{red}{S}^{-1/2}, \ \widehat{F} = F \circ \color{blue}{T}^{1/2}. \\ \text{Solve: } \max_{\widehat{p}} \min_{\widehat{u}} \langle \widehat{p}, \widehat{K}\widehat{u} \rangle + \widehat{G}(\widehat{u}) - \widehat{F}^*(\widehat{p}). \end{cases}$$

- PDHG on $(\widehat{u}, \widehat{p})$:

$$0 \in \partial \widehat{G}(\widehat{u}^{k+1}) + \widehat{K}^\top \widehat{p}^k + (\widehat{u}^{k+1} - \widehat{u}^k),$$
$$0 \in \partial \widehat{F}^*(\widehat{p}^{k+1}) - \widehat{K}(2\widehat{u}^{k+1} - \widehat{u}^k) + (\widehat{p}^{k+1} - \widehat{p}^k).$$

- Compact-form PDHG on $(\widehat{u}, \widehat{p})$:

$$0 \in \begin{bmatrix} I & -\widehat{K}^\top \\ -\widehat{K} & I \end{bmatrix} \left(\begin{bmatrix} \widehat{u}^{k+1} \\ \widehat{p}^{k+1} \end{bmatrix} - \begin{bmatrix} \widehat{u}^{k} \\ \widehat{p}^{k} \end{bmatrix} \right) + \begin{bmatrix} \partial \widehat{G} & \widehat{K}^\top \\ -\widehat{K} & \partial \widehat{F}^* \end{bmatrix} \begin{bmatrix} \widehat{u}^{k+1} \\ \widehat{p}^{k+1} \end{bmatrix}.$$

Preconditioning PDHG

- Here S is primal preconditioner, T is dual preconditioner:

$$\begin{cases} \widehat{u} = S^{1/2}u, \ \widehat{p} = T^{1/2}p, \ \widehat{K} = T^{-1/2}KS^{-1/2}, \\ \widehat{G} = G \circ S^{-1/2}, \ \widehat{F} = F \circ T^{1/2}. \\ \text{Solve: } \max\limits_{\widehat{p}} \min\limits_{\widehat{u}} \langle \widehat{p}, \widehat{K}\widehat{u} \rangle + \widehat{G}(\widehat{u}) - \widehat{F}^*(\widehat{p}). \end{cases}$$

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Proposition

Assume S, T are spd matrices. Then

$$M_{S,T} = \begin{bmatrix} S & -K^\top \\ -K & T \end{bmatrix} \succ 0 \Leftrightarrow \begin{bmatrix} I & -\widehat{K}^\top \\ -\widehat{K} & I \end{bmatrix} \succ 0$$

$$\Leftrightarrow \ \|T^{-1/2}KS^{-1/2}\| < 1.$$

Proof: Argue with *Schur complement*.

Gradient Methods

Proximal Algorithms

Convergence Theory

Acceleration

Summary

Choices of preconditioners

- Scaled PDHG:

$$\begin{cases} 0 \in \partial G(u^{k+1}) + K^\top p^k + S(u^{k+1} - u^k), \\ 0 \in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + T(p^{k+1} - p^k). \end{cases}$$

- Expectations on S and T:
  1. S and T shall fulfill $M_{S,T} \succ 0$.
  2. (Scaled) resolvents $(S + \partial G)^{-1}$ and $(T + \partial F^*)^{-1}$ are easy to compute.
  3. $\widehat{K} = T^{-1/2} K S^{-1/2}$ has smaller condition number than K.
     - The theory for why this accelerates convergence is open.
     - Empirical evidences of acceleration are observed.

- Goal: Design S and T that balance (1), (2), (3).

Gradient Methods
Proximal Algorithms
Convergence Theory
Acceleration
Summary

Diagonal preconditioner

- Diagonal preconditioners [Pock/Chambolle, 2011]:

$$S = \mathrm{diag}(\{s_j\}),\ s_j = \sum_i |K_{ij}|^{2-\theta},$$
$$T = \mathrm{diag}(\{t_i\}),\ t_i = \sum_j |K_{ij}|^{\theta},$$

  where $\theta \in [0, 2]$.

- $\widehat{K} = T^{-1/2} K S^{-1/2}$ suggests that S (resp. T) normalizes columns (resp. rows) of K by row (resp. column) sums.

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- Convergence is (almost) justified by the following result:

Proposition

Given matrix K, the diagonal preconditioners S and T above satisfy $M_{S,T} \succeq 0$.

Proof: on board.

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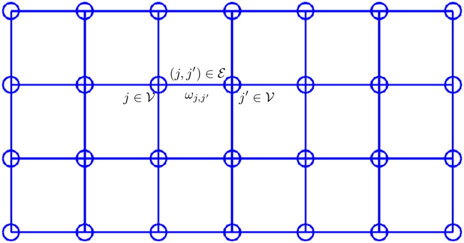
- Particularly interesting for problems on *weighted graphs*...

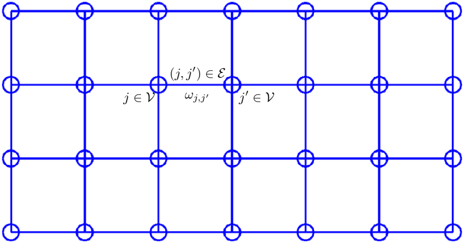
Convex optimization on weighted graphs



- Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \omega)$ be a weighted graph, with $\mathcal{V}$ set of vertices, $\mathcal{E}$ set of edges, $\omega : \mathcal{E} \to \mathbb{R}_+$ weight for edges.
- $\nabla \in \mathbb{R}^{|\mathcal{E}| \times |\mathcal{V}|}$ is the *incidence matrix* s.t. for each $(j, j') \in \mathcal{E}$:

$$\nabla_{(j,j'),j} = 1, \ \nabla_{(j,j'),j'} = -1, \ \nabla_{(j,j'),j''} = 0 \ \text{ whenever } j'' \notin \{j, j'\}.$$

Convex optimization on weighted graphs



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  $\nabla_{(j,j'),j} = 1, \ \nabla_{(j,j'),j'} = -1, \ \nabla_{(j,j'),j''} = 0$ whenever $j'' \notin \{j, j'\}$.
- Convex optimization on weighted graphs:

$$\min_{u:\mathcal{V}\to\mathbb{R}} F(Ku) + G(u).$$

  where $F : \mathbb{R}^{\mathcal{E}} \to \mathbb{R}$, $G : \mathbb{R}^{\mathcal{V}} \to \mathbb{R}$ are convex functions, and $K = \mathrm{diag}(\omega)\nabla$.

Example: Image segmentation on 2D grid

- Segment images represented on the 2D grid:

$$\min_{u:\mathcal{V}\to\mathbb{R}^L} \underbrace{\sum_{j\in\mathcal{V}} \Big(\delta\{u_j \in \Delta^{L-1}\} + \langle u_j, f_j\rangle\Big)}_{G(u)} + \underbrace{\alpha \sum_{l=1}^{L} \sum_{(j,j')\in\mathcal{E}} \omega_{j,j'} |u_j^l - u_{j'}^l|}_{F(Ku)},$$

- $\mathcal{V}$ contains image pixels; $\mathcal{E}$, ω are model-dependent.
- Pointwise constraint: Δ^{L-1} is the probability simplex in $\mathbb{R}^L$.
- Unary term: $f : \mathcal{V} \to \mathbb{R}^L$ is the pixelwise prediction.
- Pairwise term: $\omega_{j,j'}$ models pairwise similarities, e.g.
  - Edges are forged among spatially neighbored pixels; or
  - Use Gaussian similarity measure: $\omega_{j,j'} = \exp\left(-\frac{|j-j'|^2}{\sigma^2}\right)$.

Empirical study

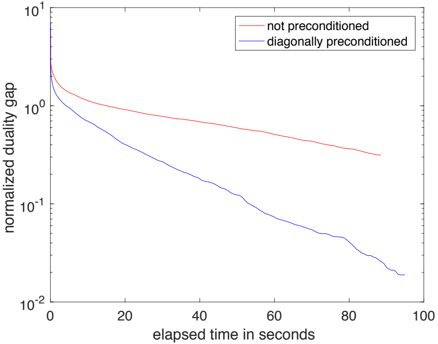
On the image segmentation example, we compare PDHG

$$\begin{cases} 0 \in \partial G(u^{k+1}) + K^\top p^k + S(u^{k+1} - u^k), \\ 0 \in \partial F^*(p^{k+1}) - K(2u^{k+1} - u^k) + T(p^{k+1} - p^k), \end{cases}$$

(i) without preconditioning and (ii) with preconditioning:

(i) $S = sI,\ T = tI,\ s = t = \|K\|$.

(ii) $S = \mathrm{diag}(\{s_j\}),\ T = \mathrm{diag}(\{t_i\}),\ s_j = \sum_i |K_{ij}|,\ t_i = \sum_j |K_{ij}|$.



What you should know from this chapter

- Gradient methods:
  - What is a descent method? (descent direction & step size)
  - How to guarantee convergence? (descent method with line search, majorize-minimize)
- Proximal algorithms:
  - How to derive proximal algorithms (FBS, ADMM, PDHG, DRS) on model problems?
  - When / how to apply a specific proximal algorithm to a specific problem?
  - What is an averaged operator?
  - How to interpret proximal algorithms as customized proximal iterations?
  - How to prove convergence of averaged-operator fixed-point iterations? (under general / special assumptions)
- Acceleration techniques (not for exam):
  - How to accelerate gradient steps in proximal algorithms? (Second-order, multistep)
  - How to precondition PDHG?
  - Some intuitions on why such acceleration techniques work.