

Chapter 2

Optimization Algorithms

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

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Optimization
Algorithms

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Gradient Methods

Proximal Algorithms

Convergence Theory

Acceleration

Summary



Gradient-based Methods

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Summary

Overview of this section

Unconstrained, differentiable, possibly nonconvex optimization

Problem setting:

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

Assume:

- 1 $J : \mathbb{E} \rightarrow \mathbb{R}$ is continuously differentiable.
- 2 There exists a global minimizer u^* . (Typically, an optimization 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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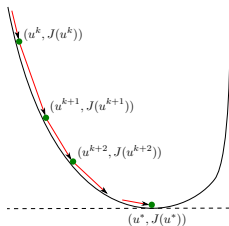
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- 2 Line search method.
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Analytical questions:

- 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 $k = 0, 1, 2, \dots$

- 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.

$$\langle \nabla J(u^k), d^k \rangle < 0.$$

- 3 Choose an “appropriate” step size $\tau^k > 0$, and update

$$u^{k+1} = u^k + \tau^k d^k.$$



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

Proof: Use the Taylor expansion:

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



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Choices of descent direction

- 1 Gradient/Steepest descent:
 $d^k = -\nabla J(u^k) = \arg \min_{d \in \mathbb{E}, \|d\| \leq 1} \langle \nabla J(u^k), d \rangle$.
- 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.



Gradient Methods

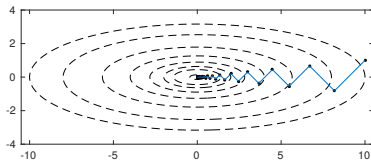
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Gradient descent with exact line search



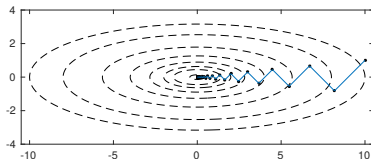
- Gradient descent with *exact* line search:

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

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



Gradient descent with exact line search



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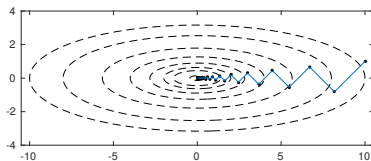
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- Case study: $J(u) = \frac{1}{2} \langle u, Qu \rangle - \langle b, u \rangle$, matrix Q is spd.
 - $\nabla J(u) = Qu - b$, $\|\cdot\|_Q^2 \equiv \langle \cdot, Q \cdot \rangle$.



Gradient descent with exact line search



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- $\tau^k = \arg \min_{\tau \geq 0} J(u^k - \tau \nabla J(u^k)) = \frac{\|\nabla J(u^k)\|_Q^2}{\|\nabla J(u^k)\|_Q^2} \Rightarrow$
$$\|u^{k+1} - u^*\|_Q^2 = \left(1 - \frac{\|\nabla J(u^k)\|_Q^4}{\|\nabla J(u^k)\|_Q^2 \|\nabla J(u^k)\|_{Q^{-1}}^2}\right) \|u^k - u^*\|_Q^2$$
$$\leq \left(\frac{\lambda_{\max}(Q) - \lambda_{\min}(Q)}{\lambda_{\max}(Q) + \lambda_{\min}(Q)}\right)^2 \|u^k - u^*\|_Q^2.$$



Backtracking line search

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

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

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

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



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

Gradient Methods

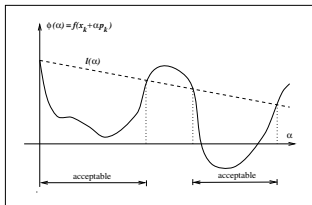
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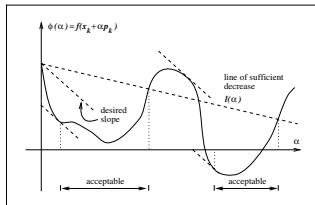
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Armijo l.s.



Wolfe-Powell l.s.



Convergence of backtracking line search

Lemma (feasibility of line search)

Assume that $J : \mathbb{E} \rightarrow \mathbb{R}$ is continuously differentiable, $\langle \nabla J(u^k), d^k \rangle < 0 \forall k$, 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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Proof: on board.

Theorem (Zoutendijk)

Assume that $J : \mathbb{E} \rightarrow \mathbb{R}$ 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

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

Proof: on board.

Remark

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



Majorize-minimize method

Majorizing function

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

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



Majorize-minimize method

Majorizing function

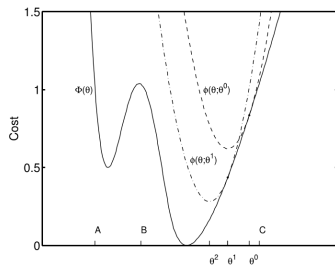
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Majorize-minimize (MM) algorithm

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

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



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

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

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



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Lemma

Assume that $J : \mathbb{E} \rightarrow \mathbb{R}$ 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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Assume that $J : \mathbb{E} \rightarrow \mathbb{R}$ is μ -Lipschitz differentiable. Then the gradient descent iteration

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

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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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Proximal Algorithms

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):**

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

- 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 $K : \mathbb{E}_1 \rightarrow \mathbb{E}_2$, find $u \in \mathbb{E}_1$ s.t. $u \in C_1$, $Ku \in C_2$.

- Variational model:

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

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



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- Optimality condition:

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

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



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- Apply FBS \Rightarrow

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



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 .



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- *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

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

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



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

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- Augmented Lagrangian:

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- Consensus ADMM:

$$u^{k+1} = \text{prox}_{F/\tau} \left(\frac{1}{n} \sum_{i=1}^n \left(v_i^k + \frac{1}{\tau} p_i^k \right) \right),$$

$$\forall i: v_i^{k+1} = \text{prox}_{G_i/\tau} \left(u^{k+1} - \frac{1}{\tau} p_i^k \right),$$

$$\forall i: p_i^{k+1} = p_i^k + \tau(v_i^{k+1} - u^{k+1}).$$

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 (PDHG)** ($st > \|K\|^2$):

$$u^{k+1} = \arg \min_u \langle u, K^\top p^k \rangle + G(u) + \frac{s}{2} \|u - u^k\|^2,$$

$$p^{k+1} = \arg \min_p - \langle K(2u^{k+1} - u^k), p \rangle + F^*(p) + \frac{t}{2} \|p - p^k\|^2.$$

- 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:

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- 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

- Recall PDGH:

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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 for convergence:

(1) M is spd matrix; (2) R is maximal monotone operator.



Interpret ADMM as customized proximal iteration

- Recall ADMM (with reordered updates):

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

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

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



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- ADMM as customized proximal iteration:

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

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

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

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

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

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

Reflection operator

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

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

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 $\text{refl}_{\tau J}$:

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



Douglas-Rachford- & Peaceman-Rachford splitting

- Consider the *monotone inclusion* problem:

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Douglas-Rachford- & Peaceman-Rachford splitting

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- Douglas-Rachford splitting (DRS):**

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

- Peaceman-Rachford splitting (PRS):**

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

- DRS & PRS in compact forms:

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

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





Fixed points of DRS & PRS:

$$v = \text{refl}_{\tau F}(\text{refl}_{\tau G}(v)) = 2 \text{prox}_{\tau F}(\text{refl}_{\tau G}(v)) - \text{refl}_{\tau G}(v)$$

$$\Leftrightarrow \text{prox}_{\tau F}(\text{refl}_{\tau G}(v)) = \text{prox}_{\tau G}(v)$$

$$\Leftrightarrow \text{refl}_{\tau G}(v) \in (I + \tau \partial F)(\text{prox}_{\tau G}(v))$$

$$\Leftrightarrow 2 \text{prox}_{\tau G}(v) - v \in \text{prox}_{\tau G}(v) + \tau \partial F(\text{prox}_{\tau G}(v))$$

$$\Leftrightarrow \text{prox}_{\tau G}(v) - v \in \tau \partial F(\text{prox}_{\tau G}(v))$$

$$\Leftrightarrow u = \text{prox}_{\tau G}(v), \quad u - v \in \tau \partial F(u)$$

$$\Leftrightarrow v \in u + \tau \partial G(u), \quad u - v \in \tau \partial F(u)$$

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

Interpret DRS as customized proximal iteration

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

$$u^{k+1} = \text{prox}_{\tau G}(v^k), \quad (1)$$

$$v^{k+1} = v^k - u^{k+1} + \text{prox}_{\tau F}(2u^{k+1} - v^k). \quad (2)$$



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

$$\begin{aligned} (1) &\Leftrightarrow u^{k+1} = \text{prox}_{\tau G}(u^k - \tau p^k) \Leftrightarrow u^k - \tau p^k \in (I + \tau \partial G)u^{k+1} \\ &\Leftrightarrow 0 \in (u^{k+1} - u^k)/\tau + p^k + \partial G(u^{k+1}), \end{aligned} \quad (3)$$

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

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

Demo: Image segmentation

- Variational model:

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

where Δ^{L-1} is the probability simplex in \mathbb{R}^L .

- Segmentation results:

image



segmentation ($L = 4$)

