Chapter 2
Optimization Algorithms

Convex Optimization for Machine Learning & Computer Vision
SS 2018

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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.
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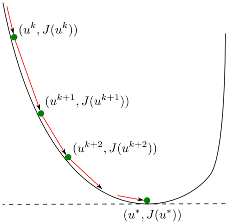
Analytical questions:

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:

$$J(u^k + \tau d^k) = J(u^k) + \tau \left\langle \nabla J(u^k), d^k \right\rangle + o(\tau)$$

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

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Choices of descent direction

1. Scaled gradient: $d^k = -(H^k)^{-1} \nabla J(u^k)$.
2. Gradient/Steepest descent: $H^k = I$.
3. Newton: $H^k = \nabla^2 J(u^k)$, assuming J is twice continuously differentiable and $\nabla^2 J(u^k) \succ 0$.
4. Quasi-Newton: $H^k \approx \nabla^2 J(u^k)$, H^k is spd.

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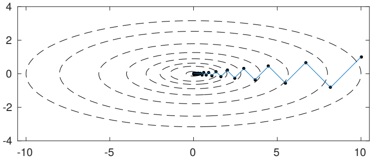
Gradient descent with exact line search



- Gradient descent with *exact* line search:

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

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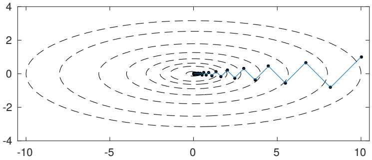

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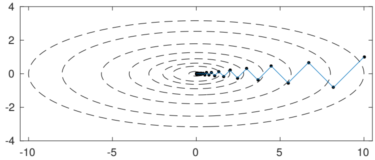
- Special case: $J(u) = \frac{1}{2}\langle u, Qu\rangle - \langle b, u\rangle$, matrix Q is spd.
  - $\nabla J(u) = Qu - b, \quad \|\cdot\|_Q^2 \equiv \langle \cdot, Q\,\cdot\rangle$.

Gradient descent with exact line search



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

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

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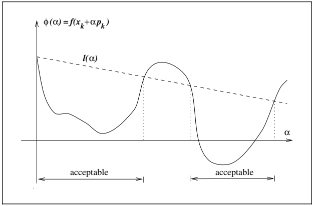
- (A) $\rightsquigarrow$ **Armijo** line search; (A) & (C) $\rightsquigarrow$ **Wolfe-Powell** l.s.

Armijo l.s.



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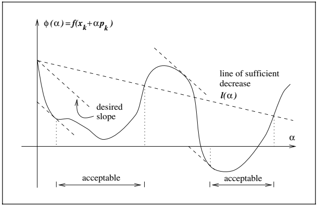

Convergence of backtracking line search

Lemma (feasibility of line search)

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

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

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Proof: 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

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

Proof: 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 $\lim_{k\to\infty} \|\nabla J(u^k)\| = 0$.

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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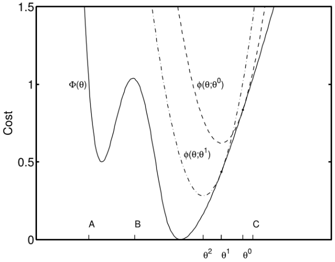
Majorize-minimize (MM) algorithm

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 $J(u^k) + \langle \nabla J(u^k), \cdot - u^k \rangle + \frac{1}{2\tau} \| \cdot - u^k \|^2 \geq J(\cdot)$ 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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Theorem (convergence of gradient descent)

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

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

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

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Proof: 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.

Proximal Algorithms

Agenda for the rest of the chapter

- Proximal algorithms for 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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- Application on examples.
- Equivalence between proximal algorithms.
- (Unified) convergence analysis.
- Acceleration techniques.

Forward-backward splitting

- Consider

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

whose minimizer is characterized by

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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 $\Rightarrow$

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

Example: Regularized least squares

Regularized least squares

$$\min_u F(u) + \frac{1}{2}\|A(u) - b\|^2,$$

where

- A: differentiable operator (modeling the *forward* process).
- b: observation.
- F: regularization/prior term.
  - $\text{prox}_{\tau F}$ is easy to compute.
  - e.g., $F(\cdot) = \|\cdot\|_2^2$, $F(\cdot) = \|\cdot\|_1$, or $F(\cdot) = \|\cdot\|_{\text{nuclear}}$.

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- Optimality condition:

$$0 \in \partial F(u) + \nabla A(u)^\top (A(u) - b).$$

- Apply FBS $\Rightarrow$

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

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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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

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

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

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

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

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

- 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:

$$0 \in \partial G(u^{k+1}) + K^\top p^k + s(u^{k+1} - u^k),$$
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- 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):

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

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

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

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- ADMM as customized proximal iteration:

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

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

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

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

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

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

Reflection operator

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

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

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

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

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Douglas-Rachford- & Peaceman-Rachford splitting

- Consider the monotone inclusion problem:

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

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

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

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- DRS & PRS in compact form:

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

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

Douglas-Rachford- & Peaceman-Rachford splitting

Fixed points of DRS & PRS:

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

Interpret DRS as customized proximal iteration

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

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

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

$$(1) \Leftrightarrow u^{k+1} = \mathrm{prox}_{\tau G}(u^k - \tau w^k) \Leftrightarrow u^k - \tau w^k \in (I + \tau \partial G) u^{k+1}$$
$$\Leftrightarrow 0 \in (u^{k+1} - u^k)/\tau + w^k + \partial G(u^{k+1}), \tag{3}$$

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

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