ORF522 – Linear and Nonlinear Optimization

16. Proximal methods and introduction to operator theory

Ed Forum

- Since there might be multiple subgradients that are very different, is there way
 to sometimes choose a 'best' subgradient for a given function that helps the
 algorithm converges faster?
- In Page 41 of Lecture 15, for the first fraction in this page, how do we conclude that it attains minimum when all t_k are equal based on the fact that the fraction is convex and symmetric in (t_1,...,t_k)?

Recap

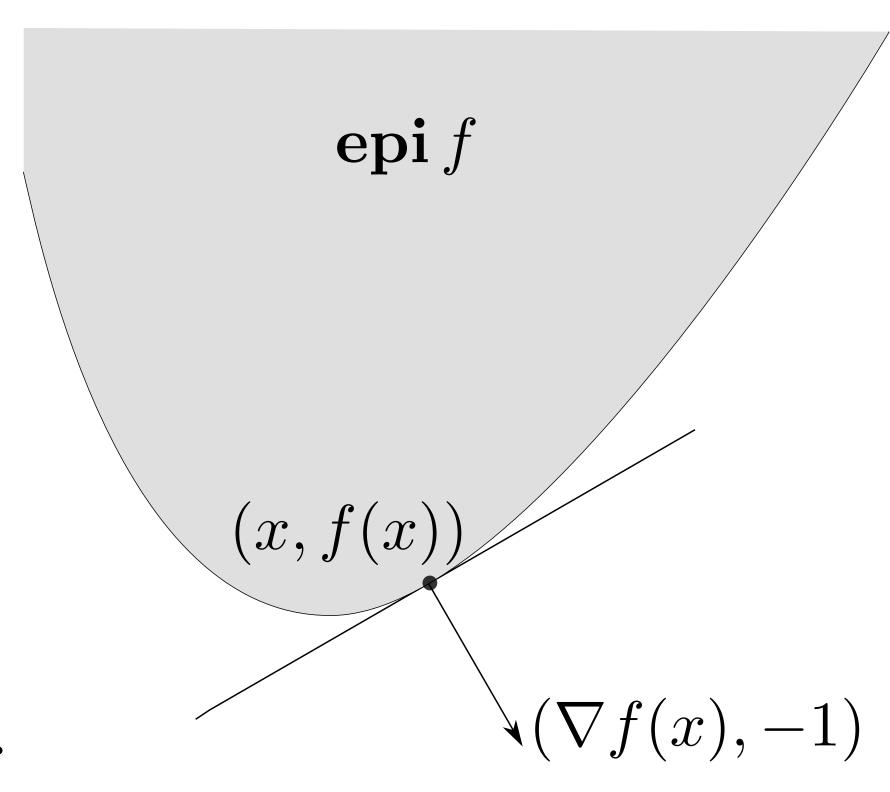
Gradients and epigraphs

For a convex differentiable function f, i.e.

$$f(y) \ge f(x) + \nabla f(x)^T (y - x), \quad \forall y \in \mathbf{dom} f$$

 $(\nabla f(x), -1)$ defines a supporting hyperplane to epigraph of f at (x, f(x))

$$\begin{bmatrix} \nabla f(x) \\ -1 \end{bmatrix}^T \left(\begin{bmatrix} y \\ t \end{bmatrix} - \begin{bmatrix} x \\ f(x) \end{bmatrix} \right) \le 0, \quad \forall (y, t) \in \mathbf{epi} f$$



Fermat's optimality condition

For any (not necessarily convex) function f where $\partial f(x^*) \neq \emptyset$,

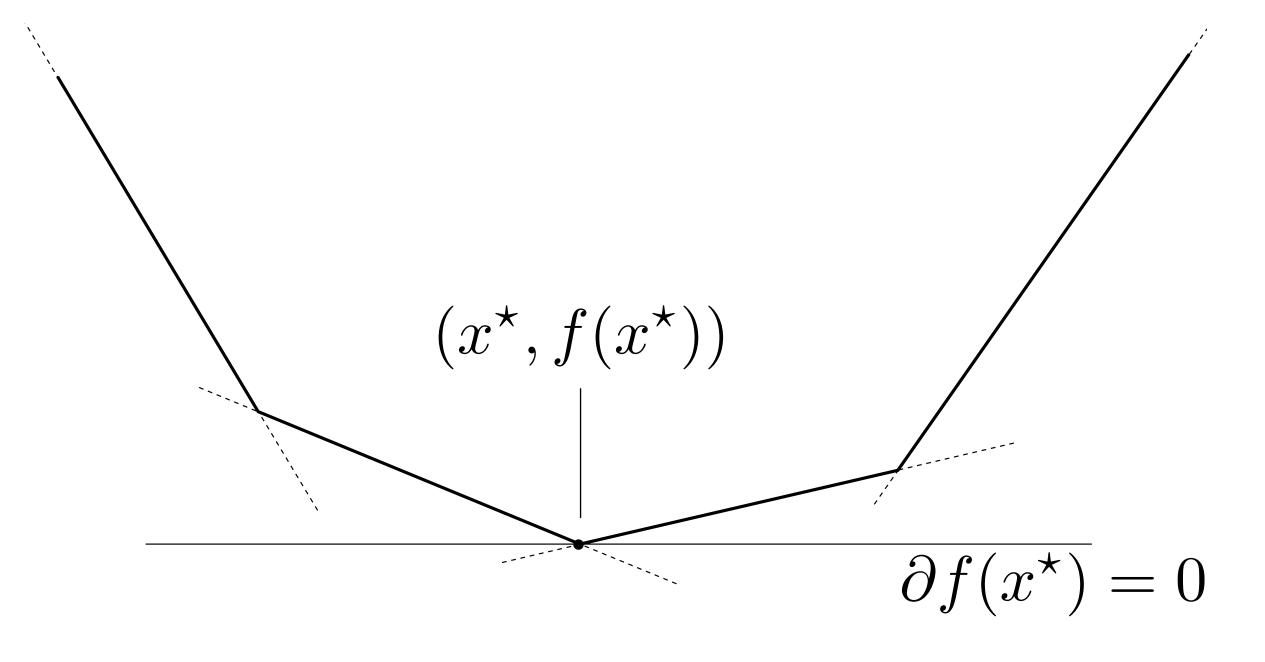
 x^{\star} is a global minimizer if and only if

$$0 \in \partial f(x^{\star})$$

Proof

A subgradient g=0 means that, for all y

$$f(y) \ge f(x^*) + 0^T (y - x^*) = f(x^*)$$



Note differentiable case with $\partial f(x) = \{\nabla f(x)\}$

Subgradient method

Convex optimization problem

minimize f(x) (optimal cost f^*)

Iterations

$$x^{k+1} = x^k - t_k g^k, \qquad g^k \in \partial f(x^k)$$

 g^k is any subgradient of f at x^k

Not a descent method, keep track of the best point

$$f_{\text{best}}^k = \min_{i=1,\dots,k} f(x^i)$$

Implications for step size rules

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2 \sum_{i=0}^k t_i^2}{2 \sum_{i=0}^k t_i}$$

Fixed:

$$t_k = t$$
 for $k = 0, \dots$

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2(k+1)t^2}{2(k+1)t}$$

May be suboptimal

$$\lim_{k \to \infty} f_{\text{best}}^k \le f^* + \frac{G^2 t}{2}$$

Diminishing:
$$\sum_{k=0}^{\infty} t_k^2 < \infty, \quad \sum_{k=0}^{\infty} t_k = \infty$$

e.g.,
$$t_k = \tau/(k+1)$$
 or $t_k = \tau/\sqrt{k+1}$

Optimal

$$\lim_{k \to \infty} f_{\text{best}}^k = f^*$$

Summary subgradient method

- Simple
- Handles general nondifferentiable convex functions
- Very slow convergence $O(1/\epsilon^2)$
- No good stopping criterion

Can we do better?

Can we incorporate constraints?

Today's lecture [Chapter 3 and 6, FMO] [PA] [PMO]

Proximal methods and introduction to operators

- Optimality conditions with subdifferentials
- Proximal operators
- Proximal gradient method
- Operator theory
- Fixed point iterations

Optimality conditions with subdifferentials

Subgradient of indicator function

 $\mathcal{N}_C(x)$

The subdifferential of the indicator function is the normal cone

$$\partial \mathcal{I}_C(x) = \mathcal{N}_C(x)$$

where,

$$\mathcal{N}_C(x) = \left\{ g \mid g^T(y - x) \le 0, \text{ for all } y \in C \right\}$$



By definition of subgradient g, $\mathcal{I}_C(y) \geq \mathcal{I}_C(x) + g^T(y-x)$, $\forall x \in \mathcal{I}_C(x)$

$$y \notin C \implies \mathcal{I}_C(y) = \infty$$

$$y \in C \implies 0 \ge g^T(y-x)$$

Constrained optimization

Indicator function

of a convex set

$$\mathcal{I}_C(x) = \begin{cases} 0 & x \in C \\ \infty & x \notin C \end{cases}$$

Constrained form

 $\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C \end{array}$

Unconstrained form

minimize $f(x) + \mathcal{I}_C(x)$

First-order optimality conditions from subdifferentials

minimize
$$f(x) + \mathcal{I}_C(x)$$

f convex smooth, C convex

Fermat's optimality condition

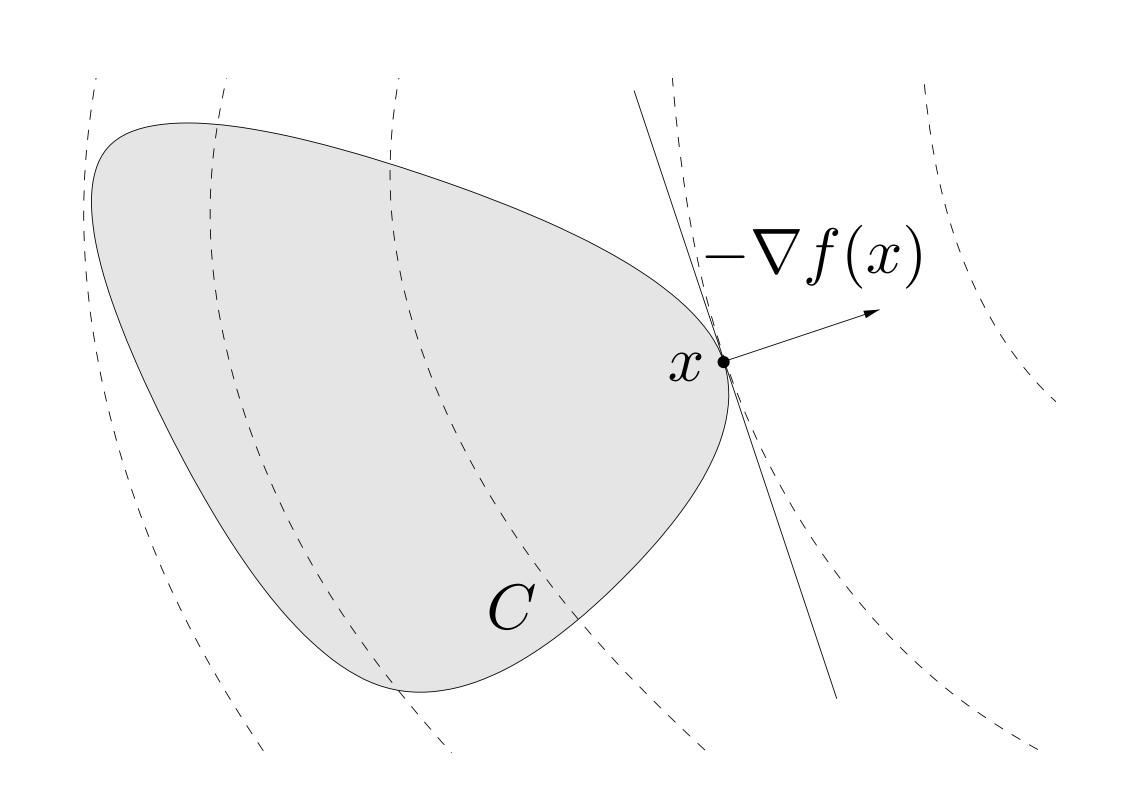
$$0 \in \partial(f(x) + \mathcal{I}_C(x))$$

$$\iff 0 \in \{\nabla f(x)\} + \mathcal{N}_C(x)$$

$$\iff -\nabla f(x) \in \mathcal{N}_C(x)$$

Equivalent to

$$\nabla f(x)^T (y - x) \ge 0, \quad \forall y \in C$$



Example: KKT of a quadratic program

Gradient

$$\nabla f(x) = Px + q$$

Normal cone to polyhedron Proof: [Theorem 6.46, Variational Analysis,

$$\mathcal{N}_{\{Ax \le b\}}(x) = \{A^T y \mid y \ge 0 \text{ and } y_i(a_i^T x - b_i) = 0\}$$

First-order optimality condition

$-\nabla f(x) \in \partial \mathcal{I}_{\{Ax < b\}}(x) = \mathcal{N}_{\{Ax < b\}}(x)$

KKT Optimality conditions

$$Px + q + A^{T}y = 0$$

$$y \ge 0$$

$$Ax - b \le 0$$

$$y_{i}(a_{i}^{T}x - b_{i}) = 0, \quad i = 1, ..., m$$

Idea: [Lecture 13].

Rockafellar & Wets]

Proximal operators

Composite models

minimize
$$f(x) + g(x)$$

f(x) convex and smooth g(x) convex (may be not differentiable)

Examples

- Regularized regression: $g(x) = ||x||_1$
- Constrained optimization: $g(x) = \mathcal{I}_C(x)$

Proximal operator

Definition

The proximal operator of the function $g: \mathbf{R}^n \to \mathbf{R}$ is

$$\mathbf{prox}_g(x) = \operatorname*{argmin}_z \left(g(z) + \frac{1}{2} ||z - x||_2^2 \right)$$

Optimality conditions of prox

$$0 \in \partial g(z) + z - x \implies x - z \in \partial g(z)$$

Properties

- It involves solving an optimization problem (not always easy!)
- Easy to evaluate for many standard functions, i.e. proxable functions
- · Generalizes many well-known algorithms

Generalized projection

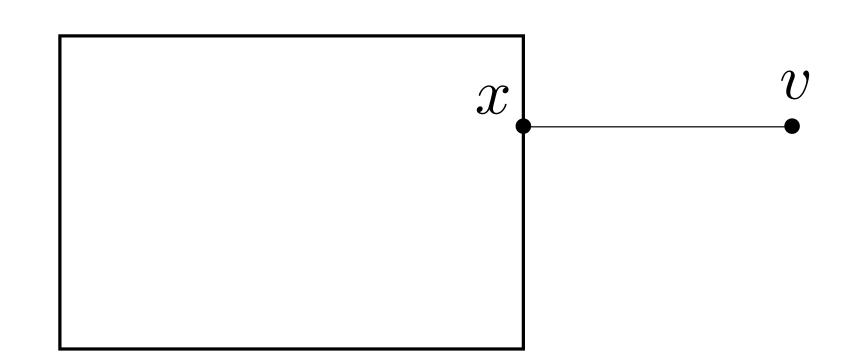
The prox operator of the indicator function \mathcal{I}_C is the projection onto C

$$\mathbf{prox}_{\mathcal{I}_C}(v) = \underset{x \in C}{\operatorname{argmin}} \|x - v\|_2 = \Pi_C(v)$$

Example projection onto a box $C = \{x \mid l \le x \le u\}$

$$\Pi_C(v)_i = \begin{cases} l_i & v_i \le l_i \\ v_i & l_i \le v_i \le u_i \end{cases}$$

$$u_i & v_i \ge u_i$$



Remarks

- Easy for many common sets (e.g., closed form)
- Can be hard for surprisingly simple lets, e.g., $C = \{Ax \leq b\}$

Quadratic functions

If
$$g(x) = (1/2)x^T P x + q^T x + r$$
 with $P \succeq 0$, then

$$\mathbf{prox}_g(v) = (I+P)^{-1}(v-q)$$

Remarks

- Closed-form always solvable (even with P not full rank)
- Symmetric, positive definite and usually sparse linear system
- Can prefactor I+P and solve for different v

Separable sum

If
$$g(x)$$
 is block separable, i.e., $g(x) = \sum_{i=1}^{N} g_i(x_i)$

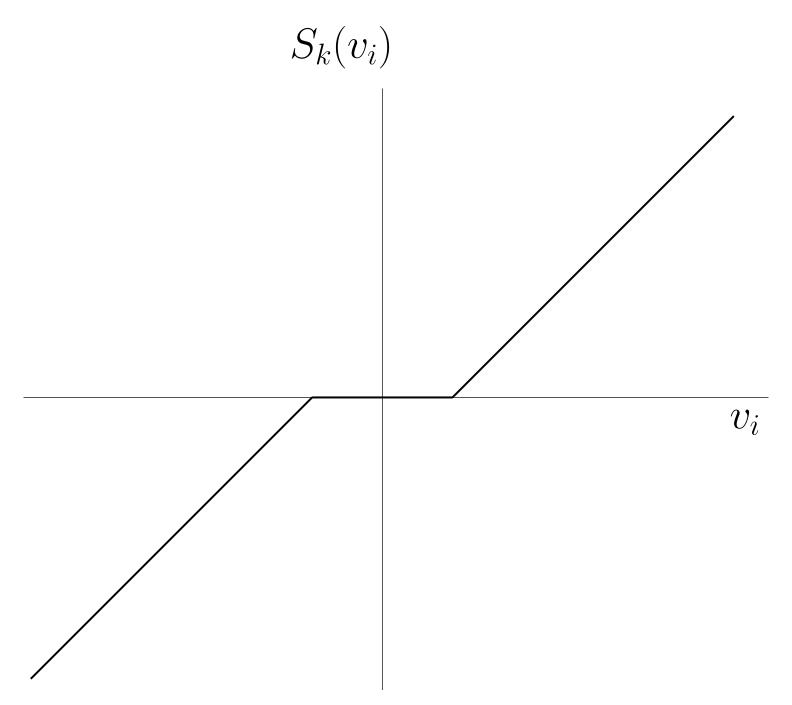
then,
$$(\mathbf{prox}_g(v))_i = \mathbf{prox}_{g_i}(v_i), \quad i = 1, \dots, N$$

(key to parallel/distributed proximal algorithms)

Example:
$$g(x) = \lambda ||x||_1 = \sum_{i=1}^{n} \lambda |x_i|$$

soft-thresholding

$$(\mathbf{prox}_g(v))_i = \mathbf{prox}_{\lambda|\cdot|}(v_i) = S_{\lambda}(v_i) = \begin{cases} v_i - \lambda & v_i > \lambda \\ 0 & |v_i| \le \lambda \\ v_i + \lambda & v_i < -\lambda \end{cases}$$



Basic rules

• Scaling and translation: g(x) = ah(x) + b with a > 0, then $\mathbf{prox}_{q}(x) = \mathbf{prox}_{ah}(x)$

Examples

- Affine addition: $g(x) = h(x) + a^T x + b$, then $\mathbf{prox}_{q}(x) = \mathbf{prox}_{h}(x-a)$
- Affine transformation: g(x) = h(ax + b), with $a \neq 0, a \in \mathbb{R}$,

$$\mathbf{prox}_g(x) = \frac{1}{a} \left(\mathbf{prox}_{a^2h}(ax + b) - b \right)$$

Proofs (exercise):

- Rearrange proximal term: $(1/2)||z-x||_2^2$
- Apply prox optimality conditions

Proximal gradient method

Gradient descent interpretation

Problem

minimize f(x)

Iterations

$$x^{k+1} = x^k - t\nabla f(x^k)$$

Quadratic approximation, replacing Hessian $\nabla^2 f(x^k)$ with $\frac{1}{t}I$ $x^{k+1} = \operatorname*{argmin} f(x^k) + \nabla f(x^k)^T (z-x^k) + \frac{1}{2t} \|z-x^k\|_2^2$

Let's exploit the smooth part

minimize
$$f(x) + g(x)$$

f(x) convex and smooth g(x) convex (may be not differentiable)

Quadratic approximation of f while keeping g

$$x^{k+1} = \operatorname*{argmin}_z g(z) + f(x^k) + \nabla f(x^k)^T (z-x^k) + \frac{1}{2t} \|z-x^k\|_2^2 \hspace{0.2cm} \longleftarrow \hspace{0.2cm} \underset{\text{gradient descent}}{\operatorname{same as}}$$

Equivalent to

Proximal operator

$$x^{k+1} = \underset{z}{\operatorname{argmin}} \ \frac{tg(z)}{t} + \frac{1}{2} \left\| z - (x^k - t\nabla f(x^k)) \right\|_2^2 = \mathbf{prox}_{tg} \left(x^k - t\nabla f(x^k) \right)$$

$$\underset{z}{\uparrow} \qquad \qquad \uparrow$$

$$\underset{z}{\uparrow} \qquad \qquad \uparrow$$

$$\underset{z}{\text{make } g} \qquad \text{stay close to }$$

$$\underset{z}{\text{small}} \qquad \underset{z}{\text{gradient update}}$$

Proximal gradient method

minimize
$$f(x) + g(x)$$

f(x) convex and smooth g(x) convex (may be not differentiable)

Iterations

$$x^{k+1} = \mathbf{prox}_{tg} \left(x^k - t\nabla f(x^k) \right)$$

Properties

- Alternates between gradient updates of f and proximal updates on g
- Useful if \mathbf{prox}_{tg} is inespensive
- Can handle nonsmooth and constrained problems

Special cases

Generalized gradient descent

Smooth

$$g(x) = 0 \implies \mathbf{prox}_{tq}(x) = x$$

Constraints

$$g(x) = \mathcal{I}_C(x) \implies \mathbf{prox}_{tg}(x) = \Pi_C(x)$$

Non smooth

$$f(x) = 0$$

Problem

minimize f(x) + g(x)

Iterations

$$x^{k+1} = \mathbf{prox}_{tg} \left(x^k - t \nabla f(x^k) \right)$$

Gradient descent

$$\implies x^{k+1} = x^k - t\nabla f(x^k)$$

Projected gradient descent

$$\implies x^{k+1} = \Pi_C(x^k - t\nabla f(x^k))$$

Proximal minimization

$$\implies x^{k+1} = \mathbf{prox}_{tg}(x^k)$$

Note: useful if \mathbf{prox}_{tq} is cheap ²⁶

What happens if we cannot evaluate the prox?

At every iteration, it can be very expensive to evaluate

$$\mathbf{prox}_g(x) = \operatorname*{argmin}_z \left(g(z) + \frac{1}{2} ||z - x||_2^2 \right)$$

Idea: solve it approximately!

If you precisely control the $\mathbf{prox}_g(x)$ evaluation errors you can obtain the same convergence guarantees (and rates) as the exact evaluations.

Example: Lasso

Iterative Soft Thresholding Algorithm (ISTA)

minimize
$$(1/2) ||Ax - b||_2^2 + \lambda ||x||_1$$
 $f(x)$ $g(x)$

Proximal gradient descent

$$x^{k+1} = \mathbf{prox}_{tg} \left(x^k - t\nabla f(x^k) \right)$$

$$\nabla f(x) = A^T (Ax - b)$$

$$\mathbf{prox}_{tg}(x) = S_{\lambda t}(x)$$
 (component wise soft-thresholding)

Closed-form iterations

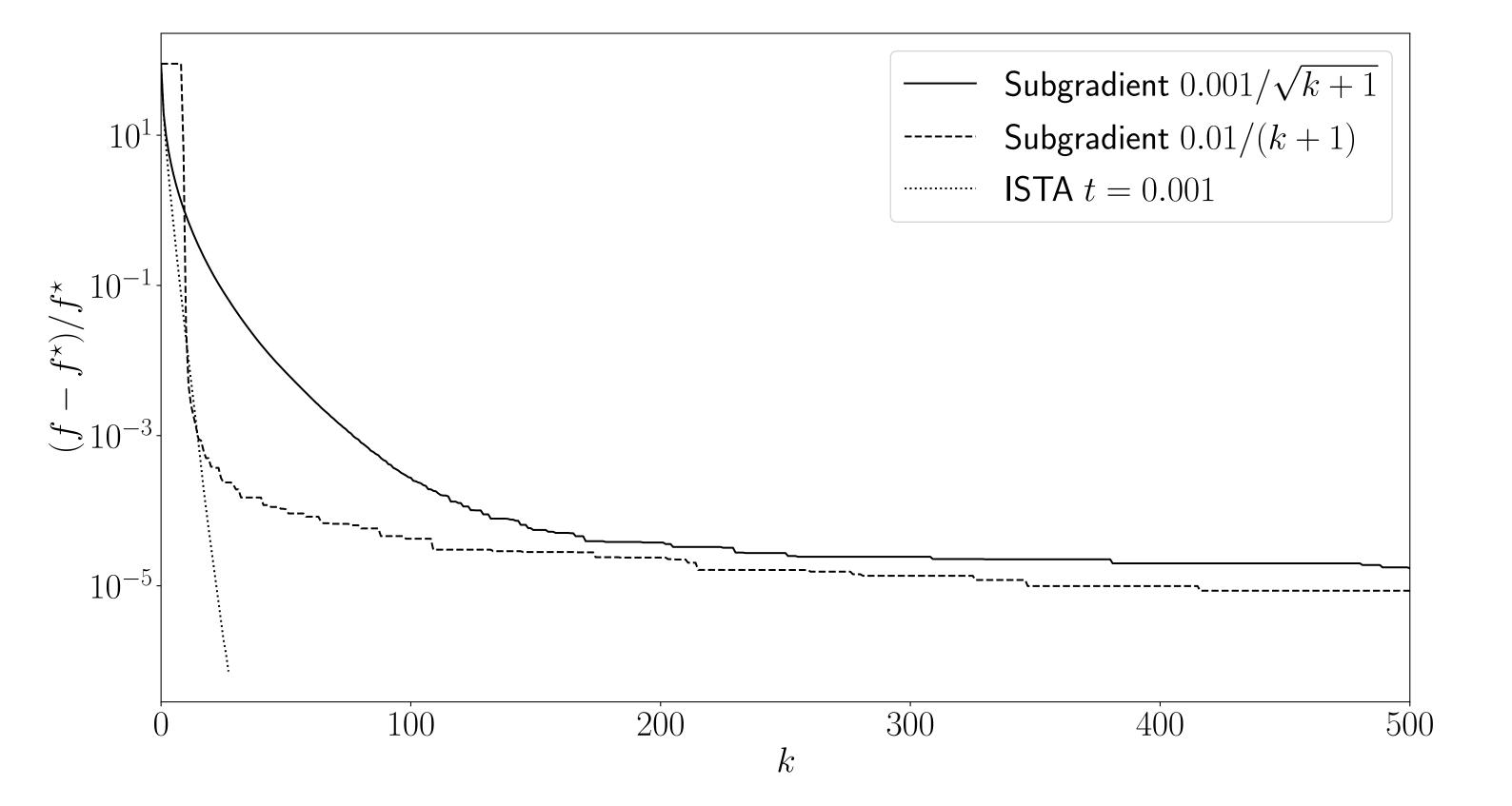
$$x^{k+1} = S_{\lambda t} (x^k - tA^T (Ax^k - b))$$

Example: Lasso

Iterative Soft Thresholding Algorithm (ISTA)

 $A \in \mathbf{R}^{500 \times 100}$

minimize
$$(1/2)||Ax - b||_2^2 + \lambda ||x||_1$$



Closed-form iterations

$$x^{k+1} = S_{\lambda t} \left(x^k - tA^T (Ax^k - b) \right)$$

Better convergence

Can we prove convergence generally?

Can we combine different operators?

Introduction to operators

Operators

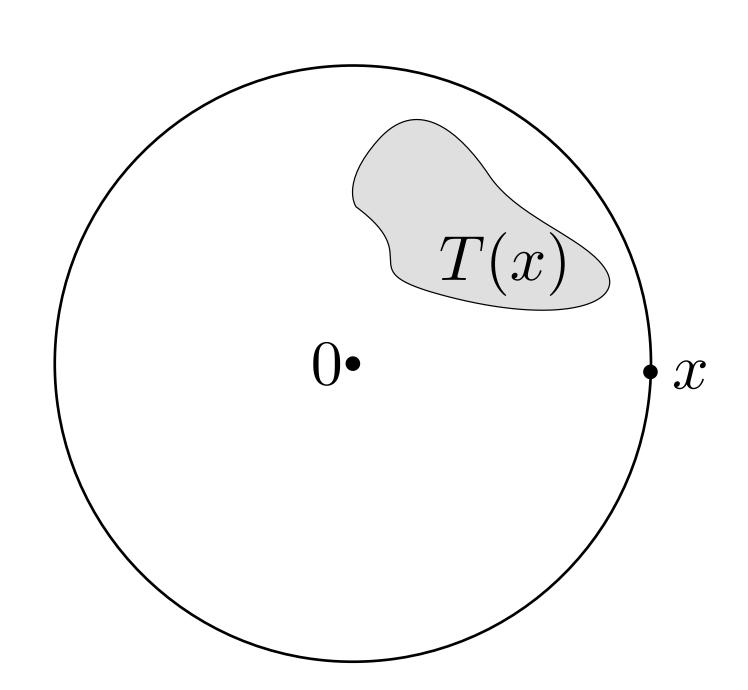
An operator T maps each point in \mathbf{R}^n to a subset of \mathbf{R}^n

- set valued T(x) returns a set
- single-valued T(x) (function) returns a singleton

The domain of T is the set $\operatorname{dom} T = \{x \mid T(x) \neq \emptyset\}$

Example

- The subdifferential ∂f is a set-valued operator
- The gradient ∇f is a single-valued operator



Graph and inverse operators

Graph

The graph of an operator T is defined as

$$\mathbf{gph}T = \{(x, y) \mid y \in T(x)\}$$

In other words, all the pairs of points (x, y) such that $y \in T(x)$.

Inverse

The graph of the inverse operator T^{-1} is defined as

$$gphT^{-1} = \{(y, x) \mid (x, y) \in gphT\}$$

Therefore, $y \in T(x)$ if and only if $x \in T^{-1}(y)$.

Zeros

Zero

x is a **zero** of T if

$$0 \in T(x)$$

Zero set

The set of all the zeros

$$T^{-1}(0) = \{x \mid 0 \in T(x)\}$$

Example

If $T=\partial f$ and $f:\mathbf{R}^n\to\mathbf{R}$, then $0\in T(x)$ means that x minimizes f

Many problems can be posed as finding zeros of an operator

Fixed points

 \bar{x} is a **fixed-point** of a single-valued operator T if

$$\bar{x} = T(\bar{x})$$

Set of fixed points
$$\operatorname{fix} T = \{x \in \operatorname{dom} T \mid x = T(x)\} = (I - T)^{-1}(0)$$

Examples

- Identity T(x) = x. Any point is a fixed point
- Zero operator T(x) = 0. Only 0 is a fixed point

Lipschitz operators

An operator T is L-Lipschitz if

$$||T(x) - T(y)|| \le L||x - y||, \quad \forall x, y \in \text{dom } T$$

Fact If T is Lipschitz, then it is single-valued

Proof If
$$y = T(x), z = T(x)$$
, then $||y - z|| \le L||x - x|| = 0 \Longrightarrow y = z$

For L=1 we say T is nonexpansive

For L < 1 we say T is **contractive** (with contraction factor L)

Lipschitz operators examples

Lipschitz affine functions

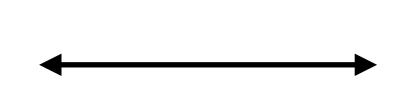
$$T(x) = Ax + b$$



maximum singular value $L = ||A||_2 = \sqrt{\lambda_{\max}(A^T A)}$

Lipschitz differentiable functions

T such that there exists derivative DT



derivative is bounded

$$||DT||_2 \leq L$$

Lipschitz operators and fixed points

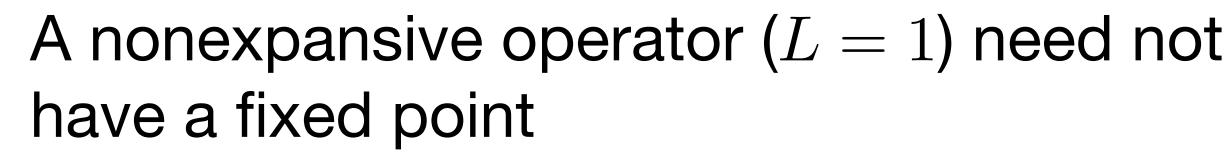
Given a L-Lipschitz operator T and a fixed point $\bar{x}=T\bar{x}$,

$$||Tx - \bar{x}|| = ||Tx - T\bar{x}|| \le L||x - \bar{x}||$$

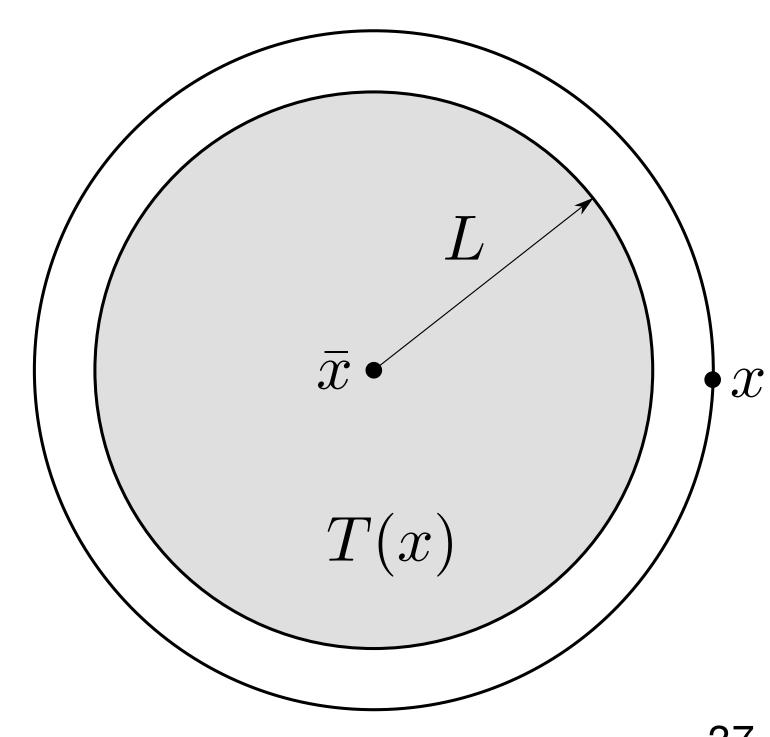
A contractive operator (L<1) can have at most one fixed point, i.e., fix $T=\{\bar{x}\}$

Proof

If $\bar x, \bar y \in \operatorname{fix} T$ and $\bar x \neq \bar y$ then $\|\bar x - \bar y\| = \|T(\bar x) - T(\bar y)\| < \|\bar x - \bar y\|$ (contradiction)



Example
$$T(x) = x + 2$$



Combining Lipschitz operators

 T_1 is L_1 -Lipschitz and T_2 is L_2 -Lipschitz

The composition T_1T_2 is L_1L_2 -Lipschitz

Proof
$$||T_1T_2x - T_1T_2y||_2 \le L_1||T_2x - T_2y||_2 \le L_1L_2||x - y||_2$$

- Composition of nonexpansive is nonexpansive
- Composition of nonexpansive and contractive is contractive

The weighted average $\theta T_1 + (1-\theta)T_2, \ \theta \in (0,1)$ is $(\theta L_1 + (1-\theta)L_2)$ -Lipschitz **Proof** (exercise)

- Weighted average of nonexpansive is nonexpansive
- Weighted average of nonexpansive and contractive is contractive

Fixed point iterations

Fixed point iteration

Apply operator

$$x^{k+1} = T(x^k)$$

until you reach $\bar{x} \in \operatorname{fix} T$

Main approach

- 1. Find a suitable T such that $\bar{x} \in \operatorname{fix} T$ solve your problem
- 2. Show that the fixed point iteration converges

Fixed point residual to terminate

$$r^k = T(x^k) - x^k$$

Contractive fixed point iterations

Contraction mapping theorem

If T is L-Lipschitz with L < 1 (contraction), the iteration

$$x^{k+1} = T(x^k)$$

converges to \bar{x} , the unique fixed point of T

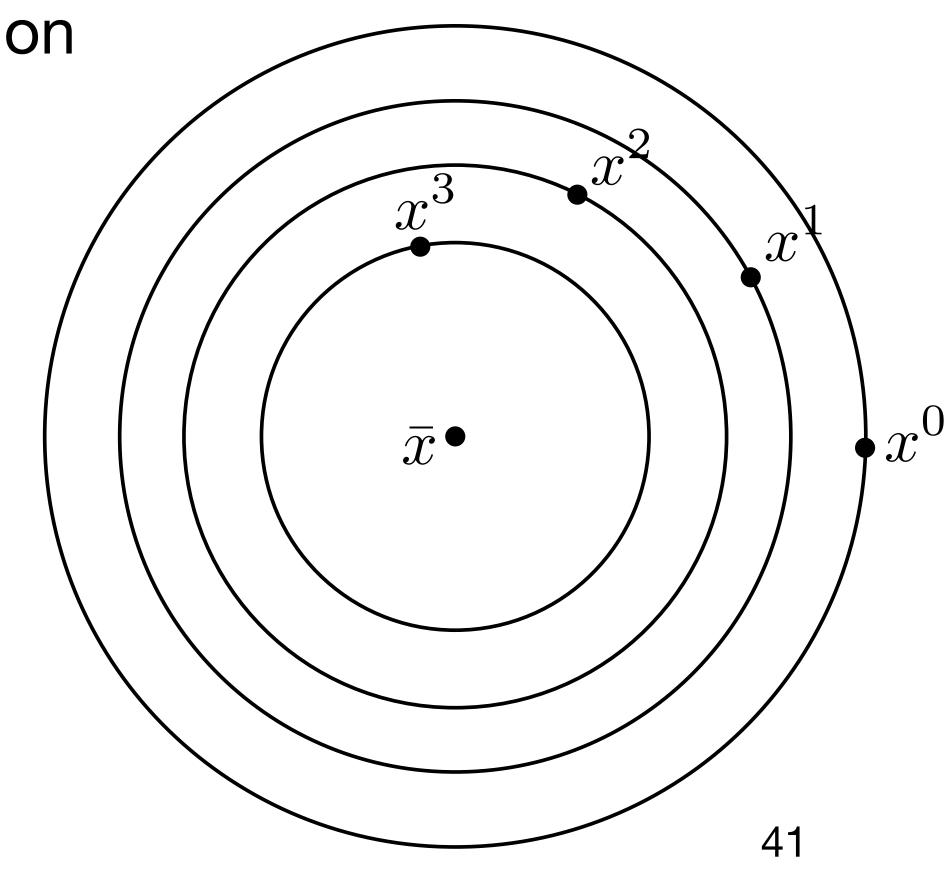
Properties

• Distance to \bar{x} decreases at each step

$$||x^{k+1} - \bar{x}|| \le L||x^k - \bar{x}||$$

(iteration is Fejer monotone)

• Linear convergence rate ${\cal L}$



Contraction mapping theorem

Proof

The sequence x^k is Cauchy

$$\begin{split} \|x^{k+\ell} - x^k\| &\leq \|x^{k+\ell} - x^{k+\ell-1}\| + \dots + \|x^{k+1} - x^k\| \\ &\leq (L^{\ell-1} + \dots + 1) \|x^{k+1} - x^k\| \\ &\leq \frac{1}{1-L} \|x^{k+1} - x^k\| \\ &\leq \frac{L^k}{1-L} \|x^1 - x^0\| \end{split} \tag{Lipschitz constant)}$$

Therefore it converges to a point \bar{x} which must be the (unique) fixed point of T

The convergence is linear (geometric) with rate L

$$||x^k - \bar{x}|| = ||T(x^{k-1}) - T(\bar{x})|| \le L||x^{k-1} - \bar{x}|| \le L^k||x^0 - x^*||$$



Nonexpansive fixed point iterations

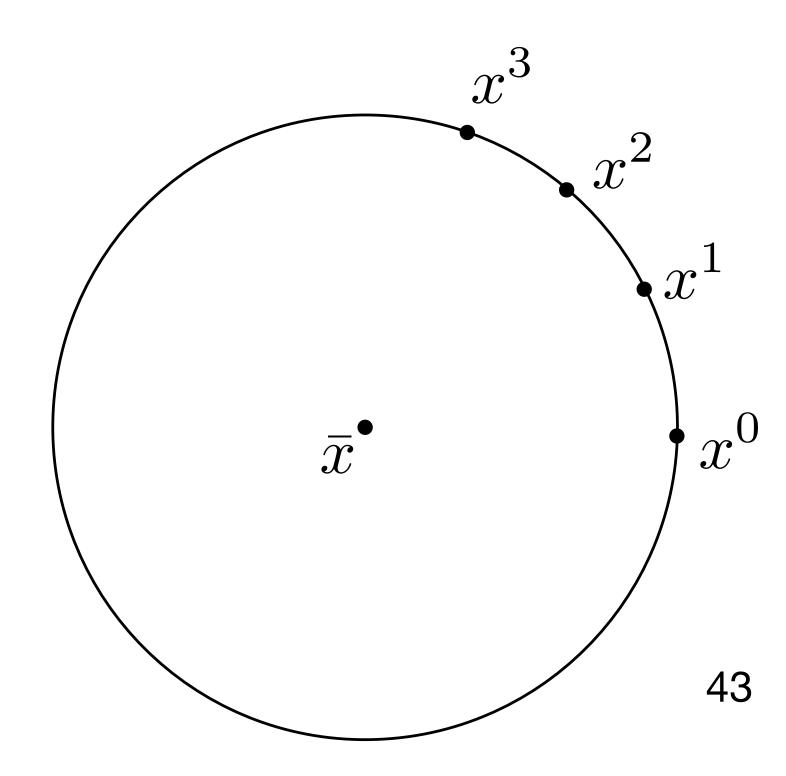
If T is L-Lipschitz with L=1 (nonexpansive), the iteration

$$x^{k+1} = T(x^k)$$

need not converge to a fixed point, even if one exists.

Example

- Let T be a rotation around the origin
- T is nonexpansive and has a fixed point $\bar{x}=0$
- $||x^k||$ never decreases



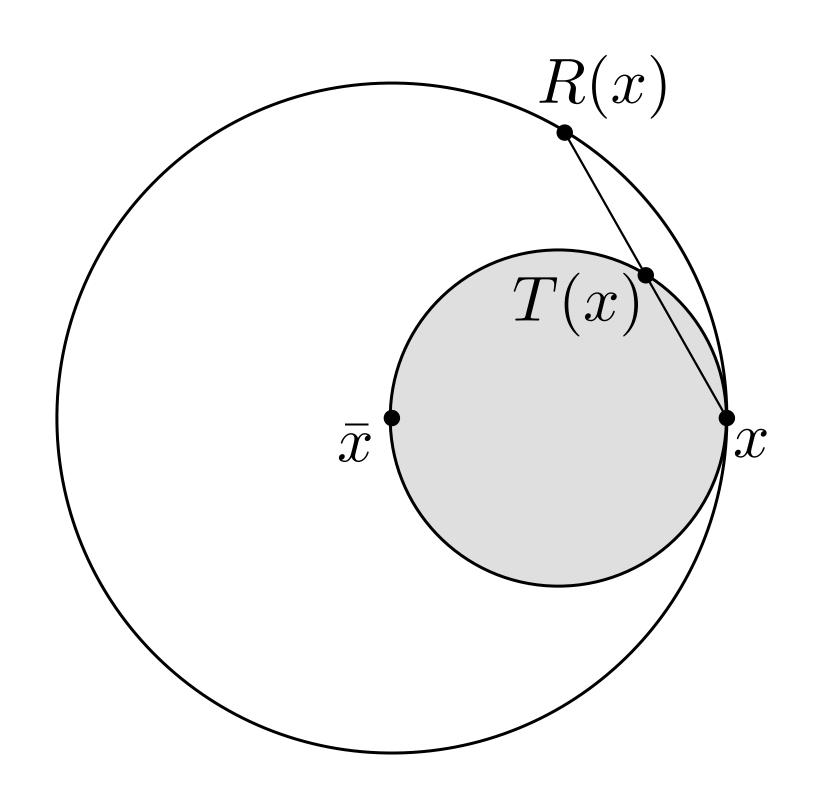
Example $\alpha = 1/2, \bar{x} = 0$

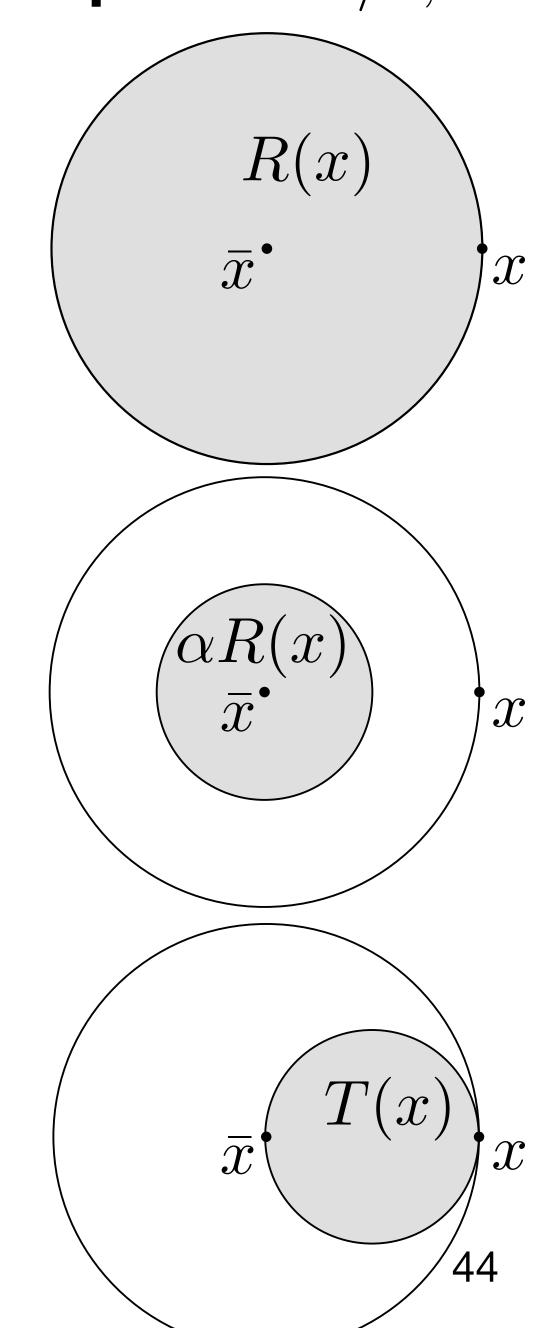
Averaged operators

We say that an operator T is α -averaged with $\alpha \in (0,1)$ if

$$T = (1 - \alpha)I + \alpha R$$

and R is nonexpansive.





Averaged operators fixed points

We say that an operator T is α -averaged with $\alpha \in (0,1)$ if

$$T = (1 - \alpha)I + \alpha R$$

Fact If T is α -averaged, then $\operatorname{fix} T = \operatorname{fix} R$

Proof
$$\bar{x} = T(\bar{x}) = (1 - \alpha)I(\bar{x}) + \alpha R(\bar{x})$$

 $= (1 - \alpha)\bar{x} + \alpha R(\bar{x})$
 $\iff \alpha \bar{x} = \alpha R(\bar{x})$
 $\iff \bar{x} = R(\bar{x})$

Averaged fixed point iterations

If $T=(1-\alpha)I+\alpha R$ is α -averaged ($\alpha\in(0,1)$ and R nonexpansive), the iteration

$$x^{k+1} = T(x^k)$$

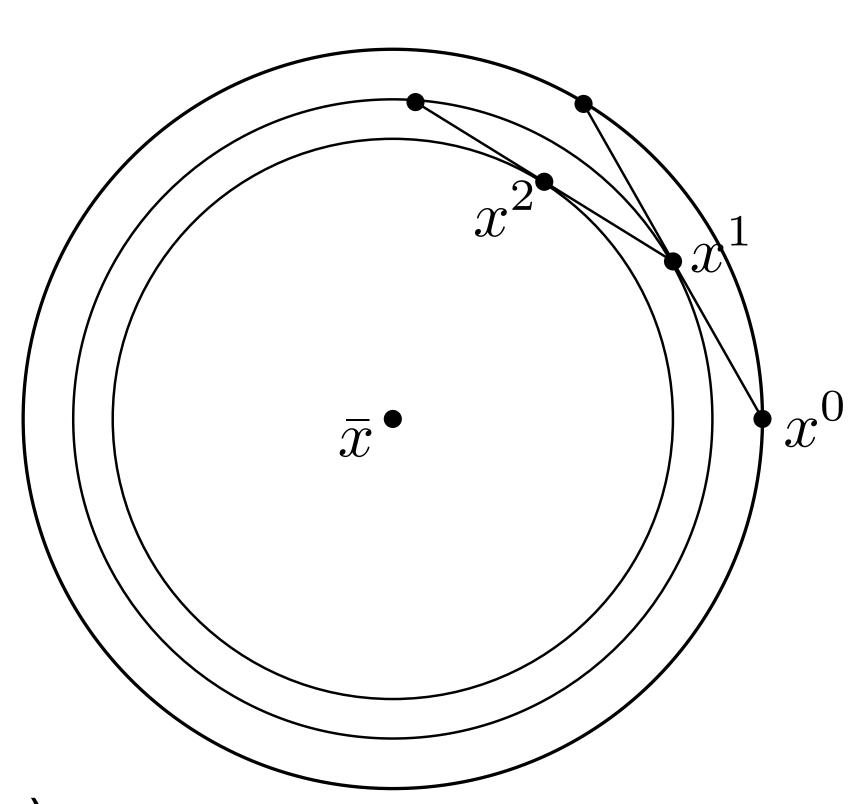
converges to $\bar{x} \in \operatorname{fix} T$

(also called damped, averaged or Mann-Krasnosel'skii iteration)

Properties

- Distance to \bar{x} decreases at each step (Fejer monotone)
- Sublinear convergence to fixed-point residual

$$||R(x^k) - x^k|| \le \frac{1}{\sqrt{(k+1)\alpha(1-\alpha)}} ||x^0 - \bar{x}||$$



Averaged fixed point iterationsProof

Use the identity (proof by expanding)

$$||(1-\alpha)a + \alpha b||^2 = (1-\alpha)||a||^2 + \alpha||b||^2 - \alpha(1-\alpha)||a-b||^2$$

and apply it to

$$x^{k+1} - \bar{x} = (1 - \alpha)(x^k - \bar{x}) + \alpha(R(x^k) - \bar{x})$$

obtaining

$$\begin{split} \|x^{k+1} - \bar{x}\|^2 &= (1-\alpha)\|x^k - \bar{x}\|^2 + \alpha \|R(x^k) - \bar{x}\|^2 - \alpha (1-\alpha)\|x^k - R(x^k)\|^2 \\ &\leq (1-\alpha)\|x^k - \bar{x}\|^2 + \alpha \|x^k - \bar{x}\|^2 - \alpha (1-\alpha)\|x^k - R(x^k)\|^2 \text{ (nonexpansive)} \\ &= \|x^k - \bar{x}\|^2 - \alpha (1-\alpha)\|x^k - R(x^k)\|^2 \\ &< 0 \end{split}$$

Iterations are Fejer monotone

Averaged fixed point iterations

Proof (continued)

iterate righthand side over $k_{_{\! L}}$ steps

$$||x^{k+1} - \bar{x}||^2 \le ||x^0 - \bar{x}||^2 - \alpha(1 - \alpha) \sum_{i=0}^{\infty} ||x^i - R(x^i)||^2$$

Since
$$||x^{k+1} - \bar{x}||^2 \ge 0$$
, we have

Since
$$||x^{k+1} - \bar{x}||^2 \ge 0$$
, we have
$$\sum_{i=0}^k ||x^i - R(x^i)||^2 \le \frac{1}{\alpha(1-\alpha)} ||x^0 - \bar{x}||^2$$

Using
$$\sum_{i=0}^{\kappa} \|x^i - R(x^i)\|^2 \ge (k+1) \min_{i=0,\dots,k} \|x^i - R(x^i)\|^2$$
, we obtain

$$\min_{i=0,\dots,k} \|x^i - R(x^i)\|^2 \le \frac{1}{(k+1)\alpha(1-\alpha)} \|x^0 - \bar{x}\|^2$$

(R is nonexpansive
$$\rightarrow \min$$
 at k)

(R is nonexpansive
$$\to \min$$
 at k) $||x^k - R(x^k)||^2 \le \frac{1}{(k+1)\alpha(1-\alpha)}||x^0 - \bar{x}||^2$ 48

Average fixed point iteration convergence rates

$$||R(x^k) - x^k|| \le \frac{1}{\sqrt{(k+1)\alpha(1-\alpha)}} ||x^0 - \bar{x}||$$

Righthand side minimized when $\alpha = 1/2$

$$||R(x^k) - x^k|| \le \frac{2}{\sqrt{k+1}} ||x^0 - \bar{x}||$$

Iterations

$$x^{k+1} = (1/2)x^k + (1/2)R(x^k)$$

Remarks

- Sublinear convergence (same as subgrad method), in general not the actual rate
- $\alpha = 1/2$ is very common for averaged operators

How to design an algorithm

Problem

minimize f(x)

Algorithm (operator) construction

- 1. Find a suitable T such that $\bar{x} \in \operatorname{fix} T$ solve your problem
- 2. Show that the fixed point iteration converges

```
If T is contractive \implies linear convergence If T is averaged \implies sublinear convergence
```

Most first order algorithms can be constructed in this way

Proximal methods and introduction to operators

Today, we learned to:

- Derive optimality conditions for constrained optimization problems using subdifferentials
- Define and evaluate proximal operators for various common functions
- Apply proximal operators to generalize gradient descent (vanilla, projected, proximal)
- Use operator theory to construct general fixed-point iterations and prove their convergence

Next lecture

Monotone operators and operator splitting algorithms