Chapter 2

Gradient Methods

Convex Optimization for Computer Vision

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Visual
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Gradient Descent

Unconstrained and smooth optimization

Recall what the lecture is all about:

$$u^* \in \arg\min_{u \in \mathbb{R}^n} E(u),$$

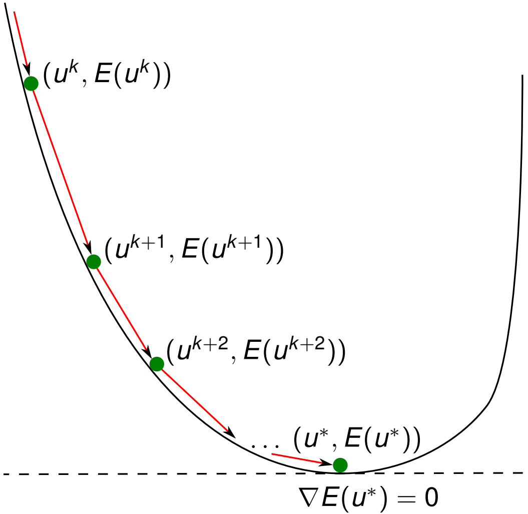
for $E : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ proper, closed, convex.

We start making our life easier:

- $\text{dom } E = \mathbb{R}^n$
- $E \in \mathcal{C}^1(\mathbb{R}^n)$
- Even more assumptions later :-)

Descent methods

$$\min E(u), \qquad u \in \mathbb{R}^n$$



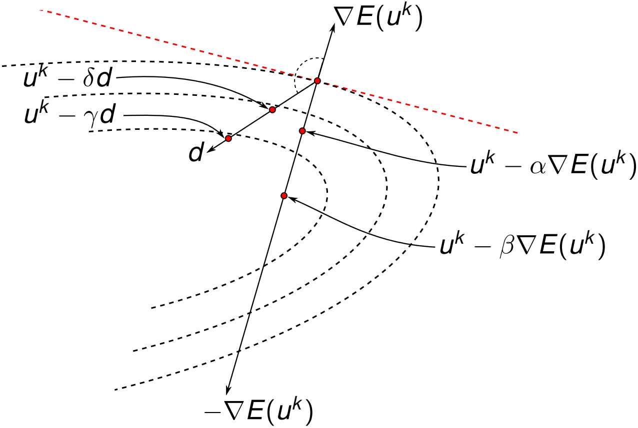
Descent methods

- Suppose we are at a point $u^k \in \mathbb{R}^n$ where $\nabla E(u^k) \neq 0$
- Consider the ray $u(\tau) = u^k + \tau d$ for some direction $d \in \mathbb{R}^n$
- Taylor expansion for E along ray

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

- The term $\tau \langle \nabla E(u^k), d \rangle$ dominates $o(\tau)$ for suff. small τ
- Pick d such that $\langle \nabla E(u^k), d \rangle < 0$, *descent direction*
- Then $E(u(\tau)) < E(u)$ for suff. small τ

Descent methods



Descent methods

- The negative gradient is the *steepest* descent direction

$$\underset{\|d\|=1}{\operatorname{argmin}} \left\{\langle d, \nabla E(u^k)\rangle\right\} = -\frac{\nabla E(u^k)}{\|\nabla E(u^k)\|}$$

- The gradient is orthogonal to the iso-contours $\gamma : I \to \mathbb{R}^n$

$$\nabla E(\gamma(t)) \perp \dot{\gamma}(t), \qquad t \in I$$

- Possible choices of descent directions
  - Scaled gradient: $d^k = -D^k \nabla E(u^k)$, $D^k \succeq 0$
  - Newton: $D^k = [\nabla^2 E(u^k)]^{-1}$
  - Quasi-Newton: $D^k \approx [\nabla^2 E(u^k)]^{-1}$
  - Steepest descent: $D^k = I$
  - ...

Gradient descent

Definition

Given a function $E \in \mathcal{C}^1(\mathbb{R}^n)$, an initial point $u^0 \in \mathbb{R}^n$ and a sequence $(\tau_k) \subset \mathbb{R}$ of step sizes, the iteration

$$u^{k+1} = u^k - \tau_k \nabla E(u^k), \qquad k = 0, 1, 2, \dots,$$

is called *gradient descent*.

Philosophy:

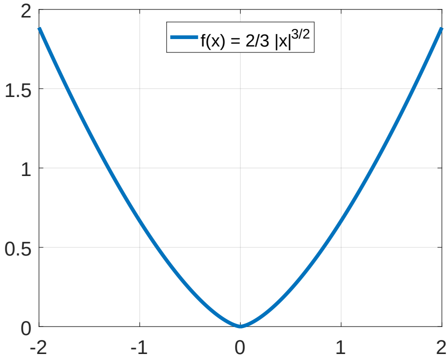
- Generate (decreasing?) sequence $\{E(u^k)\}_{k=0}^{\infty}$
- Each iteration is cheap, easy to code

Choice of τ_k:

- $\tau_k = \tau$ for some constant $\tau \in \mathbb{R}$ (this lecture)
- Exact line search $\tau_k = \arg\min_\tau \; E\left(u^k - \tau \nabla E(u^k)\right)$
- Inexact line search (more later)

Constant step size

Let us first consider a constant step size $\tau^k = \tau$. Will gradient descent work for any convex function *E*? NO!



Board: For any $\tau > 0$, the starting point $u^0 = \left(\frac{\tau}{2}\right)^2$ leads to the gradient descent sequence $u^0, -u^0, u^0, -u^0 \ldots$. In fact, gradient descent will fail to converge for almost any starting point!

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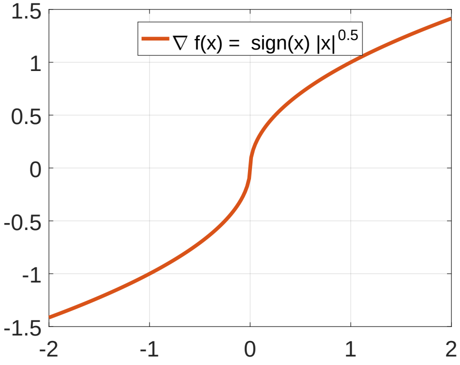

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Why can it fail?

Intuitively, an "infinitely quickly changing gradient", ∇E, seems to cause the problems!

We already know a stronger version of continuity which prevents "infinitely quick changes"!

Reminder

$f : \mathbb{R}^n \to \mathbb{R}^m$ is called Lipschitz continuous if for some $L \geq 0$

$$\|f(x) - f(y)\| \leq L \|x - y\|, \quad \forall x, y \in \mathbb{R}^n.$$

Is there a (possibly easier) characterization of Lipschitz continuous functions?

Lipschitz continuity

Theorem: Lipschitz continuity for differentiable functions

A differentiable function $E : \mathbb{R}^n \to \mathbb{R}^m$ is Lipschitz with parameter L if and only if $\|\nabla E(x)\|_{S^\infty} \leq L$ for all $x \in \mathbb{R}^n$.

Definition: *L*-smooth function

If $E : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its first derivative is Liptschitz continuous, i.e. there exists an $L \geq 0$ such that

$$\|\nabla E(u) - \nabla E(v)\| \leq L \|u - v\|, \forall u, v \in \mathbb{R}^n,$$

then E is called L-smooth (in some literature L-strongly smooth). We denote the set

- of all L-smooth functions by $\mathcal{C}_L^{1,1}(\mathbb{R}^n)$.
- of all convex L-smooth functions by $\mathcal{F}_L^{1,1}(\mathbb{R}^n)$.

How to analyze the convergence?

Conjecture

For any L-smooth proper convex function E (for which a minimizer exists) there exists a step size τ such that the gradient descent algorithm converges

But how do we proceed in proving the assertion?

If this was a research project: Using the assumptions, try to write down smart estimates until you have an inequality from which you can conclude the convergence.

Since this is a lecture: General convergence framework that applies to many convex optimization algorithms!

Fixed-point iterations

A form many algorithms can be written into:

$$u^{k+1} = G(u^k),$$

for an update function G, i.e. a **fixed-point iteration**!

Example:

$$G(u) = u - \tau \nabla E(u).$$

If the iteration converges, i.e. $\hat{u} = \lim_{k\to\infty} u^k$, then

$$\hat{u} = \hat{u} - \tau \nabla E(\hat{u}),$$

i.e. $\nabla E(\hat{u}) = 0$ (where we assumed ∇E to be continuous).

Convergence of Fixed-Point Iterations

References:

- Ryu and Boyd, *Primer on Monotone Operator Methods*, 2016.
- Burger, Sawatzky, and Steidl, *First Order Algorithms in Variational Image Processing*, 2017.
- Bauschke, and Combettes, *Convex Analysis and Monotone Operator Theory in Hilbert Spaces*, 2011.

Fixed-point iterations with contractions

When does the fixed-point iteration

$$u^{k+1} = G(u^k) \tag{1}$$

converge?

Banach fixed-point theorem

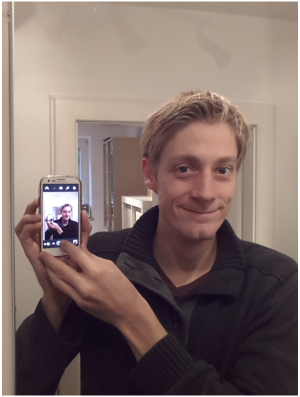
If the update rule $G : \mathbb{R}^n \to \mathbb{R}^n$ is a **contraction**, i.e. if there exists a $L < 1$ such that

$$\|G(u) - G(v)\|_2 \leq L\|u - v\|_2$$

holds for all $u,\ v \in \mathbb{R}^n$, then the iteration (1) converges to the unique fixed-point $\hat{u}$ of G. More precisely,

$$\|u^k - \hat{u}\|_2 \leq L^k\|u^0 - \hat{u}\|_2.$$

Examples for fixed-point iterations with contractions



The function $G(u) = \frac{u+\frac{1}{2}}{u+1}$ is a contraction on $[0, \infty[$. Therefore, the fixed point iteration converges to $\frac{1}{\sqrt{2}}$.

Later: The gradient descent update is a contraction for specific energies E.

Fixed-point iterations with averaged operators

As we will see, the assumption of G being a **contraction** is **too restrictive** in many cases!

One thing that often holds easily, is that G is **non-expansive**, i.e. Lipschitz continuous with constant $L = 1$.

Example: Any rotation G is non-expansive, any rotation has a fixed point (zero), but the iteration $u^{k+1} = G(u^k)$ does not converge!

$\rightarrow$ We need more!

Averaged operator

An operator $G : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is called **averaged** if there exists a non-expansive mapping $H : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and a constant $\alpha \in]0, 1[$ such that

$$G = \alpha I + (1 - \alpha)H.$$

Convergence for averaged operators

Krasnosel'skii-Mann Theorem

If the operator $G : \mathbb{R}^n \to \mathbb{R}^n$ is averaged and has a fixed-point, then the iteration

$$u^{k+1} = G(u^k)$$

converges to a fixed point of G for any starting point $u^0 \in \mathbb{R}^n$.

Proof: Board

Criteria for being averaged

We now have two loose ends: A conjecture about the conergence of the gradient descent iteration, and a theorem that states the convergence of a fixed-point iteration for averaged operators.

We need a better understanding of averaged operators!

Criteria for being averaged

Lemma about nonexpansive operators

Convex combinations as well as compositions of nonexpansive operators are nonexpansive.

Being averaged for smaller α

If a function $G : \mathbb{R}^n \to \mathbb{R}^n$ is averaged with respect to $\alpha \in]0, 1[$, then it is also averaged with respect to any other parameter $\tilde{\alpha} \in]0, \alpha[$.

Composition of averaged operators

If $G_1 : \mathbb{R}^n \to \mathbb{R}^n$ and $G_2 : \mathbb{R}^n \to \mathbb{R}^n$ are averaged, then $G_2 \circ G_1$ is also averaged.

Proofs: Board

Criteria for being averaged

Firmly non-expansive

A function $G : \mathbb{R}^n \to \mathbb{R}^n$ is called **firmly nonexpansive**, if for all $u, v \in \mathbb{R}^n$ it holds that

$$\|G(u) - G(v)\|_2^2 \leq \langle G(u) - G(v), u - v \rangle.$$

Firmly nonexpansive operators are averaged

A function $G : \mathbb{R}^n \to \mathbb{R}^n$ is firmly nonexpansive if and only if G is averaged with $\alpha = \frac{1}{2}$.

Proof: Board

Short summary

We have seen:

- An operator G is called a **contraction** if it is Lipschitz continuous with $L < 1$.
- Contractions have a unique fixed-point and their fixed-point iteration converges with $\mathcal{O}(L^k)$.
- An operator R is called a **nonexpansive** if it is Lipschitz continuous with $L = 1$.
- An operator G is called a **averaged** if $G = \alpha I + (1-\alpha)R$ for some nonexpansive operator R and $\alpha \in]0,1[$.
- If an averaged operator has a fixed-point, then the fixed-point iteration converges. The convergence rate states that $\sum_{k=1}^{n} \|G(u^k) - u^k\|_2 \leq C$ for some constant C.
- **Firmly nonexpansive** operators are the same as averaged operators with $\alpha = \frac{1}{2}$.

Relation to gradient descent

Let us use the previous results for approaching our gradient descent convergence problem:

Baillon-Haddad theorem

A continuously differentiable convex function $E : \mathbb{R}^n \to \mathbb{R}$ is L-smooth if and only if $\frac{1}{L}\nabla E$ is firmly nonexpansive, i.e.

$$\langle \nabla E(u) - \nabla E(v), u - v \rangle \geq \frac{1}{L} \|\nabla E(u) - \nabla E(v)\|_2^2$$

for all $u, v \in \mathbb{R}^n$.

Proof: Some parts on the board. Otherwise see Nesterov, *Introductory Lectures on Convex Optimization*, Theorem 2.1.5.

Tools for the proof

Theorem: characterization of convex functions

For a continuously differentiable E the following are equivalent:

1. E is convex,
2. $E(v) - E(u) - \langle \nabla E(u), v - u \rangle \geq 0 \ \ \forall u, v$,
3. $\langle \nabla E(u) - \nabla E(v), u - v \rangle \geq 0 \ \ \forall u, v$,
4. $\nabla^2 E(u) \succeq 0 \ \ \forall u$, if $E \in \mathcal{C}^2(\mathbb{R}^n)$

Proof: E.g. Ryu, Boyd, A Primer on Monotone Operator Methods, Appendix A.

Convergence of gradient descent

Gradient descent as an averaged operator

If $E : \mathbb{R}^n \to \mathbb{R}$ has a minimizer, is convex and L-smooth, and $\tau \in]0, \frac{2}{L}[$, then the gradient descent iteration converges to a minimizer.

- Sufficient: $G(u) = u - \tau \nabla E(u)$ is averaged.
- We know $\frac{1}{L}\nabla E$ is averaged with $\alpha = 1/2$, i.e., $\frac{1}{L}\nabla E = \frac{1}{2}(I + T)$ for a non-expansive T.
- It hold that

$$G(u) = u - \tau L \frac{1}{L}\nabla E(u) = \left(1 - \frac{L\tau}{2}\right) u + \frac{L\tau}{2}(-T)(u)$$

- If T is non-expansive, $(-T)$ is non-expansive, too.
  $\Rightarrow$ For $\tau \in]0, \frac{2}{L}[$, G is averaged.

Convergence rate

How fast does gradient descent converge?

Reminder: $\mathcal{O}$-notation

$$\mathcal{O}(g) = \{f \mid \exists C \geq 0, \exists n_0 \in \mathbb{N}_0, \forall n \geq n_0 : |f(n)| \leq C|g(n)|\}$$

Convergence speed of gradient descent

One can show that

$$E(u^{k+1}) \leq E(u^k) \qquad \text{and} \qquad E(u^k) - E(u^*) \in \mathcal{O}(1/k)$$

Linear convergence ($\mathcal{O}(c^k)$ for $c < 1$) would be faster. Is there no way to get a contraction?

Quick answer: Impossible in this generality! A contraction would imply the existence of a unique fixed-point!

Strong convexity

Definition: strong convexity

A function $E : \mathbb{R}^n \to \overline{\mathbb{R}}$ is called *strongly convex* with constant m or m-strongly convex if $E(u) - \frac{m}{2}\|u\|_2^2$ is still convex.

Theorem: characterization of m-strongly convex functions [a]

[a] Ryu, Boyd, A Primer on Monotone Operator Methods, Appendix A

For $E \in \mathcal{C}^1(\mathbb{R}^n)$ the following are equivalent:

1. $E(u) - \frac{m}{2}\|u\|^2$ is convex
2. $E(v) \geq E(u) + \langle \nabla E(u), v - u \rangle + \frac{m}{2}\|v - u\|^2$
3. $\langle \nabla E(u) - \nabla E(v), u - v \rangle \geq m\|u - v\|^2$
4. $\nabla^2 E(u) \succeq m \cdot I$, if $E \in \mathcal{C}^2(\mathbb{R}^n)$

L-smoothness

If a continuously differentiable function $E : \mathbb{R}^n \to \overline{\mathbb{R}}$ is L-smooth then R, $R(u) = \frac{L}{2}\|u\|^2 - E(u)$, is convex.

Strongly-convex + L-smooth

Gradient descent as an averaged operator

If $E : \mathbb{R}^n \to \mathbb{R}$ is m-strongly convex and L-smooth, and $\tau \in]0, \frac{2}{m+L}[$, then the gradient descent iteration converges to the unique minimizer u^* of E with $\|u^k - u^*\| \leq c^k \|u^0 - u^*\|$.

Partial proof on the board.

In computer vision, m-strongly convex L-smooth energies are very rare! Can one do better than the $\mathcal{O}(1/k)$ in the L-smooth case?

Optimal convergence rates

Famous analysis by Nesterov, e.g. *Introductory Lectures on Convex Optimization*, Theorem 2.1.7 and Theorem 2.1.13:

First order method:

$$u^{k+1} \in u^0 + \text{span}\{\nabla E(u^0), \dots, \nabla E(u^k)\}$$

- If E can be any convex L-smooth function (that has a minimizer), then no first order method can have a worst-case complexity less than $\mathcal{O}(1/k^2)$.
- If E can be any convex L-smooth and m-strongly convex function, then no first order method can have a worst-case complexity less than $\mathcal{O}((\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^{2k})$ for $\kappa = L/m$.

Obtaining optimal convergence rates

Nesterov's Accelerated Gradient Descent

Pick some starting point $v^0 = u^0$, set $t_0 = 1$, and iterate

1. Compute
$$u^{k+1} = v^k - \frac{1}{L}\nabla E(v^k)$$
2. Set
$$t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$$
3. Compute the extrapolation of u^{k+1} via
$$v^{k+1} = u^{k+1} + \frac{t_k - 1}{t_{k+1}}(u^{k+1} - u^k)$$

[1]

[1] Also see "A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems" by Beck and Teboulle

Backtracking line search

- Sometimes Lipschitz constant L not known
- The convergence analysis shows that one really only needs
$$E(u^{k+1}) \leq E(u^k) - \beta_k \|\nabla E(u^k)\|^2$$
for some $\beta_k \geq \beta > 0$.
- Idea: Pick $\alpha \in (0, 0.5)$, $\beta \in (0, 1)$
- Then determine τ_k each iteration by:

$\tau_k \leftarrow 1$

while $E\left(u^k - \tau_k \nabla E(u^k)\right) > E(u^k) - \alpha \tau_k \left\|\nabla E(u^k)\right\|^2$

$\quad \tau_k \leftarrow \beta \tau_k$

end

Backtracking line search

Line search...

- ... often leads to improved convergence in practice
- ... has a (slight) overhead each iteration
- ... has the same convergence rate as with constant steps

For a backtracking line search scheme for Nesterov's accelerated gradient method please see *Introductory Lectures on Convex Optimization*, page 76, scheme (2.2.6), or *A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems* by Beck and Teboulle, page 194.

Remark: Other strategies for linear search exists, e.g.

$$\tau_k = \arg\min_{\tau} E(u^k - \tau \nabla E(u^k))$$

Application: TV image denoising

Lets consider the applications of image denoising:

Via energy minimization: Let D_1 and D_2 be finite difference operators for the partial derivatives. Determine

$$\hat{u} \in \arg\min_u \quad \underbrace{\frac{\lambda}{2}\|u-f\|_2^2}_{=H_f(u) \text{stay close to input}} \quad + \underbrace{\sum_{x\in\Omega} \sqrt{(D_1 u(x))^2 + (D_2 u(x))^2}}_{=TV(u) \text{ suppress noise}}$$

Application: TV image denoising

Problem: The so called *total variation regularization*

$$TV(u) = \sum_{x \in \Omega} \sqrt{(D_1 u(x))^2 + (D_2 u(x))^2}$$

is not differentiable!

Idea: Approximate it with a differentiable function

$$TV_\epsilon(u) = \sum_{x \in \Omega} \phi \sqrt{(D_1 u(x))^2 + (D_2 u(x))^2 + \epsilon^2}$$

Exercises: Our denoising model is L-smooth for

$$L = \lambda + \frac{\|D\|_{S^\infty}}{\epsilon}$$

We expect the convergence to be better for large ϵ, but we expect $TV(u) \approx TV_\epsilon(u)$ only for small ϵ...

Image denoising

$\varepsilon = 0.1$

$\varepsilon = 0.01$

$\rightarrow$ *Motivation for non-smooth optimization!*

Convergence, backtracking line search

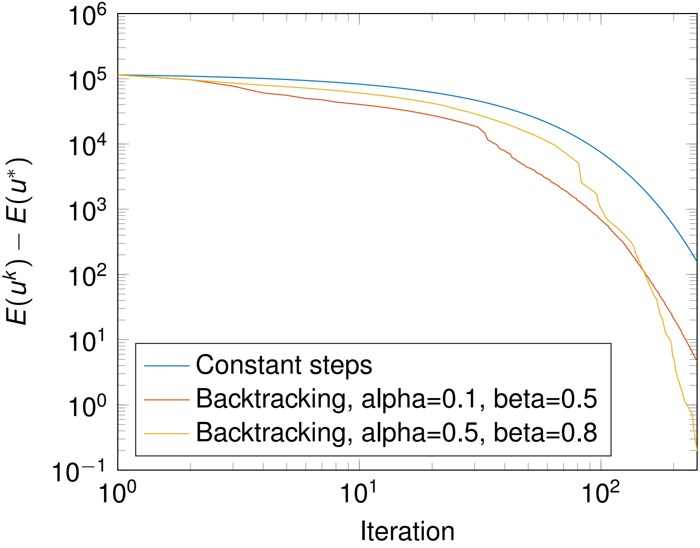
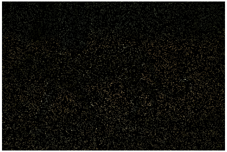
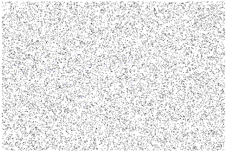


Image inpainting



$f \in \mathbb{R}^N$



$1 - m \in \mathbb{R}^N$

$u^* \in \mathbb{R}^N$

$$u^* \in \operatorname*{argmin}_u \frac{\lambda}{2} \|m \cdot (u - f)\|^2 + TV_\epsilon(u)$$

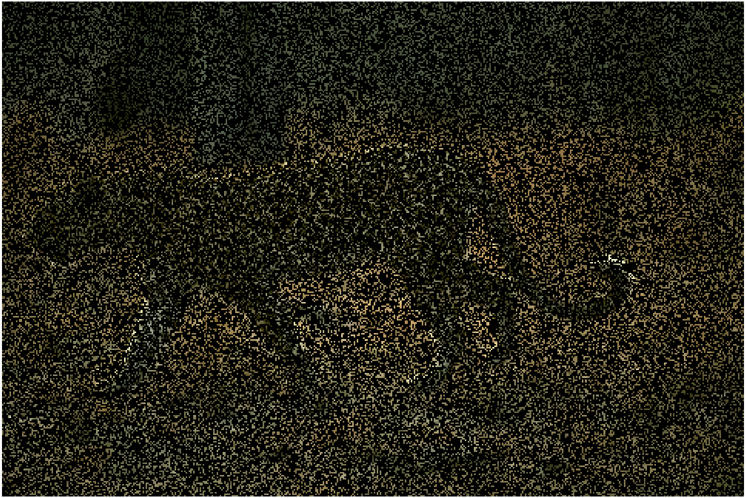
- Energy is not strongly convex, but L-smooth
- Sublinear upper bound on convergence speed

Image Inpainting

50% missing pixels

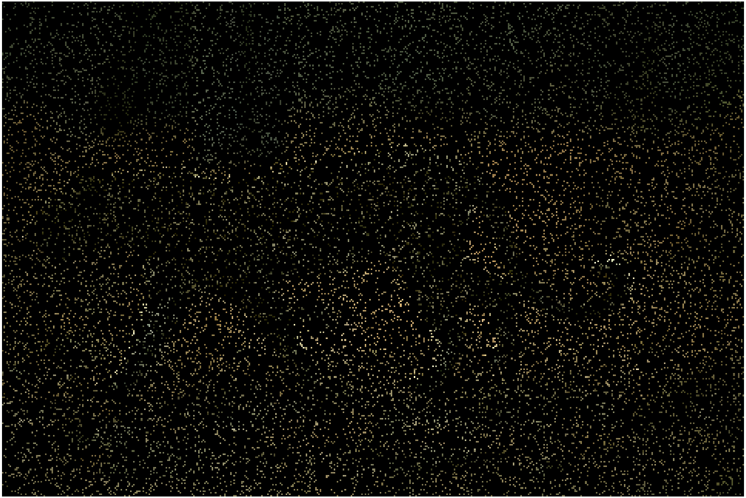
50% missing pixels

70% missing pixels



70% missing pixels

90% missing pixels



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Fast optimization challenge I

- Minimize the inpainting energy

$$E(u) = \frac{\lambda}{2}\|m \cdot (u - f)\|^2 + \sum_{i=1}^{2N} h_\varepsilon((Du)_i) + \beta\|u\|^2$$

- Huber penalty $h_\varepsilon(x) = \begin{cases} \frac{x^2}{2\varepsilon} & \text{if } |x| \leq \varepsilon, \\ |x| - \frac{\varepsilon}{2} & \text{otherwise.} \end{cases}$
- Given all the parameters, return the solution once

$$\frac{E(u^k) - E(u^*)}{E(u^*)} < \delta$$

- See template `challenge_huber_inpainting.m`
- Live leaderboard on homepage
- Fastest solution at end of semester receives a prize!

Handwritten digit recognition

- MNIST dataset[2], handwritten digit recognition
- $K = 10$ digits, 28×28 grayscale images
- $n = 60000$ training images $X \in \mathbb{R}^{n \times 768}$, with ground-truth labels $Y \in \{1, \dots, 10\}^n$
- Learn simple *linear* model $W \in \mathbb{R}^{10 \times 768}$ on raw pixel data
- Softmax regression (multinomial logistic regression)

$$p(y_i = k | x_i, W) = \frac{\exp(\langle w_k, x_i \rangle)}{\sum_{j=1}^{K} \exp(\langle w_j, x_i \rangle)}$$

[2] http://yann.lecun.com/exdb/mnist/

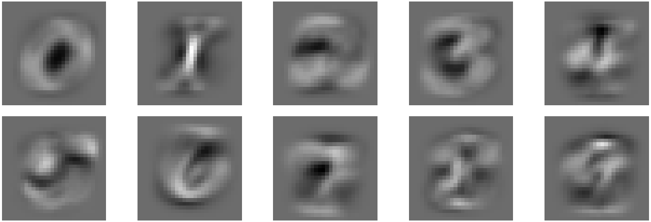
Multinomial logistic regression

- Minimize negative log-likelihood

$$
\begin{aligned}
E(W) &= -\log \frac{1}{n}\prod_{i=1}^{n} p(y_i = k|x_i, W)p(W) \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log p(y_i = k|x_i, W) + \lambda \|W\|_F^2
\end{aligned}
$$

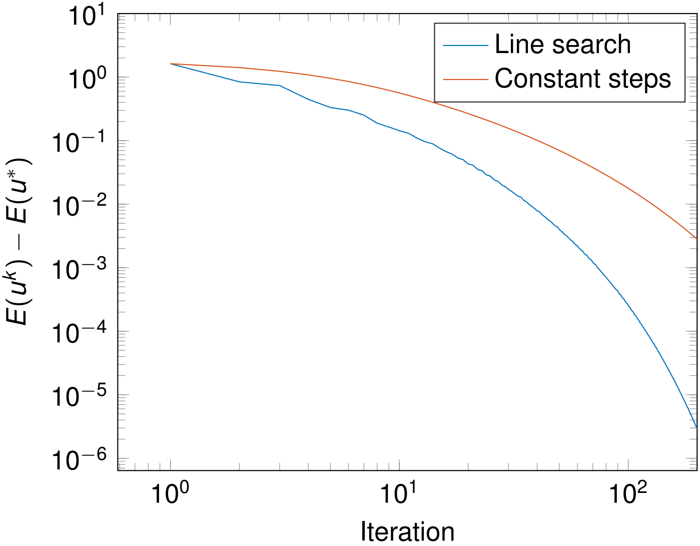
- It can be shown that $E(W)$ is λ-strongly convex
- $E(W)$ is also L-smooth (bound: $\lambda + \frac{\|X\|^2}{4n}$)
- Minimize using gradient descent with $\tau = \frac{2}{2\lambda + \|X\|^2/4n}$
- Gradient computation expensive $\rightarrow$ *stochastic* methods! (we won't cover them)

Multinomial logistic regression



- Classifier gives around 10% error on test set
- Current best: 0.21% (convolutional neural networks)

Multinomial logistic regression



Concluding remarks and outlook

- GD is still popular to date due to its simplicity and flexibility
- Various theoretically optimal extensions (Heavy-ball acceleration, Nesterov momentum) exist
- *Envelope approach:* many advanced algorithms for non-smooth optimization are just gradient descent on a particular (albeit complicated) energy
- Endless of variants and modifications of descent methods
- conjugate, accelerated, preconditioned, projected, conditional, mirrored, stochastic, coordinate, continuous, online, variable metric, subgradient, proximal, ...

Subgradient descent in one slide

We have seen in the exercises, that even for functions that are not L-smooth, gradient descent with a small step size reduces the energy up to some point where it starts oscillating.

Possible convergent variant: **Subgradient descent**

$$u^{k+1} = u^k - \tau_k p^k, \qquad \text{for any } p^k \in \partial E(u^k).$$

If it holds that

- E has a minimizer
- E is Lipschitz continuous
- $\tau_k \to 0$, but $\sum_{k=1}^n \tau_k \to \infty$, e.g. $\tau_k = 1/k$

then the subgradient descent iteration converges with

$$E(u^k) - E(u^*) \in \mathcal{O}(1/\sqrt{k})$$

Summary

This lecture is about

$$u^* \in \arg\min_{u \in \mathbb{R}^n} E(u),$$

for $E : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ proper, closed, convex.

Gradient descent:

- dom $E = \mathbb{R}^n$
- For L-smooth E (that has a minimizer)
  - energy convergence in $\mathcal{O}(1/k)$ for constant step sizes
  - energy convergence in $\mathcal{O}(1/k^2)$ for Nesterov's method.
- For L-smooth m-strongly convex E: energy and iterate convergence in $\mathcal{O}(c^k)$
- Line search strategies for unknown Lipschitz constant L.

Up next: **Gradient projection!** Generalizes gradient descent to arbitrary (nonempty, closed, convex) dom(E).

Gradient Projection

Gradient projection

Type of problem:

$$u^* \in \arg\min_{u \in C} E(u), \tag{2}$$

for an L-smooth E, and a nonempty, closed, convex set C.

What is the *projection* onto the set C?

Definition: Projection

For a (nonempty) closed convex set $C \subset \mathbb{R}^n$,

$$\pi_C(v) = \operatorname*{argmin}_{u \in C} \|u - v\|_2^2$$

is called the projection of v onto the set C.

Projections

Existence and Uniqueness of the Projection

For any (nonempty) closed convex set $C \subset \mathbb{R}^n$ and any v the projection $\pi_C(v)$ exists and is single valued.

Proof: Board.

Abuse of notation: Although $\pi_C(v)$ is (by definition) a set, we also identify $\pi_C(v)$ with the single element in the set.

Example projections

What is the projection of $v \in \mathbb{R}^n$ onto

- $C = \{u \in \mathbb{R}^n \mid \|u\|_2 \leq 1\}$?
- $C = \{u \in \mathbb{R}^n \mid \|u\|_\infty := \max_i |u_i| \leq 1\}$?
- $C = \{u \in \mathbb{R}^n \mid u_i \in [a, b]\}$?
- $C = \{u \in \mathbb{R}^n \mid u_i \geq a\}$?

Idea of gradient projection

Consider a problem

$$u^* \in \arg\min_{u \in C} E(u), \tag{3}$$

for L-smooth E, and a nonempty, closed, convex set C.

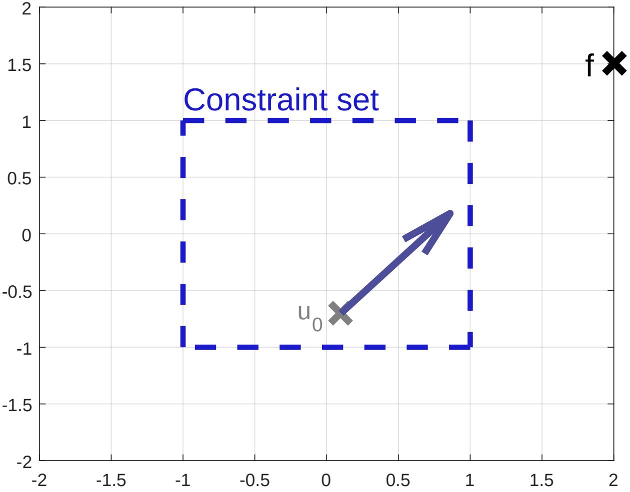
We know how gradient descent works, but updating $u^{k+1} = u^k - \tau^k \nabla E(u^k)$ may lead to $u^{k+1} \notin C$.

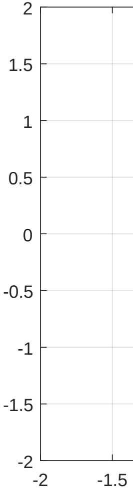
Idea: **Project every iteration back to the feasible set**, i.e.

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

Idea of gradient projection

Toy problem $\min_{|u_i|\leq 1} \|u - f\|_2^2$





Gradient projection algorithm

Gradient projection algorithm

Let $C \subset \mathbb{R}^n$ be a nonempty closed convex set and let $E : \mathbb{R}^n \to \mathbb{R} \in C^1(\mathbb{R}^n)$. Then, for $u^0 \in C$

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

is called the *gradient projection* algorithm.

When, how, why, and for which E and τ does it work?

As usual in this lecture: Analyze the **fixed-point iteration** of

$$G(u) = \pi_C(u - \tau \nabla E(u))$$

Projected GD as a fixed-point iteration

We already know that ...

1. ... for $\tau \in]0, \frac{2}{L}[$ the following operator is averaged

$$G_1(u) = u - \tau \nabla E(u)$$

2. ... compositions of averaged operators are averaged.

All we have to do is showing that π_C is averaged!

Properties of the projection

Firm Nonexpansiveness

The projection π_C onto a nonempty closed convex set $C \subset \mathbb{R}^n$ is *firmly nonexpansive*, i.e. it meets

$$\langle u - v, \pi_C(u) - \pi_C(v) \rangle \geq \|\pi_C(u) - \pi_C(v)\|^2 \qquad \forall u, v \in \mathbb{R}^n.$$

Proof: Board

This makes π_C averaged and we can immediately conclude:

Conclusion

For an L-smooth energy E that has a minimizer and a choice $\tau \in]0, \frac{2}{L}[$ the gradient projection converges!

Similar to the gradient descent case, the convergence rate is $\mathcal{O}(1/k)$ and suboptimal. We will discuss accelerations to $\mathcal{O}(1/k^2)$ of a generalized version later.

Convergence of the projected gradient descent

A simple calculation (done in the exercises) shows:

Compositions can yield contractions

The composition of a non-expansive operator with a contraction is a contraction.

The above means our gradient descent result carries over:

Conclusion

For E being L-smooth and m-strongly convex and $\tau \in]0, \frac{2}{L}[$ the gradient projection algorithm converges to the (unique) global minimizer u^* with $E(u^k) - E(u^*) \in \mathcal{O}(c^k)$ for $c < 1$.

Example Application: Solving a SUDOKU

Find the missing numbers such that each block, each row, and each column contains each number 1– 4 only once!

2			3
1	3		
		3	2
	2	4	

2	4	1	3
1	3	2	4
4	1	3	2
3	2	4	1

How can we do this with convex optimization?

Example Application: Solving a SUDOKU

In the 4×4 case we look for a matrix $u \in \{1,2,3,4\}^{4\times 4}$ such that $u_{i,j} = f_{i,j}$ for those entries $f_{i,j}$ which are given.

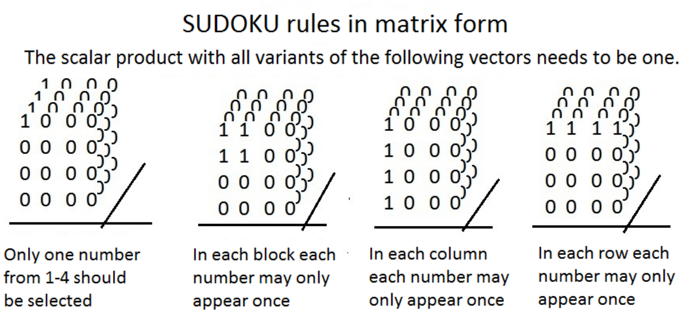
Reformulation: We look for a matrix $\boldsymbol{u} \in \{0,1\}^{4\times 4\times 4}$, where $\boldsymbol{u}_{i,j,k} = 1$ means $u_{i,j} = k$.

Rule	**Implication**	
One number for each blank spot	$\sum_k \boldsymbol{u}_{i,j,k} = 1$	$\forall i, j$
Respect given entries	$\boldsymbol{u}_{i,j,k} = 1$ if $f_{i,j} = k$	
Numbers occur in a row once	$\sum_j \boldsymbol{u}_{i,j,k} = 1$	$\forall i, k$
Numbers occur in a column once	$\sum_i \boldsymbol{u}_{i,j,k} = 1$	$\forall j, k$
Numbers occur in a block once	$\sum_{(i,j)\in B_l} \boldsymbol{u}_{i,j,k} = 1$	$\forall B_l, k$

Find $\boldsymbol{u}$ with $\boldsymbol{u}_{i,j,k} \in \{0,1\}$ subject to the above constraints!

Example Application: Solving a SUDOKU

All constraints are linear, i.e. can be expressed as $A\vec{u} = \vec{1}$.



Find $\boldsymbol{u}$ with $\boldsymbol{u}_{i,j,k} \in \{0,1\}$ is a nonconvex constraint!

Convex relaxation: Use the smallest convex set that contains the nonconvex one, $\boldsymbol{u}_{i,j,k} \in [0,1]$.

If the result meets $\boldsymbol{u}_{i,j,k} \in \{0,1\}$, we solved the nonconvex problem.

Example Application: Solving a SUDOKU

Nice thing for SUDOKU: There exists a solution to $A\vec{\boldsymbol{u}} = \vec{\boldsymbol{1}}$!

This means we may solve

$$\hat{\boldsymbol{u}} \in \underset{\boldsymbol{u}_{i,j,k} \in [0,1]}{\operatorname{argmin}} \|A\vec{\boldsymbol{u}} - \vec{\boldsymbol{1}}\|_2^2$$

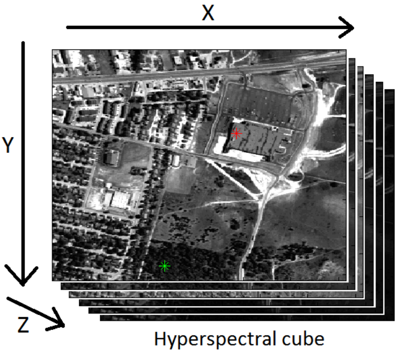
Hope that $\hat{\boldsymbol{u}}_{i,j,k} \in \{0,1\}$ in which case we solved the SUDOKU!

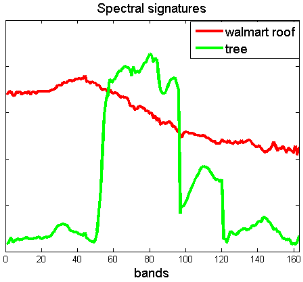
Remarks:

- Exact recovery guarantees (when is $\hat{\boldsymbol{u}}_{i,j,k} \in \{0,1\}$) are an active field of research.
- Similar constructions can be done for many computer vision problems! Look for *labeling problems*, *segmentation*, *graph cuts*, or *functional lifting*.

Example application: Unmixing and sparse recovery

Hyperspectral imagery





z-direction: Material specific reflected energy depending on the wavelength of the incoming light

Example application: Unmixing and sparse recovery

Measured signals f

Find decomposition $f = Au + n$

Dictionary of materials A, mixing coefficients u (sparse) and noise n

Example application: Unmixing and sparse recovery

General setup: Minimize a data fidelity term $H_f(v)$ which is L-smooth, such that v can be represented in a dictionary A, i.e. $v = Au$, and the representing coefficients u are sparse.

Energy minimization approach:

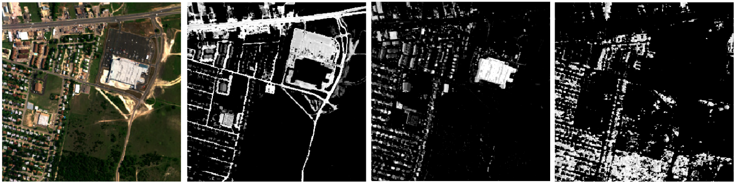
$$\min_u H_f(Au) + \alpha \|u\|_1.$$

Can we apply gradient descent/ gradient projection?

Not directly, but the problem is equivalent to

$$\min_u H_f(A(u_1 - u_2)) + \alpha\langle u_1, \mathbf{1}\rangle + \alpha\langle u_2, \mathbf{1}\rangle, \quad u_1 \geq 0, u_2 \geq 0!$$

Example application: Unmixing and sparse recovery



color image illustration | endmember "road" | endmember "roof" | endmember "trees"

The reformulation of

$$\min_u H_f(Au) + \alpha\|u\|_1,$$

$$\Leftrightarrow \min_{u_1,u_2} H_f(A(u_1-u_2)) + \alpha\langle u_1, \mathbf{1}\rangle + \alpha\langle u_2, \mathbf{1}\rangle, \quad u_1 \geq 0, u_2 \geq 0$$

possibly is a little unsatisfying. In particular, it doubles the size of our unknowns. Any other way?

Proximal Gradient

From proj to prox

Remember the theorem

Firm Nonexpansiveness

The projection π_C onto a nonempty closed convex set $C \subset \mathbb{R}^n$ is *firmly nonexpansive*.

and its proof?

$$\begin{aligned} &\langle u - v, \pi_C(u) - \pi_C(v)\rangle \\ =& \langle \pi_C(u) - \pi_C(v) + p_u - p_v, \pi_C(u) - \pi_C(v)\rangle \\ =& \|\pi_C(u) - \pi_C(v)\|^2 + \langle p_u - p_v, \pi_C(u) - \pi_C(v)\rangle \\ \geq& \|\pi_C(u) - \pi_C(v)\|^2 \end{aligned}$$

for $p_u \in \partial\delta_C(\pi_C(u)),\ p_v \in \partial\delta_C(\pi_C(v))$ denoting the subgradients.

We did not use that p_u and p_v were subgradients of an indicator function! The proof still works after replacing δ_C with an arbitrary convex function!

Proximal operators

Definition

Given a closed, proper, convex function $E : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$, the mapping $\text{prox}_E : \mathbb{R}^n \to \mathbb{R}^n$ defined as

$$\text{prox}_E(v) := \underset{u \in \mathbb{R}^n}{\text{argmin}} \; E(u) + \frac{1}{2} \|u - v\|^2$$

is called the *proximal operator* or *proximal mapping* of E.

- **Existence:** $E(u) + (1/2)\|u - v\|^2$ is closed and has bounded sublevel sets
- **Uniqueness:** $E(u) + (1/2)\|u - v\|^2$ is strongly convex
- **Generalization of the projection**: Choose $E = \delta_C$.

We have just seen

Firm Nonexpansiveness

The proximal operator prox_E for a closed, proper, convex function E is *firmly nonexpansive*.

Consider minimizing an energy

$$E(u) = F(u) + G(u),$$

for proper, closed, convex F and G such that

- $F : \mathbb{R}^n \to \mathbb{R}$ is L-smooth.
- $G : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ has an easy-to-evaluate proximity operator, which we will call *simple*.

The we can take gradient descent steps on F and proximal steps on G! This is the proximal gradient algorithm!

Proximal gradient algorithm

Definition

For a closed, proper, convex function $G : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ and a function $F \in \mathcal{C}^1(\mathbb{R}^n)$, given an initial point $u^0 \in \mathbb{R}^n$ and a step size τ, the algorithm

$$u^{k+1} = \text{prox}_{\tau G}\left(u^k - \tau \nabla F(u^k)\right), \qquad k = 0, 1, 2, \dots,$$

is called the *proximal gradient method*.

- Often referred to as *forward-backward splitting* or ISTA
- For constant G, it reduces to *gradient descent*
- For constant F, it is called *proximal point algorithm*
- For $G = \delta_C$, it reduces to *projected gradient descent*

For us (=super-duper experts on fixed point iterations) the convergence analysis is easy!

Convergence analysis

We have already seen that the prox-operator is firmly nonexpansive, i.e., averaged with $\alpha = 1/2$.

Conclusion

For F being L-smooth, $\tau \in]0, \frac{2}{L}[$, and the overall energy having a minimizer, the proximal gradient method converges.

Contractive prox-operators

If the proper, closed function G is m-strongly convex, then $\text{prox}_{\tau G} : \mathbb{R}^n \to \mathbb{R}^n$ is a contraction.

Conclusion

For F being L-smooth $\tau \in]0, \frac{2}{L}[$, and either G or F being strongly convex, the proximal gradient method converges linearly, i.e., $\|u^k - u^*\|_2^2 \in \mathcal{O}(c^k)$ for some $c < 1$.

Sanity check + examples

Sanity check: The algorithm converges, but to what?

Board: To a minimizer of $E = G + F$!

Examples of functions whose prox has a closed form:

- Quadratic functions

$$f(u) = \frac{1}{2}\|Au - b\|^2, \quad \text{prox}_{\tau f}(v) = (I + \tau A^T A)^{-1}(v + \tau A^T b)$$

- ℓ_1-norm (cf. exercise sheet 3), "soft thresholding"

$$f(u) = \|u\|_1, \quad (\text{prox}_{\tau f}(v))_i = \begin{cases} v_i + \tau & \text{if } v_i < -\tau \\ 0 & \text{if } |v_i| \leq \tau \\ v_i - \tau & \text{if } v_i > \tau. \end{cases}$$

- Euclidean norm

$$f(u) = \|u\|, \quad \text{prox}_{\tau f}(v) = \begin{cases} (1 - \tau / \|v\|)v & \text{if } \|v\| \geq \tau \\ 0 & \text{otherwise.} \end{cases}$$

Application sparse recovery

We can now solve

$$\min_u \|Au - f\|_2^2 + \alpha \|u\|_1$$

without smoothing and without the introduction of additional variables!

Convergence rates and extensions

Similar to gradient descent the proximal gradient method on

$$E = F + G$$

for L-smooth F, E having a minimizer, and choosing the step size τ to be constant converges with $E(u^k) - E(u^*) \in \mathcal{O}(1/k)$.

Similar to gradient descent one can do better and reach $E(u^k) - E(u^*) \in \mathcal{O}(1/k^2)$.

Similar to gradient descent finding the Lipschitz constant L can be annoying, and one can define line search schemes.

Gradient projection: *Introductory lectures on convex optimization* by Nesterov.
Proximal gradient: *A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems*, Beck, Teboulle, 2009.

Accelerated proximal gradient

FISTA with constant step size

Pick some starting point $v^0 = u^0$, set $t_0 = 1$, and iterate

1. Compute

$$u^{k+1} = \text{prox}_{\frac{1}{L}G}\left(v^k - \frac{1}{L}\nabla F(v^k)\right)$$

2. Determine

$$t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2},$$

3. Compute the extrapolation of u^{k+1} via

$$v^{k+1} = u^{k+1} + \frac{t_k - 1}{t_{k+1}}(u^{k+1} - u^k)$$

See Chambolle, Dossal, *On the Convergence of the Iterates of the "Fast Iterative Shrinkage/Thresholding Algorithm"*, 2015, for more general algorithms.

Accelerated gradient projection with line search

FISTA with backtracking line search

Pick $v^0 = u^0$, set $t_0 = 1$, choose $\beta < 1$, $\tau_0 > 0$, and define $Q_\tau(u,v) = F(v) + \langle u - v, \nabla F(v)\rangle + \frac{1}{2\tau}\|u-v\|^2 + G(u)$.

1. Find a suitable step size $\tau_k \leq \tau_{k-1}$ via

$$\tau_k = \tau_{k-1}, \quad u^{k+1} = \text{prox}_{\tau_k G}\left(v^k - \tau_k \nabla F(v^k)\right)$$

while $E(u^{k+1}) > Q_\tau(u^{k+1}, v^k)$

$$\tau_k \leftarrow \beta\tau_k, \quad u^{k+1} \leftarrow \text{prox}_{\tau_k G}\left(v^k - \tau_k \nabla F(v^k)\right)$$

end

2. Determine

$$t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2},$$

3. Compute the extrapolation of u^{k+1} via

$$v^{k+1} = u^{k+1} + \frac{t_k - 1}{t_{k+1}}(u^{k+1} - u^k)$$

What we can and cannot do yet

As we have seen

$$\min_u \frac{1}{2}\|Au - f\|^2 + \alpha\|u\|_1$$

does not pose a problem anymore.

But what about our TV-denoising model:

$$\min_u \frac{1}{2}\|u - f\|^2 + \alpha\|Du\|_1?$$

The minimization problem itself already is a proximal operator and not easy-to-evaluate.

Not solvable with any algorithm we did? Or maybe it is?
$\rightarrow$ Let us develop some ideas on the board!