Chapter 2

Gradient Methods

Convex Optimization for Computer Vision

SS 2016

Michael Moeller
Thomas Möllenhoff
Emanuel Laude
Computer Vision Group
Department of Computer Science
TU München

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updated 05.05.2016

Gradient Descent

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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:

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

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Emanuel Laude

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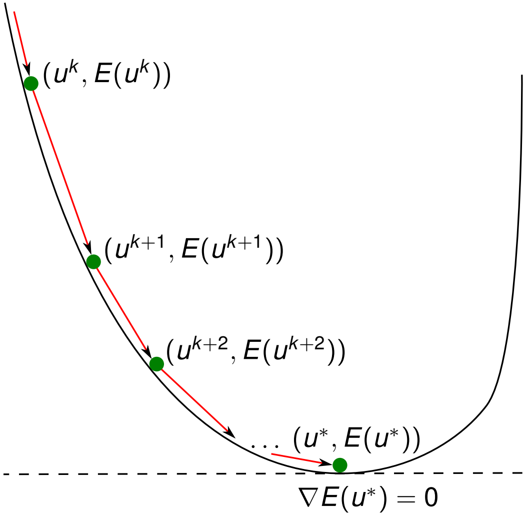
Descent methods

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



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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

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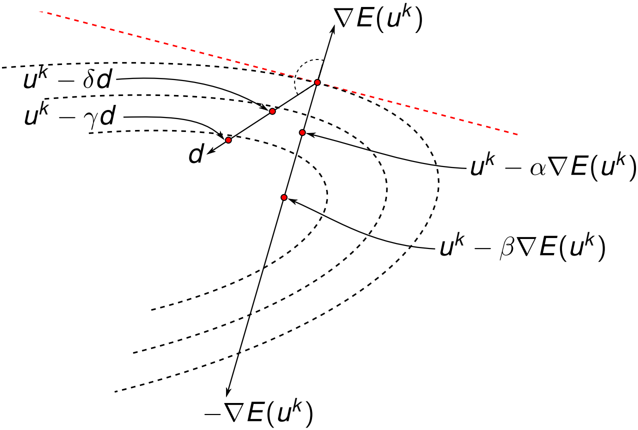
Descent methods



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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: $D^k = I$
  - ...

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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 relaxation 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)

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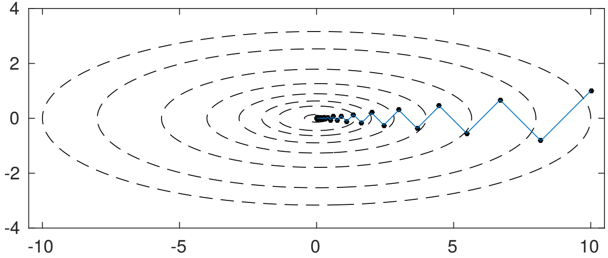
A first toy example

$$E(u) = \frac{1}{2}\left(u_1^2 + \kappa u_2^2\right) \qquad \kappa > 1$$



- Convergence rate with exact line search [1]

$$\frac{\left\| u^k - u^* \right\|^2}{\left\| u^0 - u^* \right\|^2} \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^{2k}$$

[1] Nocedal and Wright, Numerical Optimization, Theorem 3.3

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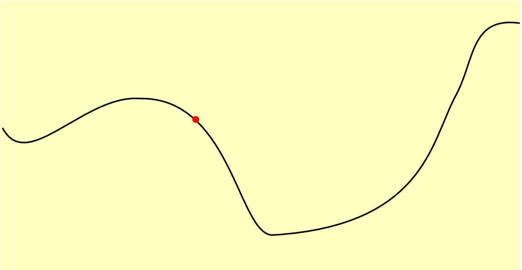
Lipschitz continuity

Definition

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

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

- If $L < 1$, then f is a *contraction*
- If $L \leq 1$, f is called *nonexpansive*



Lipschitz continuity

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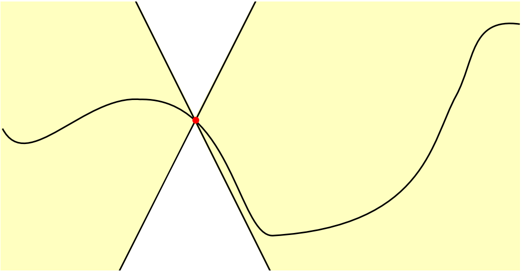

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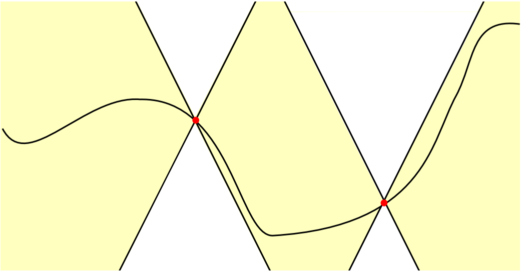

Lipschitz continuity

- Imporant special case are linear functions $f : \mathbb{R}^n \to \mathbb{R}^m$
- f can be represented by matrix $A \in \mathbb{R}^{m \times n}$
- Lipschitz constant of f is the *operator norm* or *spectral norm* of A

$$\|A\| := \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|=1} \|Ax\|$$

- A short calculation reveals

$$\|Ax\| \leq \|A\| \, \|x\| , \quad \forall x$$

- It can be shown that

$$\|A\| = \sqrt{\lambda_{\max}(A^T A)} = \sigma_{\max}(A)$$

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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 $\|\nabla E(x)\| \leq L$ for all $x \in \mathbb{R}^n$.

Proof: Board!

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Lipschitz continuity

Definition: Functions with Lipschitz derivative

Let $Q \subset \mathbb{R}^n$. We denote by $\mathcal{C}_L^{k,p}(Q)$ the class of functions with the following properties:

- any $f \in \mathcal{C}_L^{k,p}(Q)$ is k times continuously differentiable on Q.
- Its p-th derivative is Lipschitz continuous on Q with constant L.

Definition: L-smooth function

If $E : \mathbb{R}^n \to \mathbb{R}$ and $E \in \mathcal{C}_L^{1,1}(\mathbb{R}^n)$, i.e.,

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

it is called L-smooth (in some literature L-strongly smooth).

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Convexity and Lipschitz continuity

Reminder: Characterization of convex functions [2]

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

- $E(\theta u + (1-\theta)v) \leq \theta E(u) + (1-\theta)E(v), \forall u, v, \forall \theta \in [0,1]$
- $E(v) \geq E(u) + \langle \nabla E(u), v - u \rangle$
- $\nabla^2 E(u) \succeq 0$, if $E \in \mathcal{C}^2(\mathbb{R}^n)$

Definition: Convex functions with Lipschitz derivative

Let $Q \subset \mathbb{R}^n$ be convex. The functions $f \in \mathcal{C}_L^{k,p}(Q)$ which are also convex form the class $\mathcal{F}_L^{k,p}(Q)$.

[2] Boyd, Vandenberghe, Convex Optimization, Section 3.1.3

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Convexity and Lipschitz continuity

Theorem: Characterization of convex L-smooth functions [3]

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

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

Proof: See notes!

[3] Nesterov, Introductory Lectures on Convex Optimization, Theorem 2.1.5

Majorization minimization interpretation

- For $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$ it holds for all $u, v \in \mathbb{R}^n$

$$E(v) \leq E(u) + \langle \nabla E(u), v - u \rangle + \frac{L}{2} \|v - u\|^2$$

- Minimizing the quadratic upper bound at iterate u^k yields

$$\begin{aligned} u^{k+1} &= \operatorname*{argmin}_v \; E(u^k) + \langle \nabla E(u^k), v - u^k \rangle + \frac{L}{2} \left\| v - u^k \right\|^2 \\ &= u^k - \frac{1}{L} \nabla E(u^k) \end{aligned}$$

- For the minimum of the upper bound we have

$$\begin{aligned} E(u^*) &\leq \min_v \; E(u^k) + \langle \nabla E(u^k), v - u^k \rangle + \frac{L}{2} \left\| v - u^k \right\|^2 \\ &= E(u^k) - \frac{1}{2L} \left\| \nabla E(u^k) \right\|^2 \end{aligned}$$

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Divergent example

- Minimize $E(u) = u^4$ with gradient descent
- $\nabla E(u) = 4u^3$ is not Lipschitz
- Gradient descent iteration

$$u_{k+1} = u_k - \tau 4 u_k^3 = u_k(1 - 4\tau u_k^2)$$

- For $u_0 > \frac{1}{\sqrt{2\tau}}$ we have $(1 - 4\tau u_0^2) < -1$ which implies

$$u_1 < -u_0$$

- Applying the above iteratively yields divergent sequence

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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.

- Short exercise: strong convexity implies strict convexity
- Notation for cont. diff. and m-strongly convex: $E \in \mathcal{S}_m^1(\mathbb{R}^n)$
- We will also consider the classes $\mathcal{S}_{m,L}^{k,l}(\mathbb{R}^n)$ of m-strongly convex, k-times continuously differentiable functions with L-Lipschitz continuous l-th derivative

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Strong convexity

Theorem: characterization of m-strongly convex functions [4]

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

1. $E(u) - \frac{m}{2}\|u\|^2$ is convex, i.e., $E \in \mathcal{S}^1_m(\mathbb{R}^n)$
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 $E \in \mathcal{C}^2(\mathbb{R}^n)$

Proof: See literature.

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

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Strong convexity and Lipschitz continuity

- The *condition number* κ of a function $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$ is

$$\kappa = \frac{L}{m}$$

- If f is linear, i.e., $f(x) = Ax$ then

$$\kappa = \frac{\sqrt{\lambda_{max}(A^T A)}}{\sqrt{\lambda_{min}(A^T A)}} = \frac{\sigma_{max}(A)}{\sigma_{min}(A)}$$

- If f twice continuously differentiable, gives lower and upper bound on Hessian

$$m \cdot I \preceq \nabla^2 f(x) \preceq L \cdot I$$

$\rightarrow$ *Online TED.*

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What we have seen so far...

- If initialized wrong, gradient descent doesn't converge when minimizing x^4 for any fixed step size $\tau > 0$
- Need additional structure beyond convexity for convergence analysis
- Lipschitz continuity of gradient, $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$
- Strong convexity, $E \in \mathcal{S}_m^1(\mathbb{R}^n)$
- Combination of both, $E \in \mathcal{S}_{m,L}^{1,1}(\mathbb{R}^n)$
- **Today:** understand behaviour of gradient descent for these functions
- Some simple applications

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Strong convexity and Lipschitz continuity

Theorem: strongly convex + L-smooth bound

If $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$, then for any $u, v \in \mathbb{R}^n$ we have

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

Proof: Exercise!

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Gradient descent convergence

Theorem: Convergence (L-smooth + m-strongly convex)

Let $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$. For the sequence $(u^k)_k$ produced by gradient descent with step size $0 < \tau \leq 2/(m+L)$ we have

$$\left\| u^k - u^* \right\|^2 \leq c^k \left\| u^0 - u^* \right\|^2,$$

$$E(u^k) - E(u^*) \leq \frac{Lc^k}{2} \left\| u^0 - u^* \right\|^2,$$

with $c = 1 - \tau \frac{2mL}{m+L}$.

Proof: Board!

Remarks:

- Optimal choice is $\tau = 2/(m+L)$
- Results in factor $c = \left(\frac{\kappa-1}{\kappa+1}\right)^2$, $\kappa = L/m$

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Gradient descent convergence

Theorem: Convergence (L-smooth)

Let $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$ and let $u^* \in \text{argmin}_u E(u)$ exist. For the sequence $(u_k)_k$ produced by gradient descent with step size $0 < \tau \leq 1/L$ we have

$$E(u^k) - E(u^*) \leq \frac{1}{2k\tau} \left\| u^0 - u^* \right\|^2 .$$

Proof: Board!

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Rates of convergence

Reminder: $\mathcal{O}$-notation

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

Sublinear rate

- $r(k) = \mathcal{O}(\frac{1}{k^c})$, $c > 0$
- New correct digit takes the amount of computations comparable with total amount of previous work.
- Constant factor in $\mathcal{O}$-notation plays a significant role

Linear rate

- $r(k) = \mathcal{O}(c^k)$, $c < 1$
- Each new correct digit takes a constant amount of computations

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Worst-case complexities

- First order method:

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

- We have shown the following for gradient descent:
  - $E \in \mathcal{F}_L^{1,1}$ gives $\mathcal{O}(1/k)$ convergence
  - $E \in \mathcal{S}_{m,L}^{1,1}$ gives $\mathcal{O}\left(\left(\frac{\kappa-1}{\kappa+1}\right)^{2k}\right)$ convergence
- Worst-case complexity of first-order methods [5]
  - For $E \in \mathcal{F}_L^{1,1}$ there is a $\mathcal{O}(1/k^2)$ lower bound
  - For $E \in \mathcal{S}_{m,L}^{1,1}$ the lower bound is $\mathcal{O}\left(\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2k}\right)$
- It turns out that these lower bounds can be attained
- Theoretical convergence rates only tell half the story

[5] Nesterov, Introductory Lectures on Convex Optimization, Theorem 2.1.7 and Theorem 2.1.13

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Line search

- Sometimes Lipschitz constant L not known
- Use backtracking line search to estimate τ_k each iteration
- Pick $\alpha \in (0, 0.5)$, $\beta \in (0, 1)$
- Then determine τ_k each iteration by:

$$\tau_k \leftarrow 1$$

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

$$\qquad \tau_k \leftarrow \beta \tau_k$$

$$\text{end}$$

- Often leads to improved convergence in practice
- (Slight) overhead each iteration
- Theory: same convegence rate as with constant steps

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Image denoising

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

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

$$u^* \in \operatorname*{argmax}_{u \in \mathbb{R}^N} p(u|f) = \operatorname*{argmax}_{u \in \mathbb{R}^N} \frac{p(f|u)p(u)}{p(f)}$$

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Image denoising

- Gaussian noise assumption $f_i \sim \mathcal{N}(u_i, \sigma)$

$$p(f_i|u_i) \propto \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(u_i - f_i)^2}{2\sigma}\right)$$

- Impose prior distribution on image gradient $Du \in \mathbb{R}^{2N}$

$$p(u) \propto \prod_{i=1}^{2N} \exp(-\varphi((Du)_i))$$

- Natural image statistics suggest the choice

$$\varphi(x) = c_\varepsilon(x) = \sqrt{x^2 + \varepsilon^2}$$

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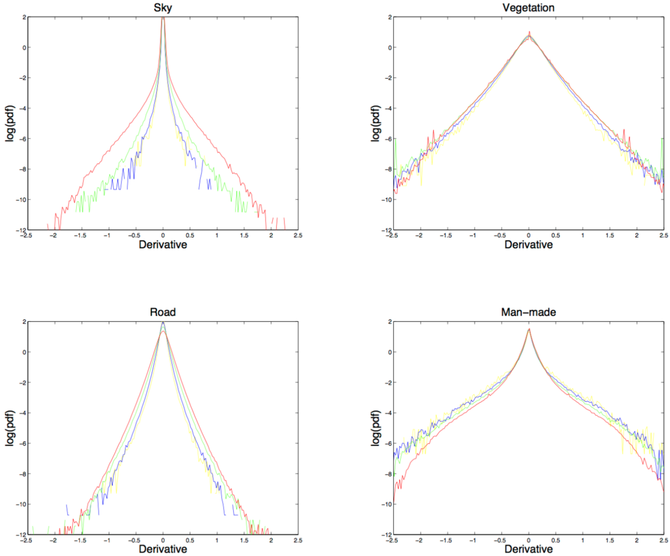
Natural image statistics [6]



[6] J. Huang, D. Mumford, Statistics of Natural Images and Models, CVPR '99

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Image denoising

- Minimize negative logarithm

$$
\begin{aligned}
u^* &\in \underset{u\in\mathbb{R}^N}{\operatorname{argmin}} \; -\log p(f|u)p(u) \\
&= \underset{u\in\mathbb{R}^N}{\operatorname{argmin}} \; -\log p(f|u) - \log p(u) \\
&= \underset{u\in\mathbb{R}^N}{\operatorname{argmin}} \; \underbrace{\frac{\lambda}{2}\|u-f\|^2 + \sum_{i=1}^{2N} c_\varepsilon((Du)_i)}_{=:E(u)}
\end{aligned}
$$

- $E(u)$ is λ-strongly convex and L-smooth with $L = \lambda + \frac{\|D\|^2}{\varepsilon}$
- Proof and implementation: last week's exercises :-)

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Evolution to global optimum via gradient descent

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$\varepsilon = 0.1$

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$\varepsilon = 0.01$

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

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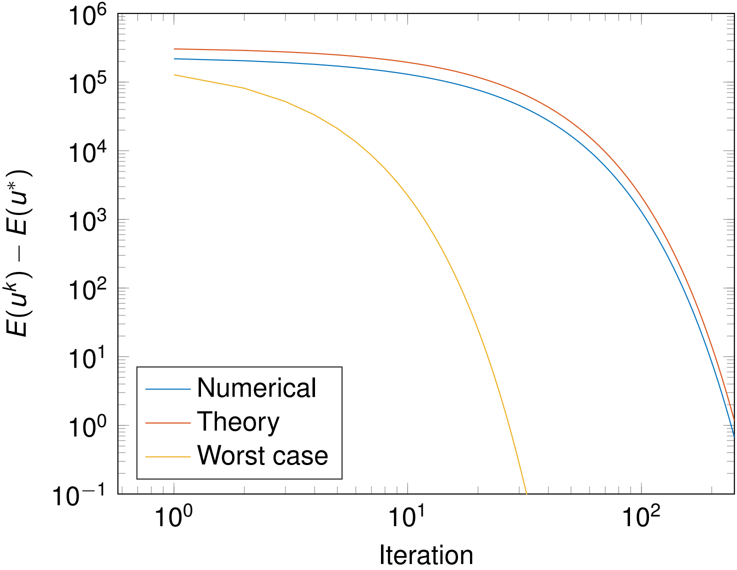
Convergence, $\tau = 2/(m + L)$



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Convergence, backtracking line search

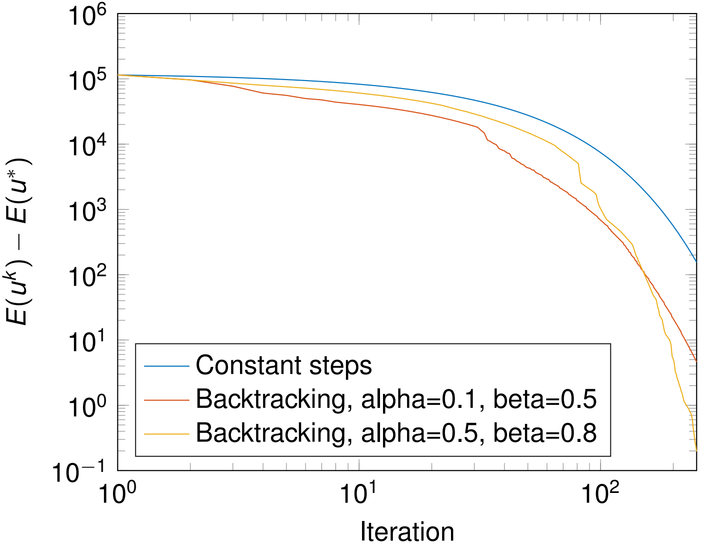

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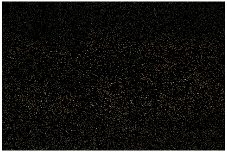
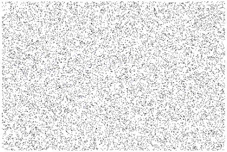
Image inpainting



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



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

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

$$u^* \in \operatorname*{argmin}_u \frac{\lambda}{2} \|m \cdot (u - f)\|^2 + \sum_{i=1}^{2N} c_\varepsilon \left((\nabla u)_i \right)$$

- Energy is not strongly convex, but L-smooth
- Sublinear $\mathcal{O}(1/k)$ upper bound on convergence speed

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50% missing pixels

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50% missing pixels

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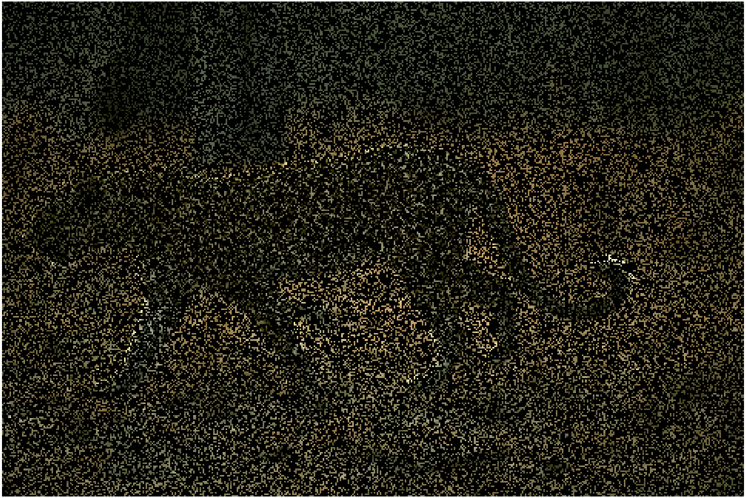
70% missing pixels



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70% missing pixels

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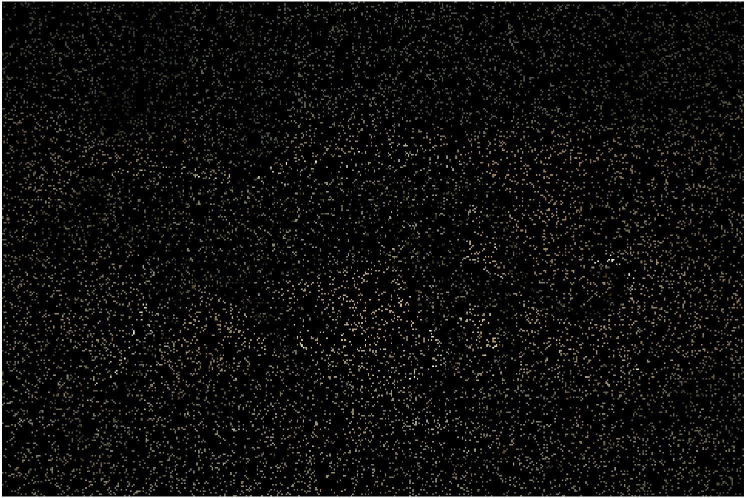
90% missing pixels



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90% missing pixels

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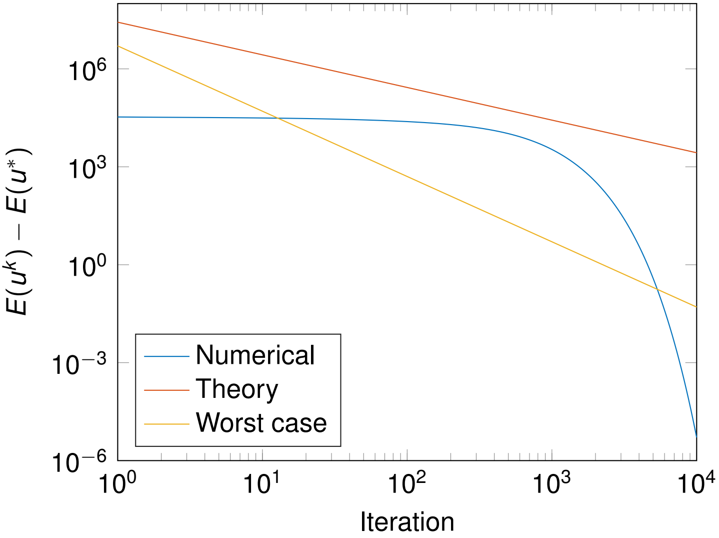
Convergence, $\tau = 1/L$



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Fast optimization challenge I

- Minimize the inpainting energy

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

- 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

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Handwritten digit recognition

- MNIST dataset[7], 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)

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

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

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Multinomial logistic regression

- Minimize negative log-likelihood

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

- 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)

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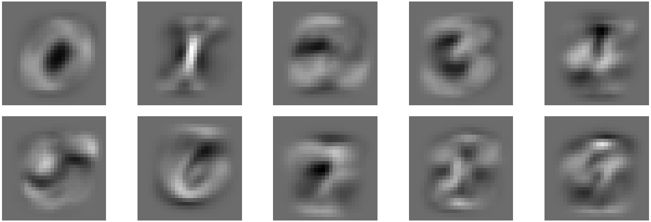
Multinomial logistic regression



- Classifier gives around 10% error on test set
- Can be easily improved to around $1 - 2\%$ with a few additional lines of MATLAB code (use features instead of raw pixels)
- Current best: 0.23% (convolutional neural networks)
- Learn more about learning:
  `https://vision.in.tum.de/teaching/ss2016/mlcv16`

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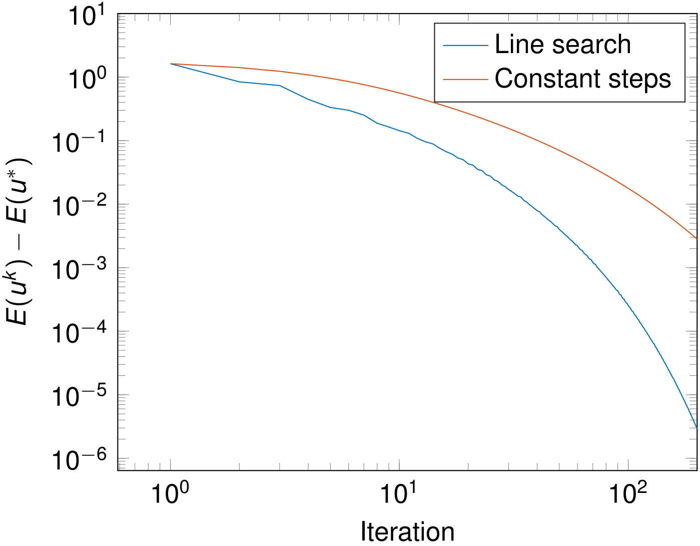

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Concluding remarks and outlook

- 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, ...

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Subgradient Method

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Non-smooth optimization

- Last lecture: analysis of gradient descent method
- Assumption: energy $E(u)$ is L-smooth
- However, many energies in practice are not even differentiable
- Smoothing the energy leads to poor approximation and high condition number
- Last week: subdifferential ∂E as a generalization of the gradient for nonsmooth functions
- Can we use it to construct an algorithm?

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Subgradient descent

Definition

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

$$u^{k+1} = u^k - \tau_k g^k, \text{ where } g^k \in \partial E(u^k), \quad k = 0, 1, 2, \dots,$$

is called *subgradient descent*.

Some remarks:

- g^k can be *any* subgradient of E at u^k
- Simple to implement
- Typically low per iteration complexity
- We'll see later: not a descent method

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Thomas Möllenhoff
Emanuel Laude

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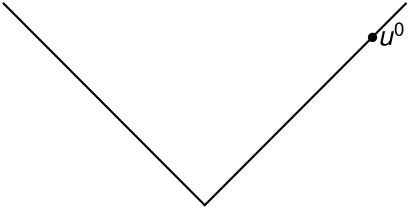
First example

- Let's use it to minimize $E(u) = |u|$ with $\tau_k = \tau$
- Iteration is given by

$$u^{k+1} = u^k - \tau \text{sign}(u^k)$$



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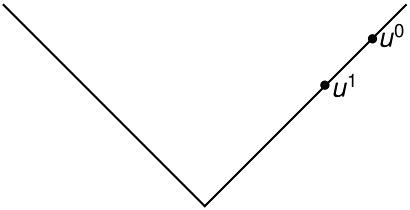

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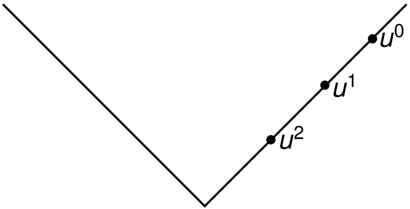

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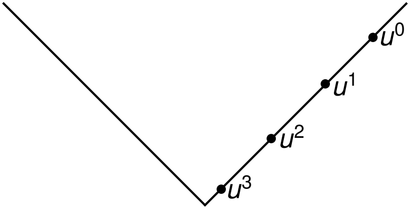

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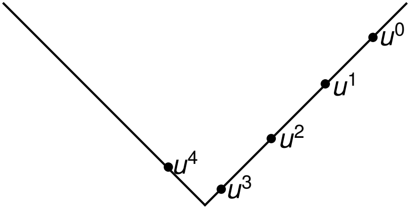

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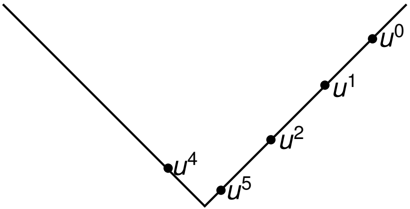

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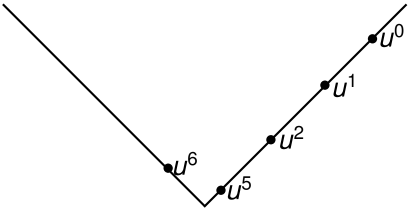

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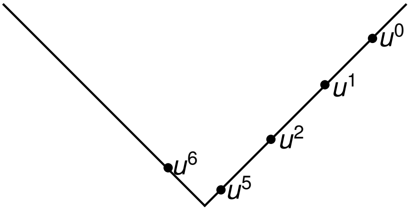

- Doesn't converge to optimum for constant step sizes

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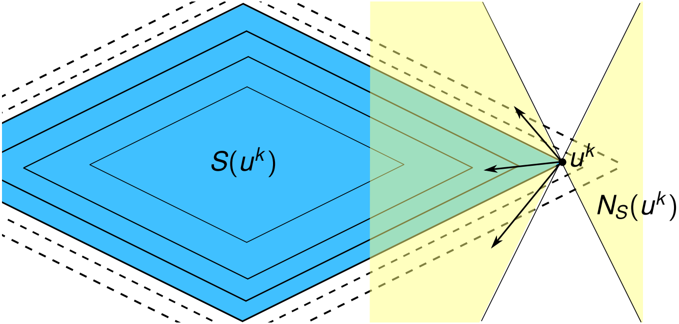
Not a descent method!

- Minimize $E(u) = |u_1| + 2|u_2|$



- Consider sub level sets at point u^k (shown in blue)

$$S(u^k) = \{u \in \mathbb{R}^n \mid E(u) \leq E(u^k)\}$$

- Subgradient method: move along vector from $-N_S(u^k)$
- These are not necessarily descent directions

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Some assumptions

- E has a minimizer u^*
- $E \in \mathcal{F}_G^0(\mathbb{R}^n)$, i.e., E is convex and Lipschitz continuous with constant G, and $\text{dom}(E) = \mathbb{R}^n$

Theorem: Bounded subdifferential

If $E : \mathbb{R}^n \to \mathbb{R}$ is convex and Lipschitz continuous with constant $G > 0$, then this is equivalent to

$$\|g\|_2 \leq G, \qquad \forall g \in \partial E(u), \forall u \in \mathbb{R}^n.$$

Proof: Board!

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Thomas Möllenhoff
Emanuel Laude

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Convergence analysis

- Consider distance to optimal set, $u^+ = u - \tau g$, $g \in \partial E(u)$

$$
\begin{aligned}
\left\|u^+ - u^*\right\|^2 &= \|u - \tau g - u^*\|^2 \\
&= \|u - u^*\|^2 - 2\tau\langle g, u - u^*\rangle + \tau^2\|g\|^2 \\
&\leq \|u - u^*\|^2 - 2\tau\left(E(u) - E(u^*)\right) + \tau^2\|g\|^2
\end{aligned}
$$

- Rearranging the above yields:

$$2\tau\left(E(u) - E(u^*)\right) \leq \|u - u^*\|^2 - \left\|u^+ - u^*\right\|^2 + \tau^2\|g\|^2$$

- Set $u^+ = u^k$, $u^- = u^{k-1}$, $\widehat{E}_N = \min_{0\leq k\leq N} E(u^k)$:

$$2\left(\sum_{k=1}^{N}\tau_k\right)\left(\widehat{E}_N - E(u^*)\right) \leq \left\|u^0 - u^*\right\|^2 + \sum_{k=1}^{N}\tau_k^2\left\|g^k\right\|^2$$

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Convergence analysis for fixed step size

- For fixed step size $\tau_k = \tau$ we have

$$\widehat{E}_N - E(u^*) \leq \frac{\left\| u^0 - u^* \right\|^2}{2N\tau} + \frac{G^2 \tau}{2}$$

- Does not guarantee convergence
- $\widehat{E}_N$ is $(G^2\tau/2)$-suboptimal for large N
- For step size $\tau_k = \tau / \left\| g^k \right\|$ we have

$$\widehat{E}_N - E(u^*) \leq \frac{G \left\| u^0 - u^* \right\|^2}{2N\tau} + \frac{G\tau}{2}$$

- Also does not guarantee convergence
- $\widehat{E}_N$ is $(G\tau/2)$-suboptimal for large N

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Diminishing step sizes

- Choose sequence $\tau_k \to 0$, $\sum_{k=1}^{\infty} \tau_k = \infty$
- Example: harmonic series $\tau_k = 1/k$
- For non-constant steps we have the following bound

$$\widehat{E}_N - E(u^*) \leq \frac{\left\| u^0 - u^* \right\|^2 + G^2 \sum_{k=1}^{N} \tau_k^2}{2 \sum_{k=1}^{N} \tau_k}$$

- For such a sequence it holds that

$$\frac{\sum_{k=1}^{N} \tau_k^2}{\sum_{k=1}^{N} \tau_k} \to 0, \quad \text{for} \quad N \to \infty$$

- Thus $\widehat{E}_N$ converges to the optimal $E(u^*)$ for $N \to \infty$

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Thomas Möllenhoff
Emanuel Laude

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Polyak step size

- Recall the inequality we started with

$$\left\|u^+ - u^*\right\|^2 \leq \|u - u^*\|^2 - 2\tau(E(u) - E(u^*)) + \tau^2 \|g\|^2$$

- Right hand side is minimized for

$$\tau = \frac{E(u) - E(u^*)}{\|g\|^2}$$

- Plugging this back in yields

$$\left\|u^+ - u^*\right\|^2 \leq \|u - u^*\|^2 - \frac{(E(u) - E(u^*))^2}{\|g\|^2}$$

- A short calculation ($\rightarrow$ board!) shows:

$$\widehat{E}_N - E(u^*) \leq \frac{G\left\|u^0 - u^*\right\|}{\sqrt{N}}$$

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Worst-case complexity

- Problem class: convex functions $E : \mathbb{R}^n \to \mathbb{R}$
- First-order method:

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

- Worst-case complexity: $E(u^k) - E(u^*) = \mathcal{O}(1/\sqrt{k})$[8]
- The subgradient method, which is amongst the simplest concievable methods is optimal
- Indicates that the problem class of general convex functions is too complicated to be solved efficiently

[8] Nesterov, Introductory Lectures on Convex Optimization, Theorem 3.2.1

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The total variation

- Consider an image $f \in \mathbb{R}^{Nc}$ with N pixels and c channels
- Many possible ways of defining the total variation for color images, one choice:

$$TV(f) = \varphi(Df)$$

- $D : \mathbb{R}^{Nc} \to \mathbb{R}^{2Nc}$ is the usual finite differencing matrix
- $\varphi(g) = \sum_{i=1}^{N} \|g_i\|_2$ is the sum of consecutive $g_i \in \mathbb{R}^{2c}$
- It is non-differentiable, since $\|\cdot\|_2$ is not differentiable at 0

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Subdifferential of the total variation

- The subdifferential follows from the chain rule

$$\partial TV(u) = (D^T \circ \partial\varphi \circ D)(u)$$

- The subdifferential of φ for $g \in \mathbb{R}^{2Nc}$ is given as a product of N sets

$$\partial\varphi(g) = I_1 \times I_2 \times \ldots \times I_N \subset \mathbb{R}^{2Nc}$$

- The individual sets are the subdifferentials of $\|\cdot\|_2$

$$\mathbb{R}^{2c} \supset I_k = \begin{cases} \left\{ \frac{g_k}{\|g_k\|_2} \right\}, & \text{if } 0 \neq g_k, \\ B(0,1), & \text{otherwise.} \end{cases}$$

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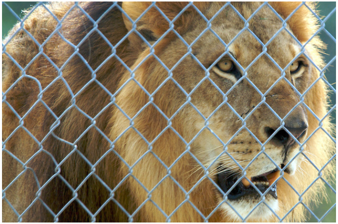
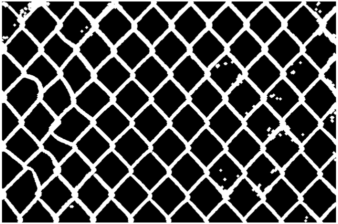
TV Inpainting



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



$m \in \mathbb{R}^{Nc}$

- Non-differentiable energy due to *TV* term

$$E(u) = \frac{\lambda}{2} \|m \cdot (u - f)\|^2 + TV(u)$$

- Subgradient can be easily computed:

$$g^k = \lambda(m \cdot (u^k - f)) + p^k, \text{ with } p^k \in \partial TV(u^k)$$

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Thomas Möllenhoff
Emanuel Laude

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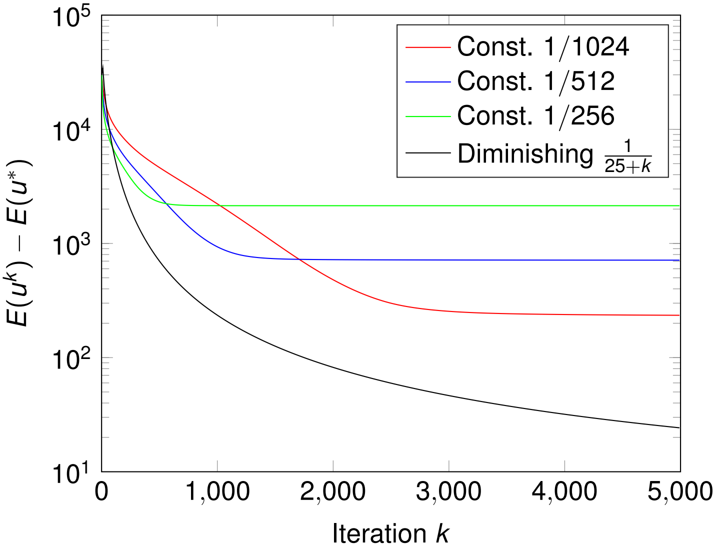
Numerical convergence results



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The TV-ℓ_1 model

- A robust model for image denoising is given by

$$E(u) = \lambda \|u - f\|_1 + TV(u)$$

- The ℓ_1-data term is less sensitive to outliers than the previous quadratic data term
- Both data term and regularizer are non-smooth
- Getting a subgradient g^k is straightforward

$$g^k = \lambda \text{sign}(u^k - f) + p^k, \text{ with } p^k \in \partial TV(u^k)$$

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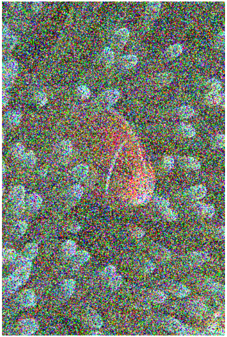
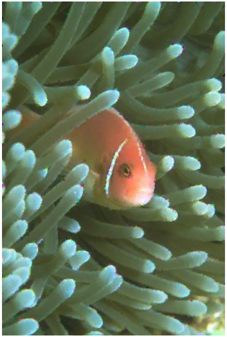
Robust denoising

Original



Noisy input



$TV - \ell_1$ denoised

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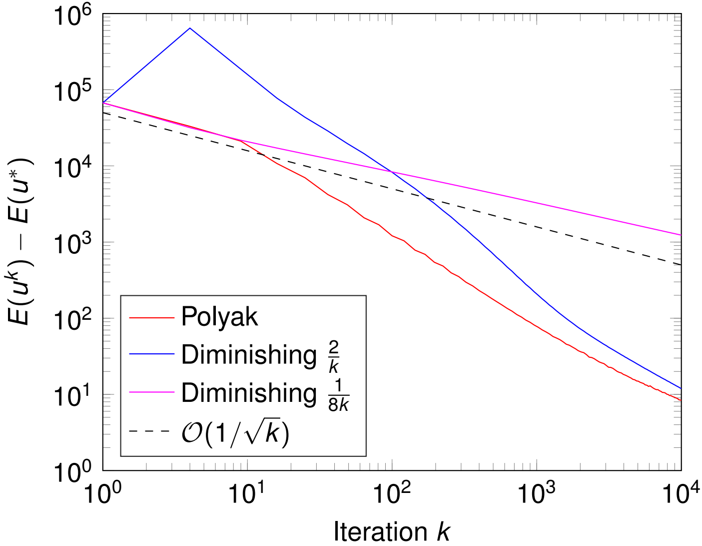

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Concluding remarks

- Why care about subgradient method?
  - Simple
  - Each iteration fast
  - Low memory requirements
- We covered only the absolute basics
- Many extensions to the subgradient method exist (acceleration, constraints, stochastic, ...)
- Next week: solving constrained problems, duality

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Thomas Möllenhoff
Emanuel Laude

Gradient Projection

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Thomas Möllenhoff
Emanuel Laude

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Gradient and subgradient descent

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

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

Gradient descent:

- $\text{dom } E = \mathbb{R}^n$
- For $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$ energy convergence in $\mathcal{O}(1/k)$
- For $E \in \mathcal{S}_{m,L}^{1,1}(\mathbb{R}^n)$ energy and iterate convergence in $\mathcal{O}(c^k)$

Subgradient descent:

- $\text{dom}(E) = \mathbb{R}^n$
- Applicable to any Lipschitz-continuous convex energy
- Usually rather slow

Gradient projection: Generalizes gradient descent to arbitrary (nonempty, closed, convex) $\text{dom}(E)$.

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Gradient projection

Type of problem:

$$u^* \in \arg\min_{u \in C} E(u), \tag{1}$$

for $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$, 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.

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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.

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Thomas Möllenhoff
Emanuel Laude

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Example projections

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

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

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Properties of the projection

Firm Nonexpansiveness

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

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

By Cauchy-Schwartz, this implies the nonexpansiveness

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

Proof: Board

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Idea of gradient projection

Consider a problem

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

for $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$, 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.

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

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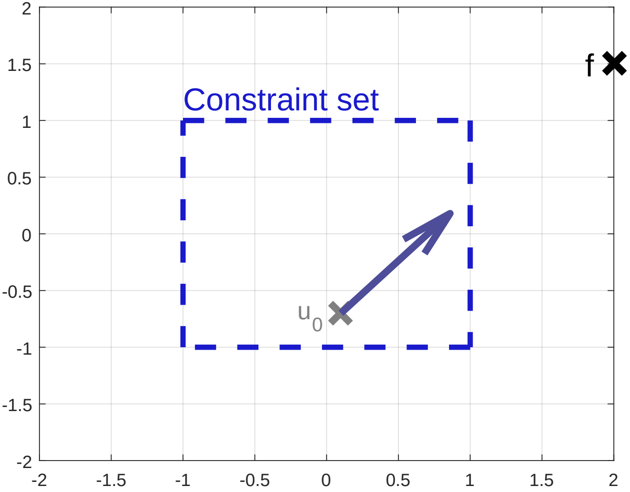
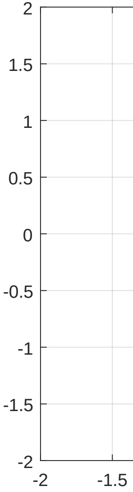
Idea of gradient projection

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 $u^0 \in C$

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

is called the *gradient projection* algorithm.

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

Remember: Gradient descent

- $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$ leads to a convergence of $\mathcal{O}(c^k)$, $c < 1$.
- $E \in \mathcal{F}^{1,1}_{L}(\mathbb{R}^n)$ leads to a convergence of $\mathcal{O}(1/k)$.

Same convergence for gradient projection?

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Gradient projection algorithm

First: $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$. Convergence proof of gradient descent

$$
\begin{aligned}
\|u^{k+1} - u^*\|^2 &= \|u^{k+1} - u^k + u^k - u^*\|^2 \\
&= \|u^k - u^*\|^2 \underbrace{+2\langle u^{k+1} - u^k, u^k - u^* \rangle + \|u^{k+1} - u^k\|^2}_{\text{bound from above by something negative} \cdot \|u^k - u^*\|^2} \\
&\leq c\|u^k - u^*\|^2
\end{aligned}
$$

To carry out a similar proof we need an upper bound on

$$\langle u^{k+1} - u^k, u^k - u^* \rangle + \|u^{k+1} - u^k\|^2$$

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Gradient projection algorithm

We will need (at least) three things:

1. E is L-smooth, i.e. for all u, v it holds that

$$E(v) - E(u) - \langle \nabla E(u), v - u \rangle - \frac{L}{2} \|v - u\|^2 \leq 0$$

2. E is m-strongly convex, i.e. for all u, v it holds that

$$E(v) - E(u) - \langle \nabla E(u), v - u \rangle - \frac{m}{2} \|v - u\|^2 \geq 0$$

3. Gradient projection equation:

$$0 = u^{k+1} - u^k + \tau \nabla E(u^k) + p^{k+1} \qquad p^{k+1} \in \partial \iota_C(u^{k+1})$$

Continue on the board.

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Gradient Projection Estimate

For $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$, $\tau = 1/L$, and $u \in C$ arbitrary it holds that

$$0 \leq E(u) - E(u^{k+1}) - \frac{L}{2}\|u - u^{k+1}\|^2 + \frac{L-m}{2}\|u - u^k\|^2$$

Corollary

In the above setting it holds that

$$0 \leq E(u^k) - E(u^{k+1}) - \frac{L}{2}\|u^{k+1} - u^k\|^2$$

$$0 \leq -\frac{L}{2}\|u^* - u^{k+1}\|^2 + \frac{L-m}{2}\|u^* - u^k\|^2$$

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Convergence of gradient projection for $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$

For $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$ the gradient projection algorithm with constant stepsize $\tau = \frac{1}{L}$ converges with

$$\|u^k - u^*\|^2 \leq \left(1 - \frac{m}{L}\right)^k \|u^0 - u^*\|^2.$$

What happens if we do not have strong convexity?

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Gradient projection algorithm

Our gradient projection estimate for $E \in \mathcal{S}^{1,1}_{m,L}(\mathbb{R}^n)$ with $m = 0$ and $u \in C$ arbitrary, yields

$$0 \leq E(u) - E(u^{k+1}) - \frac{L}{2}\|u - u^{k+1}\|^2 + \frac{L}{2}\|u - u^k\|^2$$

Picking $u = u^*$ we find

$$E(u^{k+1}) - E(u^*) \leq \frac{L}{2}\|u - u^k\|^2 - \frac{L}{2}\|u - u^{k+1}\|^2$$

$$\Rightarrow \sum_{k=0}^{K-1} \left(E(u^{k+1}) - E(u^*) \right) \leq \frac{L}{2}\|u - u^0\|^2 - \frac{L}{2}\|u - u^K\|^2$$

Similar to the gradient descent case, the monotonicity of the energy yields the convergence.

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Thomas Möllenhoff
Emanuel Laude

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Gradient projection algorithm

Did we really show convergence of $E(u)$ or did we implicitly make an additional assumption?

Convergence of gradient projection for $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$

Let $E \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$ have a global minimizer u^*. Then the gradient projection algorithm with constant stepsize $\tau = \frac{1}{L}$ yields

$$E(u^k) - E(u^*) \leq \frac{L}{2k} \|u^0 - u^*\|^2.$$

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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?

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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!

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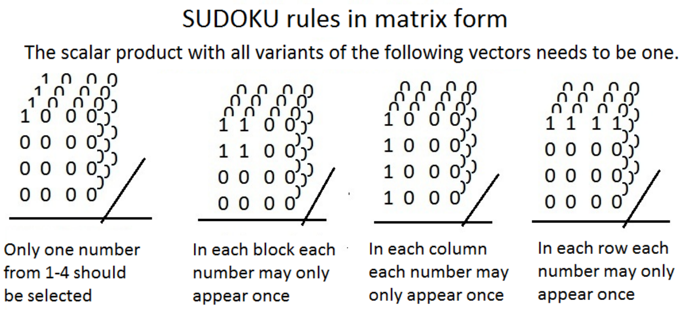
Example Application: Solving a SUDOKU

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 $A\vec{\boldsymbol{u}} = \vec{\mathbf{1}}$!

This means we may solve

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

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*.

Michael Moeller
Thomas Möllenhoff
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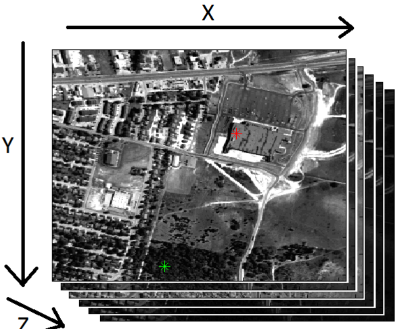
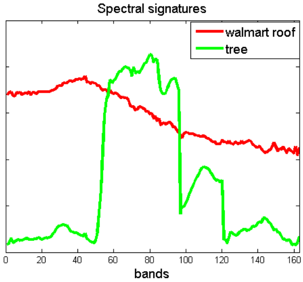
Example application: Unmixing and sparse recovery

Hyperspectral imagery



Hyperspectral cube



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

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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

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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

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

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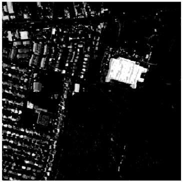
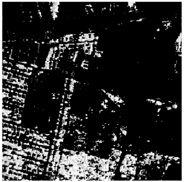
Example application: Unmixing and sparse recovery

color image illustration

endmember "road"



endmember "roof"



endmember "trees"

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Thomas Möllenhoff
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