Chapter 2

Gradient Methods

Convex Optimization for Computer Vision

SS 2016

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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:

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

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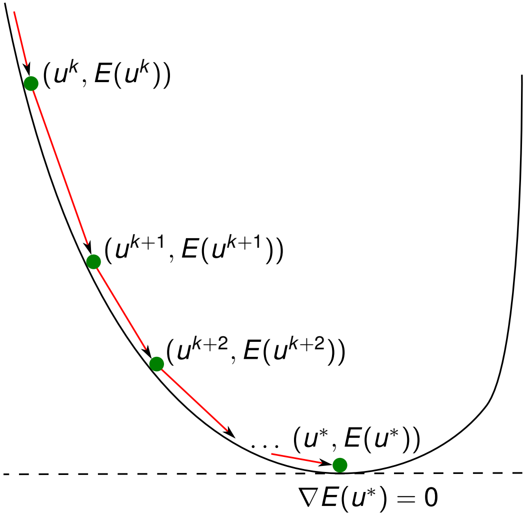
Descent methods

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



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

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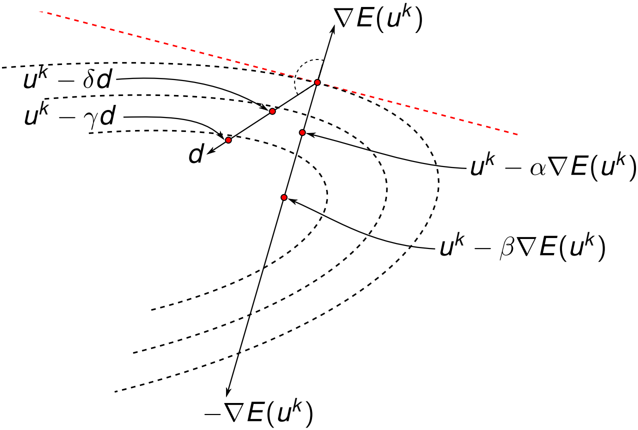
Descent methods



Descent methods

- The negative gradient is the *steepest* descent direction

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

- 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

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

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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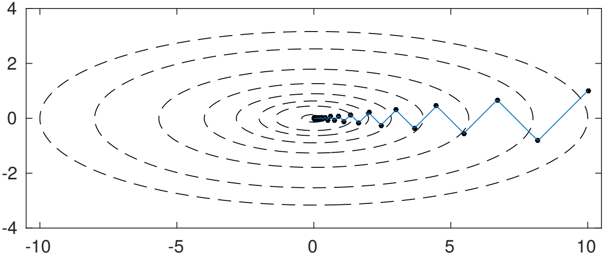
A first toy example

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



- 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

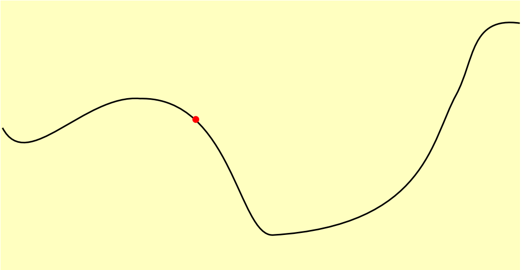
Lipschitz continuity

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*



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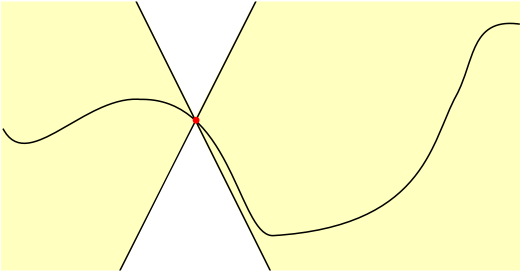

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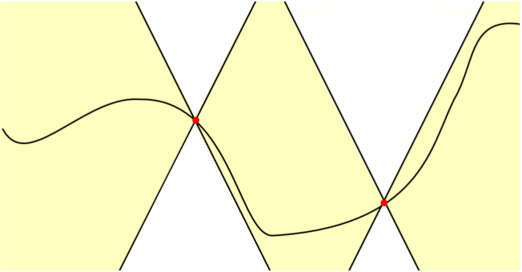

Lipschitz continuity

- 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

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

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!

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

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

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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

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

- For the minimum of the upper bound we have

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

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

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

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

- 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

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:

$$
\begin{aligned}
&\tau_k \leftarrow 1 \\
&\text{while } E\left(u^k - \tau_k \nabla E(u^k)\right) > E(u^k) - \alpha\tau_k \left\|\nabla E(u^k)\right\|^2 \\
&\qquad \tau_k \leftarrow \beta\tau_k \\
&\text{end}
\end{aligned}
$$

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

$$u^* \in \underset{u \in \mathbb{R}^N}{\text{argmax}}\; p(u|f) = \underset{u \in \mathbb{R}^N}{\text{argmax}}\; \frac{p(f|u)p(u)}{p(f)}$$

Image denoising

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

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

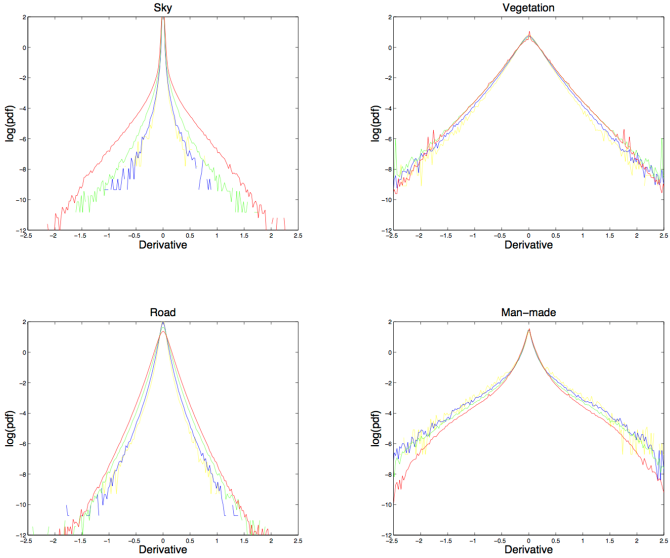
- Impose prior distribution on image gradient $Du \in \mathbb{R}^{2N}$

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

- Natural image statistics suggest the choice

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

Natural image statistics [6]



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

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 :-)

Image denoising

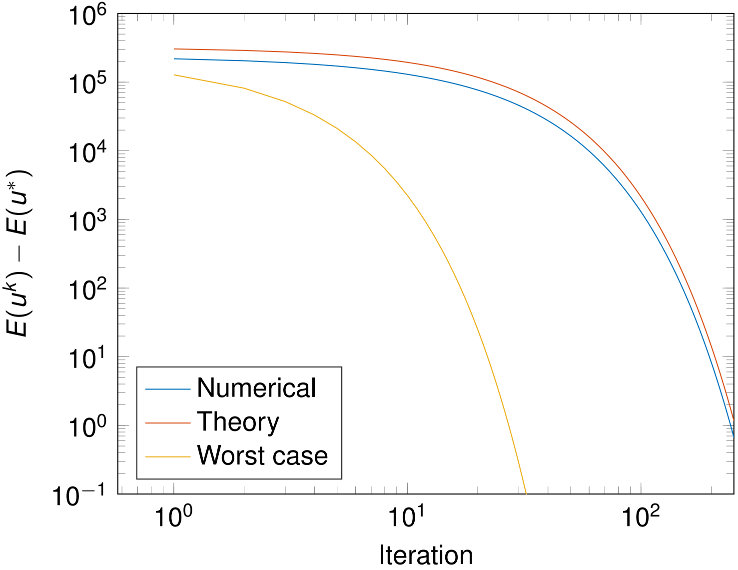
Evolution to global optimum via gradient descent

$\varepsilon = 0.1$

$\varepsilon = 0.01$

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

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



Convergence, backtracking line search

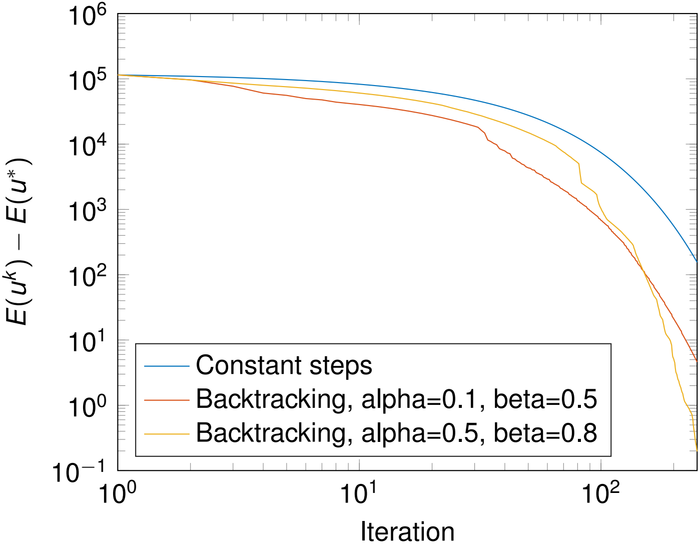
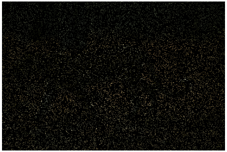
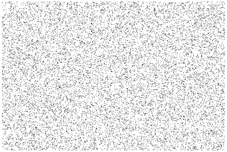


Image inpainting



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



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

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

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

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

Image Inpainting

50% missing pixels

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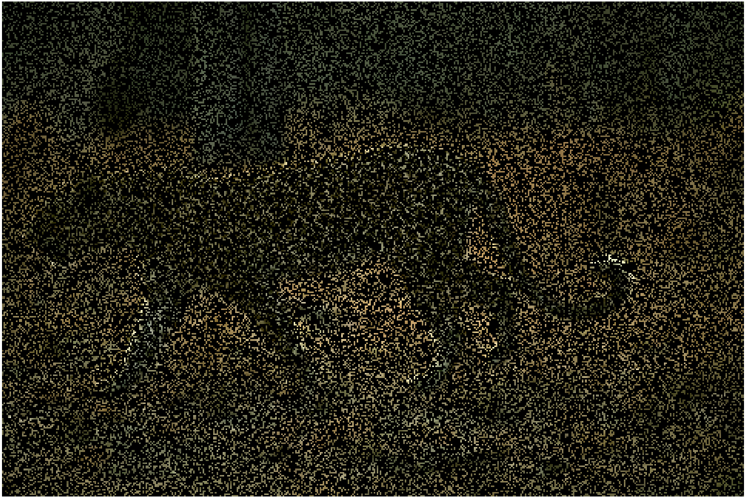
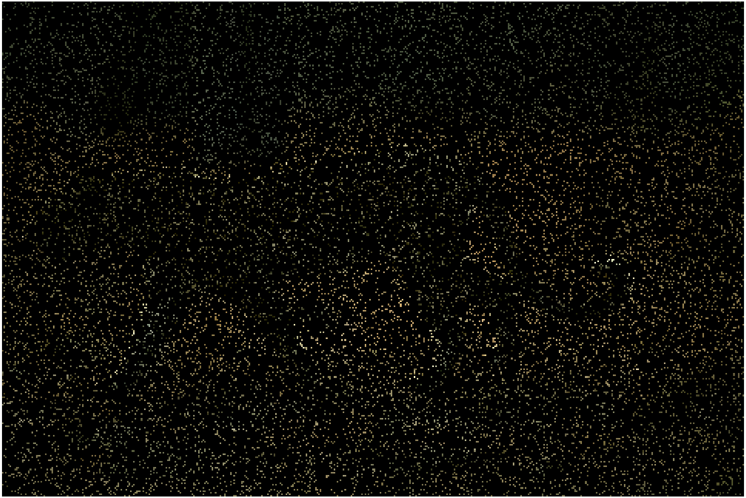
50% missing pixels

70% missing pixels



70% missing pixels

90% missing pixels



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90% missing pixels

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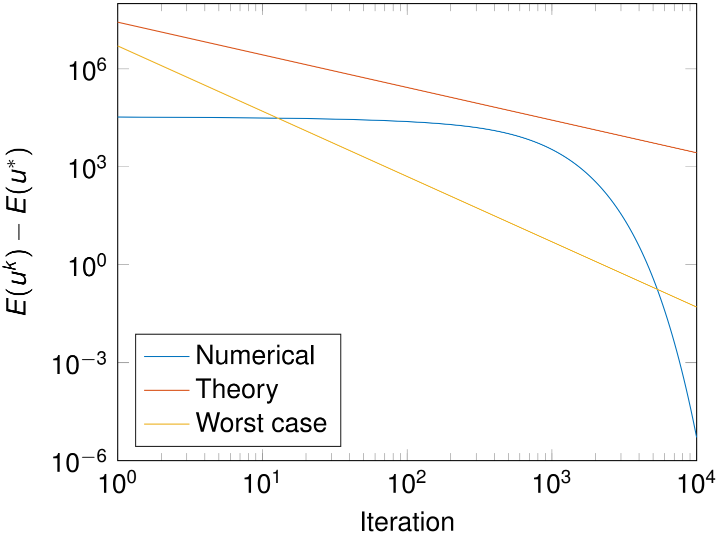
Convergence, $\tau = 1/L$



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Fast optimization challenge I

- Minimize the inpainting energy

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

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

$$\frac{E(u^k) - E(u^*)}{E(u^0)} < \delta$$

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

Handwritten digit recognition

- MNIST dataset[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/

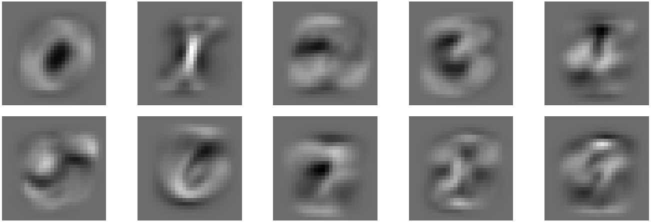
Multinomial logistic regression

- 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)

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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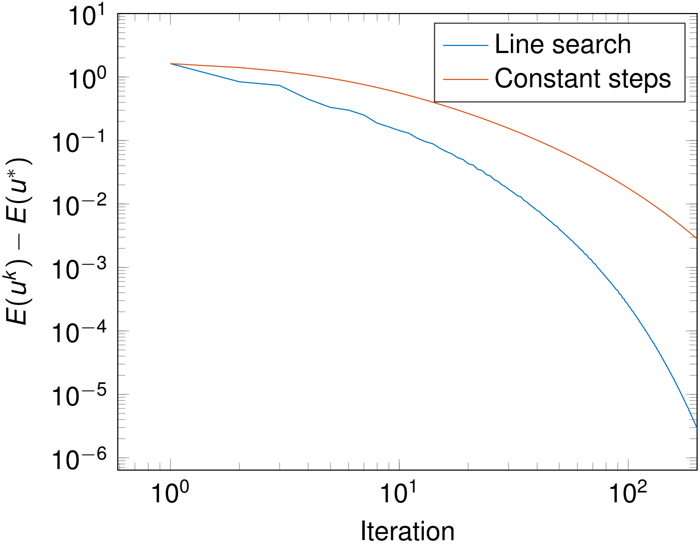
Multinomial logistic regression



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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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