Modern Optimization Techniques

2. Unconstrained Optimization / 2.5. Subgradient Methods

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Syllabus

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		2. Unconstrained Optimization
Mon. 13.11.	(2)	2.1 Gradient Descent
Mon. 20.11.	(3)	2.2 Stochastic Gradient Descent
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Mon. 4.12.	(5)	2.4 Quasi-Newton Methods
Mon. 11.12.	(6)	2.5 Subgradient Methods
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	—	— *Christmas Break* —
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Mon. 8.1.	(8)	3.1 Duality
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Outline

Outline

Motivation

- If a function is once differentiable
  we can optimize it using
  - Gradient Descent,
  - Stochastic Gradient Descent,
  - Quasi-Newton Methods

  (1st order information)

- If a function is twice differentiable
  we can optimize it using
  - Newton's method

  (2nd order information)

- What if the objective function is not differentiable?

1st-Order Condition for Convexity

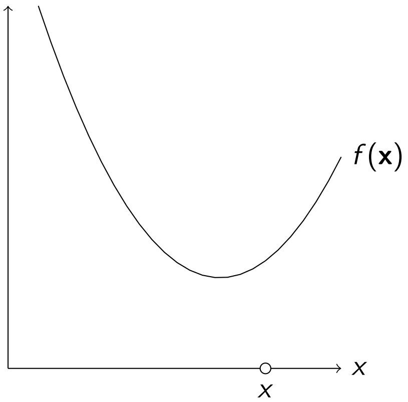
1st-order condition: a differentiable function f is convex iff

- dom f is a convex set and
- for all $\mathbf{x}, \mathbf{y} \in \text{dom } f$

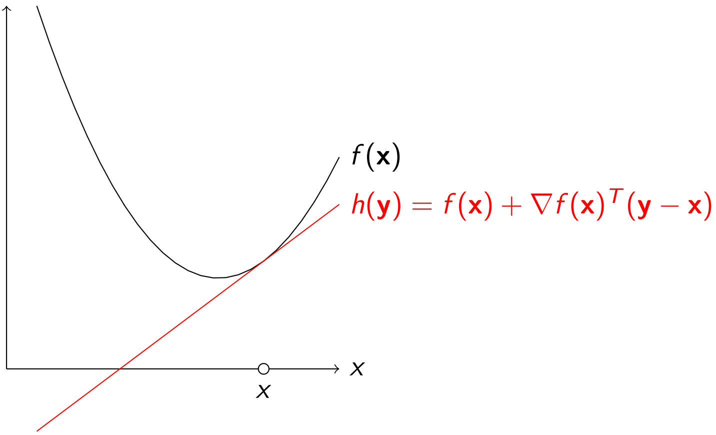
$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x})$$

  - i.e., the tangent (= first order Taylor approximation) of f at $\mathbf{x}$ is a global underestimator

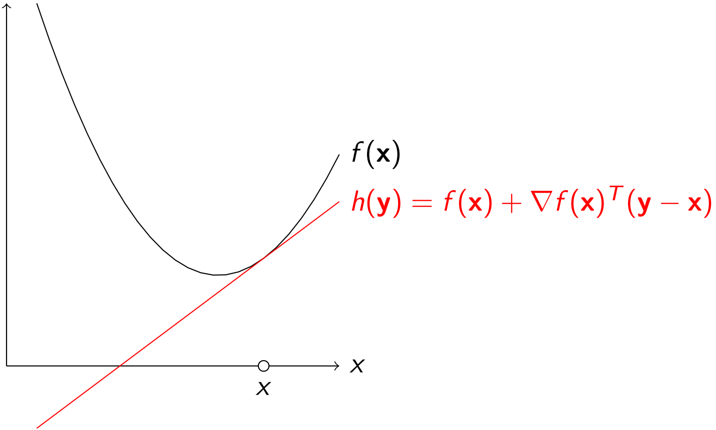
Tangent as a global underestimator



Tangent as a global underestimator



Tangent as a global underestimator

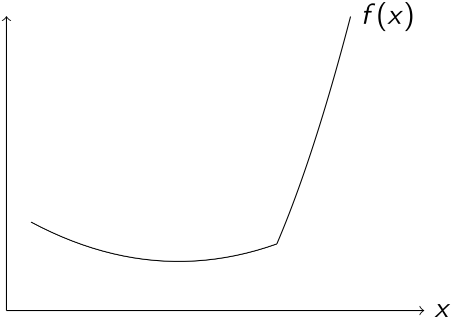


What happens if f is not differentiable?

Subgradient

Given a function f and a point $\mathbf{x} \in \operatorname{dom} f$,
$\mathbf{g} \in \mathbb{R}^n$ is called a **subgradient** of f at $\mathbf{x}$ if:
the hypersurface with slopes $\mathbf{g}$ through $(\mathbf{x}, f(\mathbf{x}))$ is a global underestimator of f, i.e.

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^T(\mathbf{y} - \mathbf{x}), \quad \text{for all } \mathbf{y} \in \operatorname{dom} f$$



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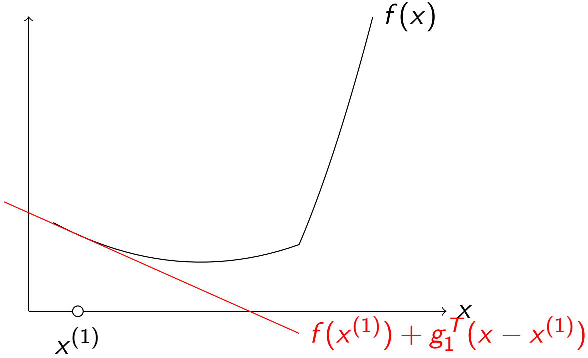

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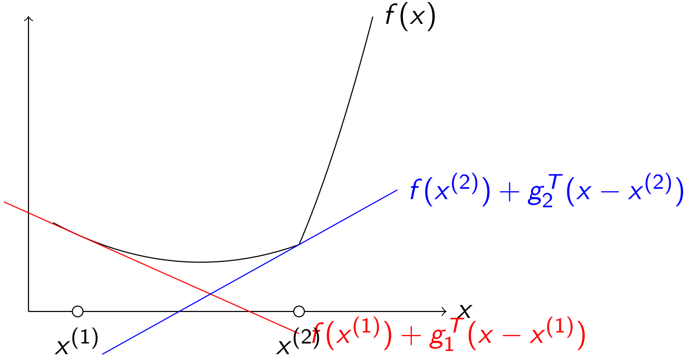

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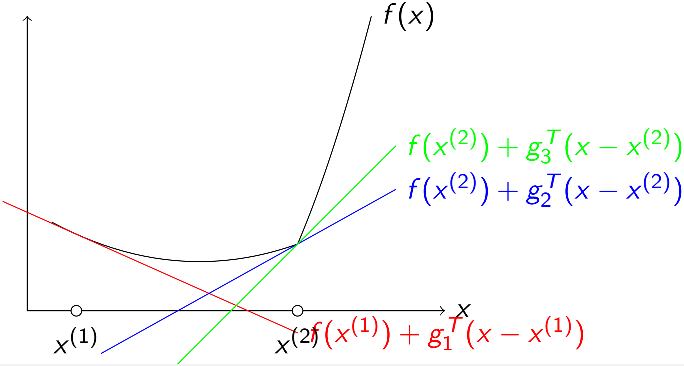


Subgradient

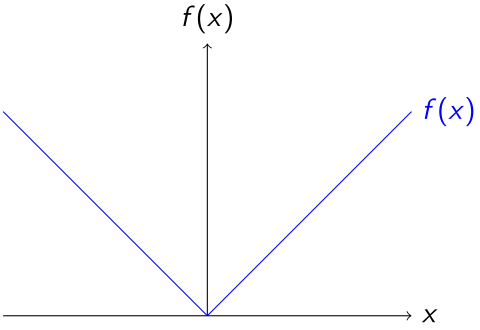
In the last example,

- $\mathbf{g_1}$ is a subgradient of f at $x^{(1)}$
- g_2 and g_3 are subgradients of f at $x^{(2)}$

Example

For $f : \mathbb{R} \to \mathbb{R}$ and $f(x) = |x|$:

- For $x \neq 0$ there is one subgradient $g = \nabla f(x) = \text{sign}(x)$
- For $x = 0$ the subgradient is $g \in [-1, 1]$



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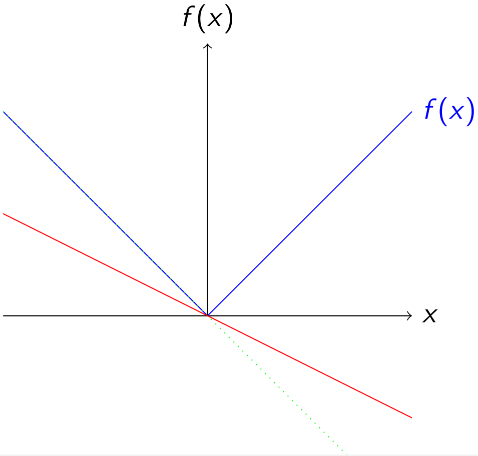

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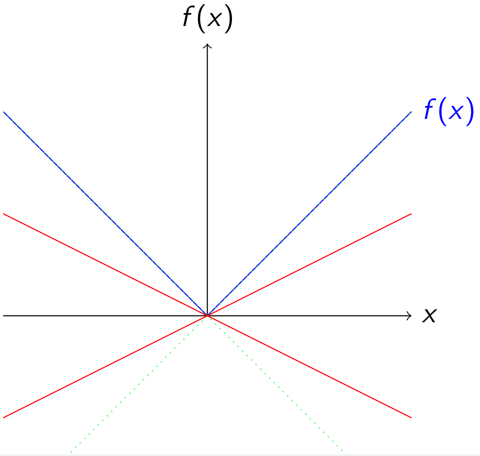


Subdifferential

Subdifferential $\partial f(\mathbf{x})$: set of all subgradients of f at $\mathbf{x}$

$$\partial f(\mathbf{x}) := \{\mathbf{g} \in \mathbb{R}^n \mid f(\mathbf{y}) \geq f(\mathbf{x}) + g^T(\mathbf{y} - \mathbf{x}) \; \forall \mathbf{y} \in \operatorname{dom} f\}$$

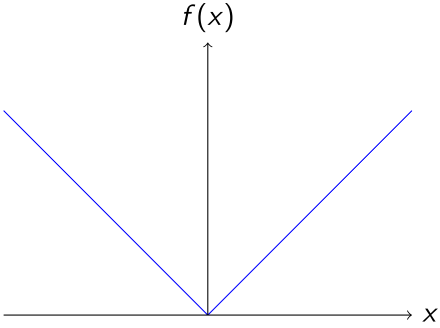
For a **convex** function f:

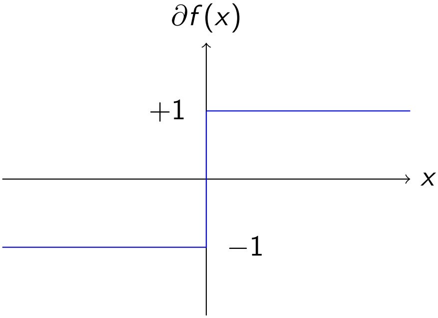
- subgradients always exist: $\partial f(\mathbf{x}) \neq \emptyset$
- f is differentiable at x
  iff the subdifferential contains a single element (the gradient)

$$f \text{ differentiable at } x \Longleftrightarrow \partial f(x) = \{\nabla f(x)\}$$

Example

For $f(x) = |x|$:





Subdifferential

For a **non-convex** function f:

- subgradients make less sense
  - see generalized subgradients, defined on local information

Outline

Subgradient Calculus

Assume f convex and $\mathbf{x} \in \operatorname{dom} f$

Some algorithms require only **one** subgradient for optimizing nondifferentiable functions f

Other algorithms, and optimality conditions require the *whole* subdifferential at $\mathbf{x}$

Tools for finding subgradients:

- **Weak subgradient calculus**: finding *one* subgradient $\mathbf{g} \in \partial f(\mathbf{x})$
- **Strong subgradient calculus**: finding the *whole* subdifferential $\partial f(\mathbf{x})$

Subgradient Calculus

We know that if f is differentiable at $\mathbf{x}$ then $\partial f(\mathbf{x}) = \{\nabla f(\mathbf{x})\}$
There are a couple of additional rules:

- **Scaling**: for $a > 0$: $\partial(a \cdot f) = \{a \cdot \mathbf{g} \mid \mathbf{g} \in \partial(f)\}$
- **Addition**: $\partial(f_1 + f_2) = \partial f_1 + \partial f_2$
- **Affine composition**: for $h(\mathbf{x}) = f(A\mathbf{x} + \mathbf{b})$ then

$$\partial h(\mathbf{x}) = A^T \partial f(A\mathbf{x} + \mathbf{b})$$

- **Finite pointwise maximum**: if $f(\mathbf{x}) = \max_{m=1\,\ldots,M} f_m(\mathbf{x})$ then

$$\partial f(\mathbf{x}) = \text{conv} \bigcup_{m: f_m(\mathbf{x}) = f(\mathbf{x})} \partial f_m(\mathbf{x})$$

  the subdifferential is the convex hull of the union of subdifferentials of all active functions at $\mathbf{x}$

Subgradients / More Examples

$$f(x) := ||x||_2$$

$$\partial f(x) =$$

Subgradients / More Examples

$$f(x) := ||x||_2$$

$$\partial f(x) = \begin{cases} \{\frac{x}{||x||_2}\}, & \text{if } x \neq 0_N \\ \{g \in \mathbb{R}^N \mid ||g||_2 \leq 1\}. & \text{if } x = 0_N \end{cases}$$

proof:

$$\begin{aligned} \partial(||x||_2) &= \partial(\max_{z:||z||_2\leq 1} z^T x) \\ &= \text{conv} \bigcup_{z:||z||_2\leq 1, z^T x \text{ max.}} z, \quad \text{for } x = 0 \\ &= \text{conv} \bigcup_{z:||z||_2\leq 1} z \\ &= \{z \in \mathbb{R}^N \mid ||z||_2 \leq 1\} \end{aligned}$$

Outline

Descent Direction

- idea:
  - choose an arbitrary subgradient $g \in \partial f$
  - use its negative $-g$ as next direction
- negative subgradients are in general no descent directions
  - example:

$$f(x) := |x|$$
$$x^{(0)} := 0$$

Optimality Condition

For a convex $f : \mathbb{R}^n \rightarrow \mathbb{R}$:

$$\mathbf{x}^* \text{ is a global minimizer} \quad \Leftrightarrow \quad \mathbf{0} \text{ is a subgradient of } f \text{ at } \mathbf{x}^*$$

$$f(\mathbf{x}^*) = \min_{\mathbf{x} \in \text{dom}\, f} f(\mathbf{x}) \qquad \mathbf{0} \in \partial f(\mathbf{x}^*)$$

Proof:

If $\mathbf{0}$ is a subgradient of f at $\mathbf{x}^*$, then for all $\mathbf{y} \in \mathbb{R}^n$:

$$f(\mathbf{y}) \geq f(\mathbf{x}^*) + \mathbf{0}^T(\mathbf{y} - \mathbf{x}^*)$$
$$f(\mathbf{y}) \geq f(\mathbf{x}^*)$$

Gradient Descent (Review)

min-gd$(f, \nabla f, x^{(0)}, \mu, \epsilon, K)$:
    for $k := 1, \ldots, K$:
        $\Delta x^{(k-1)} := -\nabla f(x^{(k-1)})$
        if $||\nabla f(x^{(k-1)})||_2 < \epsilon$:
            return $x^{(k-1)}$
        $\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$
        $x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$
    return "not converged"

where

- f objective function
- ∇f gradient of objective function f
- $x^{(0)}$ starting value
- μ step length controller
- ϵ convergence threshold for gradient norm
- K maximal number of iterations

Subgradient Method

min-subgrad$(f, \partial f, x^{(0)}, \mu, K)$:

$\quad x_{\text{best}}^{(0)} := x^{(0)}$

$\quad$ for $k := 1, \ldots, K$:

$\quad\quad$ if $0 \in \partial f(x^{(k-1)})$:

$\quad\quad\quad$ return $x_{\text{best}}^{(k-1)}$

$\quad\quad$ choose $g \in \partial f(x^{(k-1)})$ arbitrarily

$\quad\quad \Delta x^{(k-1)} := -g$

$\quad\quad \mu^{(k-1)} := \mu_{k-1}$

$\quad\quad x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$

$$x_{\text{best}}^{(k)} := \begin{cases} x^{(k)}, & \text{if } f(x^{(k)}) < f(x_{\text{best}}^{(k-1)}) \\ x_{\text{best}}^{(k-1)}), & \text{else} \end{cases}$$

$\quad$ return "not converged"

where

- $\mu \in \mathbb{R}^*$ step length schedule

Outline

Slowly Diminishing Stepsizes

Proof of convergence requires **slowly diminishing stepsizes**:

$$\lim_{k\to\infty} \mu^{(k)} = 0, \quad \sum_{j=0}^{\infty} \mu^{(j)} = \infty, \quad \sum_{j=0}^{\infty} (\mu^{(j)})^2 < \infty$$

for example:

$$\mu^{(k)} := \frac{1}{k+1}$$

but not:

- constant stepsizes $\mu^{(k)} := \mu \in \mathbb{R}$
- too fast shrinking stepsizes, e.g., $\mu^{(k)} := \frac{1}{(k+1)^2}$
- adaptive stepsize chosen by a step length controller

Convergence

Theorem (convergence of subgradient method)

Under the assumptions

I. $f : X \to \mathbb{R}$ *is convex,* $X \subseteq \mathbb{R}^n$ *is open*

II. f *is Lipschitz-continuous with constant* $G > 0$*, i.e.*

$$|f(\mathbf{x}) - f(\mathbf{y})| \leq G||\mathbf{x} - \mathbf{y}||_2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$$

- *Equivalently:* $||\mathbf{g}||_2 \leq G$ *for any subgradient of* f *at any* $\mathbf{x}$

III. *slowly diminishing stepsizes* $\mu^{(k)}$*, i.e.,*

$$\lim_{k \to \infty} \mu^{(k)} = 0, \quad \sum_{j=0}^{\infty} \mu^{(j)} = \infty, \quad \sum_{j=0}^{\infty} (\mu^{(j)})^2 < \infty$$

the subgradient method converges and

$$f_{best}^{(k)} - f(\mathbf{x}^*) \leq \frac{||\mathbf{x}^{(0)} - \mathbf{x}^*||^2 + G^2 \sum_{j=0}^{k} (\mu^{(j)})^2}{2 \sum_{j=0}^{k} \mu^{(j)}}$$

Convergence / Proof (1/2)

$$
\begin{aligned}
||\mathbf{x}^{(k+1)} - \mathbf{x}^*||_2^2 \\
&= ||\mathbf{x}^{(k)} - \mu^{(k)}\mathbf{g}^{(k)} - \mathbf{x}^*||_2^2 \\
&= ||\mathbf{x}^{(k)} - \mathbf{x}^*||_2^2 - 2\mu^{(k)}(\mathbf{g}^{(k)})^T(\mathbf{x}^{(k)} - \mathbf{x}^*) + (\mu^{(k)})^2||\mathbf{g}^{(k)}||_2^2 \\
&\underset{\text{SG}}{\leq} ||\mathbf{x}^{(k)} - \mathbf{x}^*||_2^2 - 2\mu^{(k)}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^*)) + (\mu^{(k)})^2||\mathbf{g}^{(k)}||_2^2 \\
&\underset{\text{rec}}{\leq} ||\mathbf{x}^{(0)} - \mathbf{x}^*||_2^2 - 2\sum_{j=0}^{k}\mu^{(j)}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*)) + \sum_{j=0}^{k}(\mu^{(j)})^2||\mathbf{g}^{(j)}||_2^2 \\
&\underset{\text{II}}{\leq} ||\mathbf{x}^{(0)} - \mathbf{x}^*||_2^2 - 2\sum_{j=0}^{k}\mu^{(j)}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*)) + G\sum_{j=0}^{k}(\mu^{(j)})^2 \qquad (1)
\end{aligned}
$$

Convergence / Proof (2/2)

$$f_{\text{best}}^{(k)} - f(\mathbf{x}^*) \leq \frac{\sum_{j=0}^{k}(f_{\text{best}}^{(k)} - f(\mathbf{x}^*))\mu^{(j)}}{\sum_{j=0}^{k} \mu^{(j)}}$$

$$\leq \frac{\sum_{j=0}^{k}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*))\mu^{(j)}}{\sum_{j=0}^{k} \mu^{(j)}}$$

$$\leq \frac{2\sum_{j=0}^{k}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*))\mu^{(j)} + ||\mathbf{x}^{(k+1)} - \mathbf{x}^*||_2^2}{2\sum_{j=0}^{k} \mu^{(j)}}$$

$$\underset{(1)}{\leq} \frac{||\mathbf{x}^{(0)} - \mathbf{x}^*||_2^2 + G\sum_{j=0}^{k}(\mu^{(j)})^2}{2\sum_{j=0}^{k} \mu^{(j)}}$$

$$\lim_{k\to\infty} f_{\text{best}}^{(k)} - f(\mathbf{x}^*) \leq \lim_{k\to\infty} \frac{||\mathbf{x}^{(0)} - \mathbf{x}^*||_2^2 + G\sum_{j=0}^{k}(\mu^{(j)})^2}{2\sum_{j=0}^{k} \mu^{(j)}} \underset{\text{III}}{=} 0$$

Further Readings

- Subgradient methods are not covered by Boyd and Vandenberghe [2004]
- Subgradients:
  - [Bertsekas, 1999, ch. B.5 and 6.1]
- Subgradient methods:
  - [Bertsekas, 1999, ch. 6.3.1]

References I

Dimitri P. Bertsekas. *Nonlinear Programming*. Springer, 1999.

Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge Univ Press, 2004.

Example: Text Classification

Features **A**: normalized word frequecies in text documents

Category **y**: topic of the text documents

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 1 & a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,1} & a_{m,2} & a_{m,3} & a_{m,4} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

$$\hat{y}_i = \sigma(\mathbf{x}^T \mathbf{a_i})$$

Text Classification: L1-Regularized Logistic Regression

For $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$ and $\mathbf{A} \in \mathbb{R}^{m \times n}$ we have the following problem

$$\text{minimize} \quad -\sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i})) + \lambda ||\mathbf{x}||_1$$

Which can be rewritten as:

$$\text{minimize} \quad -\sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i})) + \lambda \sum_{k=1}^{n} |x_k|$$

f is convex and non-smooth

Example: L1-Regularized Logistic Regression

The subgradients of
$f(\mathbf{x}) = -\sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i})) + \lambda ||\mathbf{x}||_1$ are:

$$\mathbf{g} = -\mathbf{A}^T(\mathbf{y} - \hat{\mathbf{y}}) + \lambda \mathbf{s}$$

where $\mathbf{s} \in \partial ||\mathbf{x}||_1$, i.e.:

- $s_k = \text{sign}(\mathbf{x}_k)$ if $\mathbf{x}_k \neq 0$
- $s_k \in [-1, 1]$ if $\mathbf{x}_k = 0$

Example - The algorithm

For $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$ and $\mathbf{A} \in \mathbb{R}^{m \times n}$ we have the following the problem

$$\text{minimize} \quad -\sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i})) + \lambda \sum_{k=1}^{n} |x_k|$$

1. Start with an initial solution $\mathbf{x}^{(0)}$
2. $t \leftarrow 0$
3. $f_{\text{best}} \leftarrow f(\mathbf{x}^{(0)})$
4. Repeat until convergence
   - 4.1 $\mathbf{x}^{(k+1)} \leftarrow \mathbf{x}^{(k)} - \mu^{(k)}(-\mathbf{A}^T(\mathbf{y} - \hat{\mathbf{y}}) + \lambda \mathbf{s})$
   - 4.2 $t \leftarrow t + 1$
   - 4.3 $f_{\text{best}} \leftarrow \min(f(\mathbf{x}^{(k)}), f_{\text{best}})$
5. Return f_{best}

where $\mathbf{s} \in \partial ||\mathbf{x}||_1$, i.e.:

- $s_k = \text{sign}(\mathbf{x}_k)$ if $\mathbf{x}_k \neq 0$
- $s_k \in [-1, 1]$ if $\mathbf{x}_k = 0$