Modern Optimization Techniques

2. Unconstrained Optimization / 2.5. Subgradient Methods

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Syllabus

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		1. Theory
Mon. 6.11.	(2)	1. Convex Sets and Functions
		2. Unconstrained Optimization
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Mon. 20.11.	(4)	2.2 Stochastic Gradient Descent
Mon. 27.11.	(5)	2.3 Newton's Method
Mon. 4.12.	(6)	2.4 Quasi-Newton Methods
Mon. 11.12.	(7)	2.5 Subgradient Methods
Mon. 18.12.	(8)	2.6 Coordinate Descent
	—	— *Christmas Break* —
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Outline

1. Subgradients

2. Subgradient Calculus

3. The Subgradient Method

4. Convergence

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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 (Review)

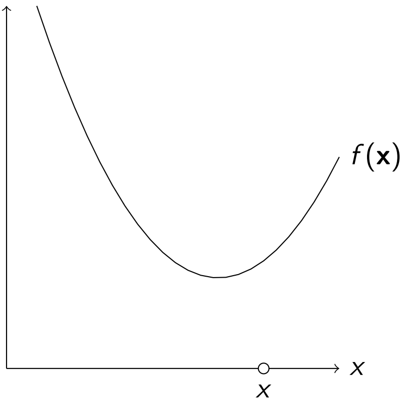
1st-order condition: a differentiable function f is convex iff

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

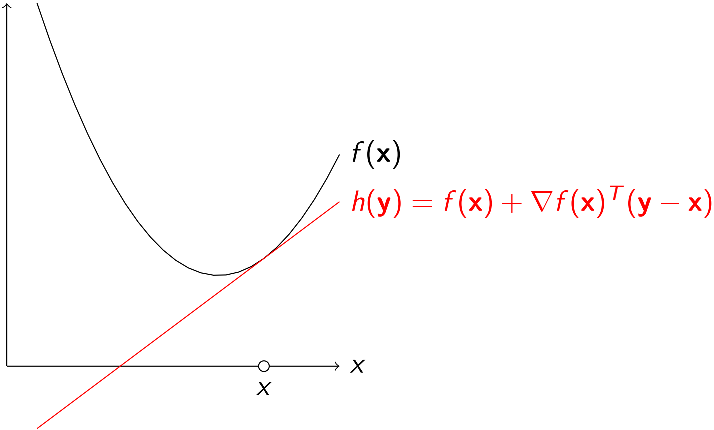
$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x})$$

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

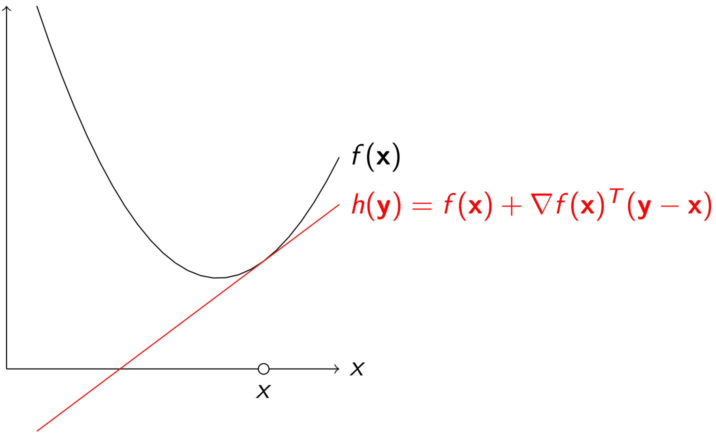
Tangent as a global underestimator



Tangent as a global underestimator



Tangent as a global underestimator

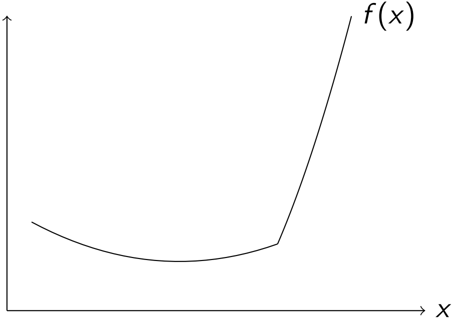


What happens if f is not differentiable?

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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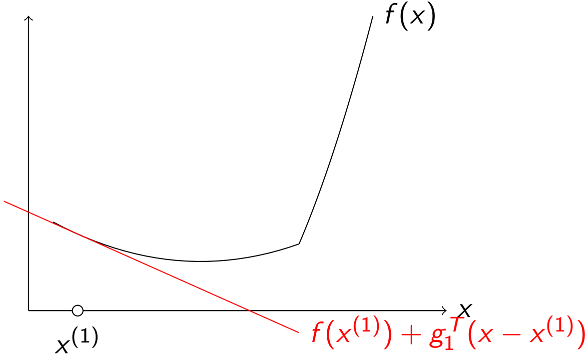

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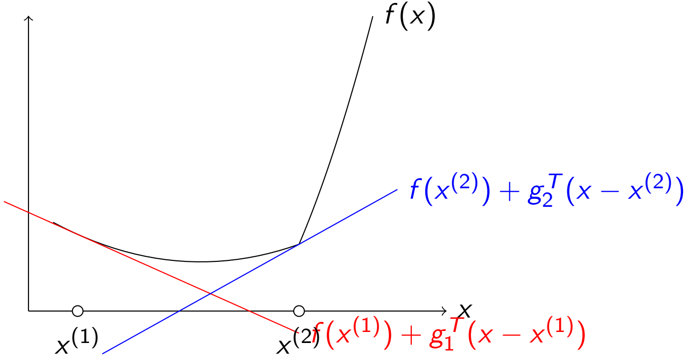

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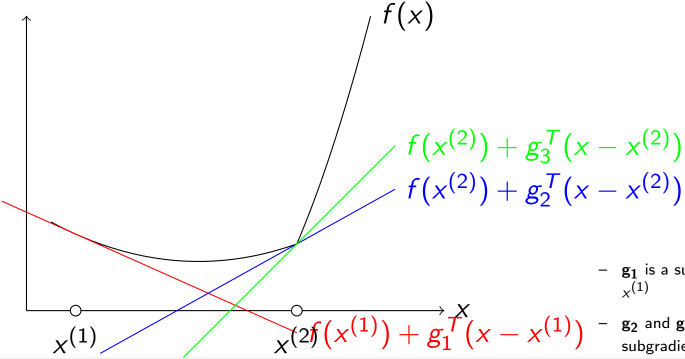
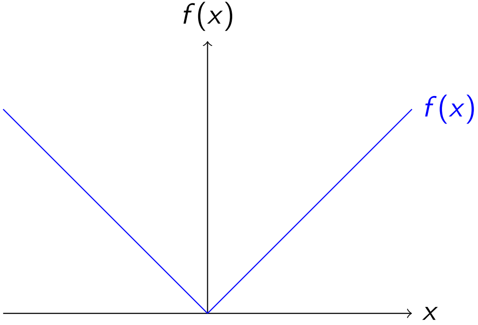


- $\mathbf{g_1}$ is a subgradient of f at $x^{(1)}$
- $\mathbf{g_2}$ and $\mathbf{g_3}$ are subgradients of f at $x^{(2)}$

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 subgradients are: $g \in [-1, 1]$



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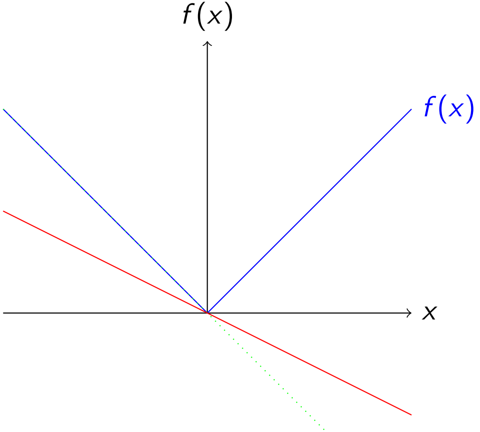

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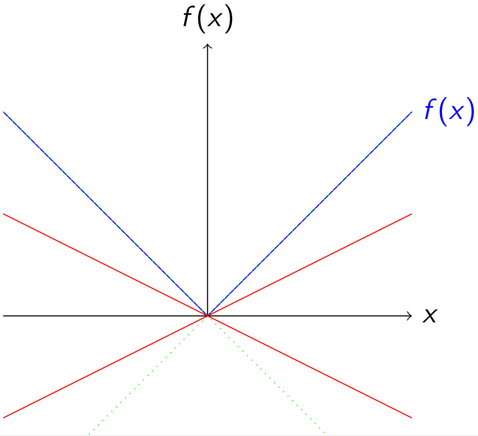


Subdifferential

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

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

- the subdifferential $\partial f(\mathbf{x})$ is a convex set.

$$\begin{aligned}(\alpha\mathbf{g} + (1-\alpha)\mathbf{h})^T(\mathbf{y} - \mathbf{x}) &= \alpha\mathbf{g}^T(\mathbf{y} - \mathbf{x}) + (1-\alpha)\mathbf{h}^T(\mathbf{y} - \mathbf{x}) \\ &\leq \alpha(f(\mathbf{y}) - f(\mathbf{x})) + (1-\alpha)(f(\mathbf{y}) - f(\mathbf{x})) \\ &= f(\mathbf{y}) - f(\mathbf{x}) \quad \rightsquigarrow (\alpha\mathbf{g} + (1-\alpha)\mathbf{h}) \in \partial f(\mathbf{x})\end{aligned}$$

- 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)

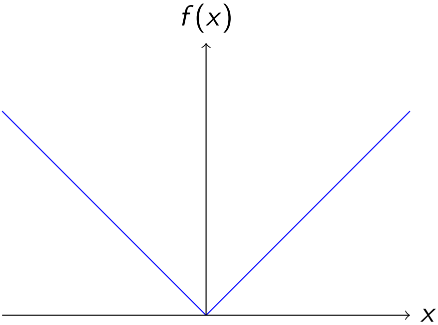
$$f \text{ differentiable at } x \iff \partial f(x) = \{\nabla f(x)\}$$

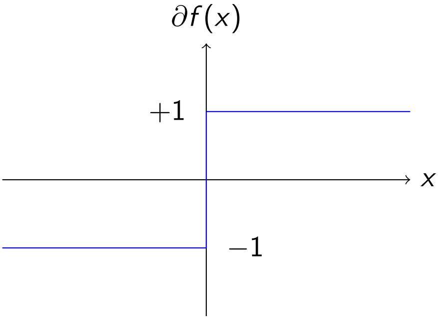
Example

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

- remember, ∂f is set valued:

$$\partial f(x) = \{1\}, \quad \forall x > 0, \quad \partial f(x) = \{-1\}, \quad \forall x < 0, \quad \partial f(0) = [-1, +1]$$





Subdifferential

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

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

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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

If f is differentiable at $\mathbf{x}$: $\partial f(\mathbf{x}) = \{\nabla f(\mathbf{x})\}$.

Additional rules:

- **Scaling**: for $a > 0$: $\partial(a \cdot f) = a \cdot \partial f = \{a \cdot \mathbf{g} \mid \mathbf{g} \in \partial(f)\}$
- **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

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

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

Subgradient Calculus / Pointwise Supremum

- **Pointwise Supremum**: if $f(\mathbf{x}) = \sup_{a \in A} f_a(\mathbf{x})$ then

$$\partial f(\mathbf{x}) \supseteq \operatorname{conv}\Big(\bigcup_{a \in A : f_a(\mathbf{x}) = f(\mathbf{x})} \partial f_a(\mathbf{x})\Big)$$

  - "$=$" if A is compact and f continuous in x and a.

Subgradient Calculus / Function Composition

- **Function Composition**: if $f(\mathbf{x}) = h(g_1(\mathbf{x}), g_2(\mathbf{x}), \ldots, g_M(\mathbf{x}))$, then

$$\partial f(\mathbf{x}) \supseteq \text{conv}\{(b_1, b_2, \ldots, b_M)a \mid b_m \in \partial g_m(x), m = 1 : M,$$
$$a \in (\partial h)(g_1(x), g_2(x), \ldots, g_M(x))\}$$

  - chain rule
  - for differentiable g_m and h:
    - $Dg(x) = (b_1, b_2, \ldots, b_M)^T$ Jacobi matrix of $g := (g_1, g_2, \ldots, g_M)$
    - $(\nabla h)(g(x)) = a$ gradient of h at $g(x)$

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:

use $||x||_2 = \max_{z:||z||_2 \leq 1} z^T x$

$$\text{“} \leq \text{”} : z := \frac{x}{||x||_2}, \quad \text{“} \geq \text{”} : z^T x \leq ||z||_2 ||x||_2 \text{ Cauchy-Schwarz}$$

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

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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:

$$f(x_1, x_2) := |x_1| + 3|x_2|$$

negative subgradients at $x := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$:

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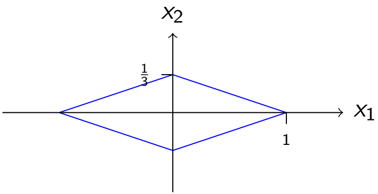

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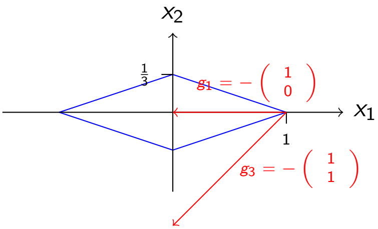

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- negative subgradients are in general no descent directions
  - example:

$$f(x_1, x_2) := |x_1| + 3|x_2|$$

negative subgradients at $x := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$:

$$-g_1 := -\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{descent direction}$$

$$-g_2 := -\begin{pmatrix} 1 \\ 3 \end{pmatrix} \quad \text{not a descent direction}$$

- thus cannot use stepsize controllers such as backtracking.

Optimality Condition

For a convex $f : \mathbb{R}^N \to \mathbb{R}$:

$$\begin{array}{ccc} \mathbf{x}^* \text{ is a global minimizer} & \Leftrightarrow & \mathbf{0} \text{ is a subgradient of } f \text{ at } \mathbf{x}^* \\ f(\mathbf{x}^*) = \min_{\mathbf{x} \in \operatorname{dom} f} f(\mathbf{x}) & & \mathbf{0} \in \partial f(\mathbf{x}^*) \end{array}$$

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

$$
\begin{array}{l}
\textbf{min-subgrad}(f, \partial f, x^{(0)}, \mu, K):\\
\quad x_{\text{best}}^{(0)} := x^{(0)}\\
\quad \text{for } \ k := 1, \ldots, K:\\
\qquad \text{if } \ 0 \in \partial f(x^{(k-1)}):\\
\qquad\quad \text{return } \ x_{\text{best}}^{(k-1)}\\
\qquad \text{choose } g \in \partial f(x^{(k-1)}) \text{ arbitrarily}\\
\qquad \Delta x^{(k-1)} := -g\\
\qquad \mu^{(k-1)} := \mu_{k-1}\\
\qquad x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}\\
\qquad x_{\text{best}}^{(k)} := \begin{cases} x^{(k)}, & \text{if } f(x^{(k)}) < f(x_{\text{best}}^{(k-1)})\\ x_{\text{best}}^{(k-1)}, & \text{else} \end{cases}\\
\quad \text{return } \ \text{"not converged"}
\end{array}
$$

where

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

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Slowly Diminishing Stepsizes

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

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

Q: Which of the following stepsizes are slowly diminishing?

- constant $\mu^{(k)} := \mu_0$
- $\mu^{(k)} := \frac{1}{k+1}$
- $\mu^{(k)} := \frac{1}{(k+1)^2}$

Slowly Diminishing Stepsizes

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

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

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

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* $\mathbf{g}$ *of* f *at any* $\mathbf{x}$

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

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

the subgradient method converges and

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

Convergence / Proof (1/2)

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

Convergence / Proof (2/2)

$$
\begin{aligned}
f(\mathbf{x}^{(k)}_{\text{best}}) - f(\mathbf{x}^*) &= \frac{\sum_{j=0}^{k}(f(\mathbf{x}^{(k)}_{\text{best}}) - f(\mathbf{x}^*))\mu^{(j)}}{\sum_{j=0}^{k}\mu^{(j)}} \\
&\leq \frac{\sum_{j=0}^{k}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*))\mu^{(j)}}{\sum_{j=0}^{k}\mu^{(j)}} \\
&\leq \frac{2\sum_{j=0}^{k}(f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*))\mu^{(j)} + ||\mathbf{x}^{(k+1)} - \mathbf{x}^*||_2^2}{2\sum_{j=0}^{k}\mu^{(j)}} \\
&\underset{(1)}{\leq} \frac{||\mathbf{x}^{(0)} - \mathbf{x}^*||_2^2 + G^2\sum_{j=0}^{k}(\mu^{(j)})^2}{2\sum_{j=0}^{k}\mu^{(j)}}
\end{aligned}
$$

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

Summary

- **Subgradients** generalize gradients (for convex functions):
  - any slope of a hypersurface that is global underestimator.
  - at a differentiable location: the gradient is the only subgradient.
- Example **absolute value**: $\partial(|x|)|(0) = [-1, +1]$
- **subgradient calculus**:
  - scalar multiplication, addition, affine composition, pointwise maximum
- The **subgradient method** generalizes gradient descent:
  - use an arbitrary subgradient
  - stop if 0 is among the subgradients
  - as subgradients generally are no descent direction, the best location so far has to be tracked.
- The subgradient method is converging.
  - for Lipschitz-continuous functions and slowly diminishing stepsizes.

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

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

Boyd, Stephen and Lieven Vandenberghe (2004). *Convex Optimization*. Cambridge University Press.

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.:

- $s_k = \mathrm{sign}(\mathbf{x}_k)$ 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 $\mathbf{x}_k = 0$