Nonsmooth optimization: beyond first order methods.

A tutorial focusing on bundle methods

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Computational NSO: what do we mean?

For the unconstrained problem

$$\min f(x),$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is convex but not differentiable at some points

Algorithms defined according on **how much** information is provided by certain oracle

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an **informative oracle**

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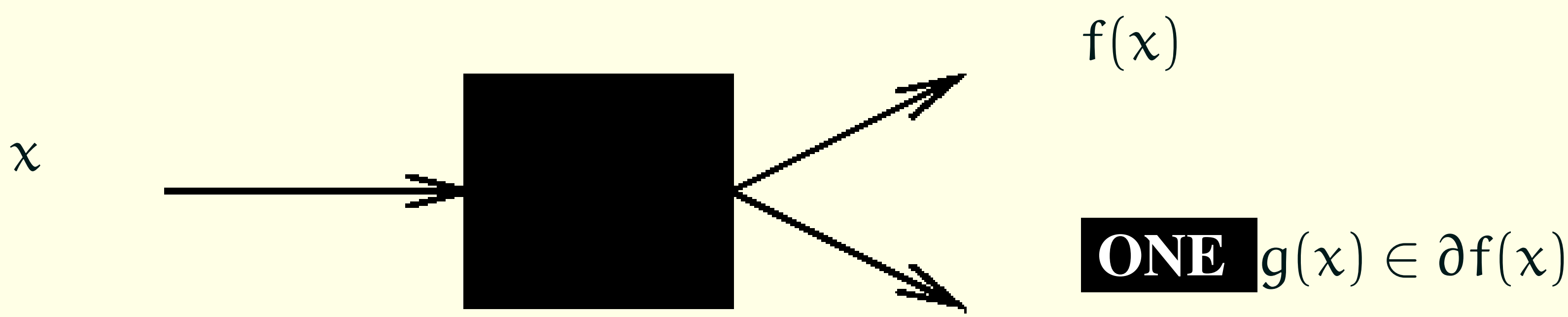
a **“black box”**



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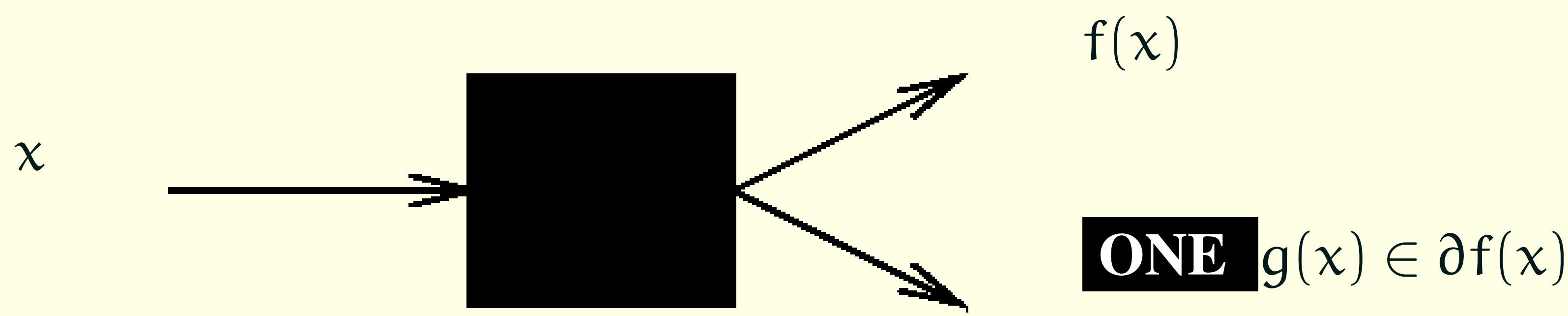


How common are nonsmooth objective functions in optimization?

When does nonsmoothness appear?

* if the **nature** of the problem imposes a nonsmooth model; or
* if **sparsity** of the solution is a concern; or
* in problems difficult to solve,

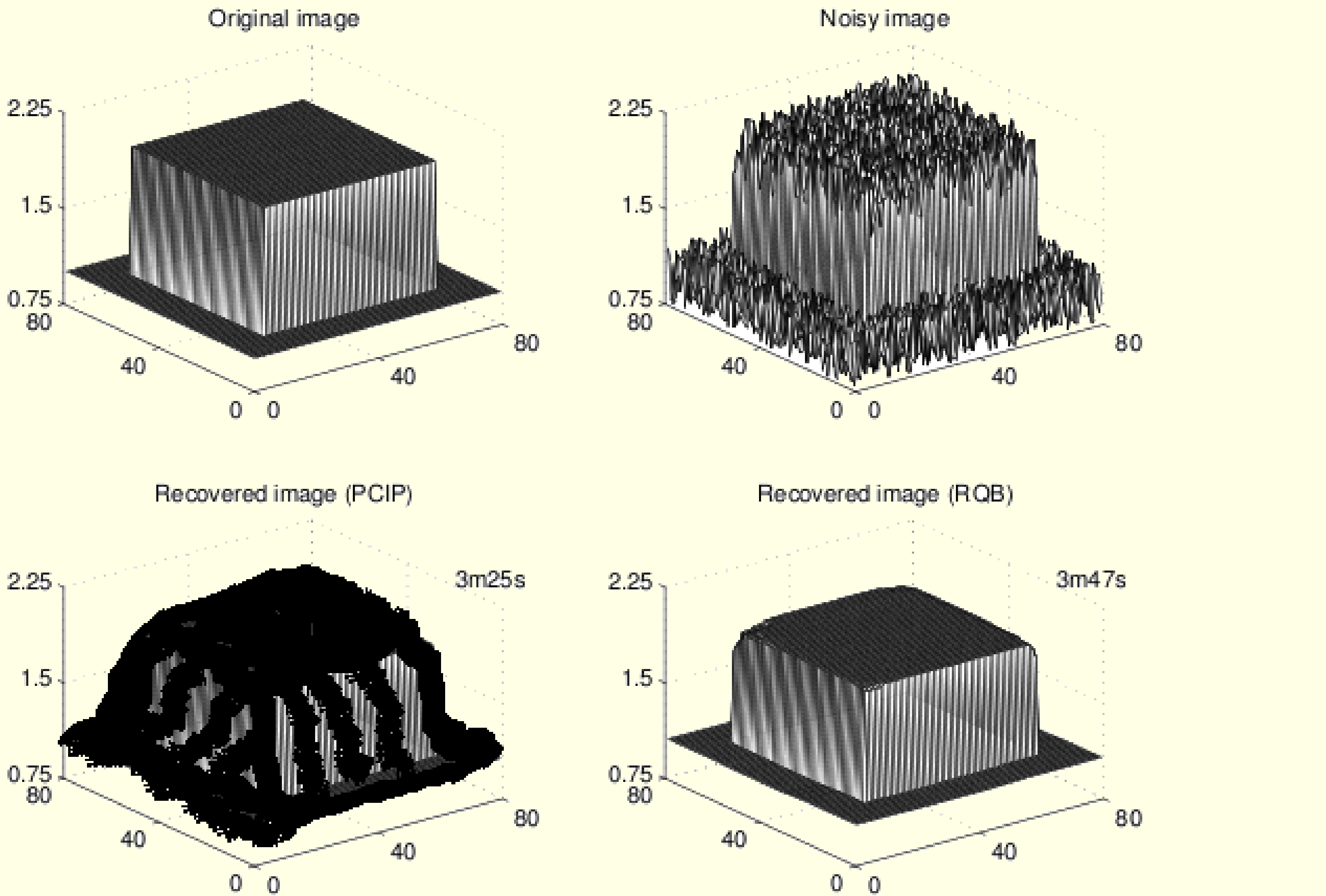
– because they are large scale

– because they are heterogeneous

sometimes the **solution method** induces nonsmoothness

Example of NS model

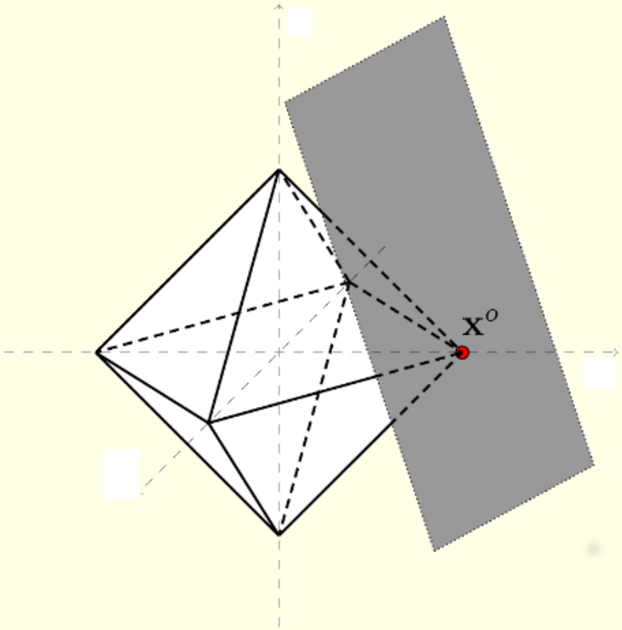
Recovery of **blocky** images (ℓ_1-regularization of TV)



Example of sparse optimization $\min\{\|x\|_1 : Ax = b\}$

Basis pursuit: find least 1-norm point on the affine plane

Tends to return a sparse point (sometimes, the sparsest)



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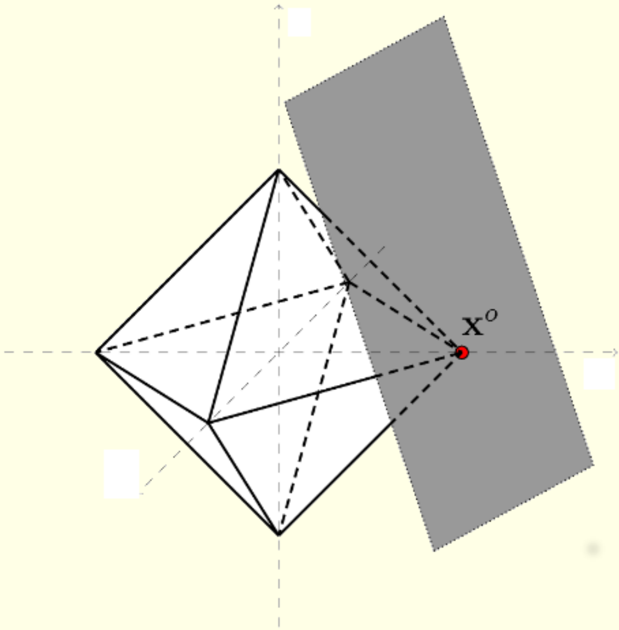

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LASSO denoises basis pursuit

$$\min\left\{\|Ax-b\|_2^2 : \|x\|_1 \le \tau\right\}$$

or

$$\min\left\{\|x\|_1 + \frac{\mu}{2}\|Ax-b\|_2^2\right\}$$

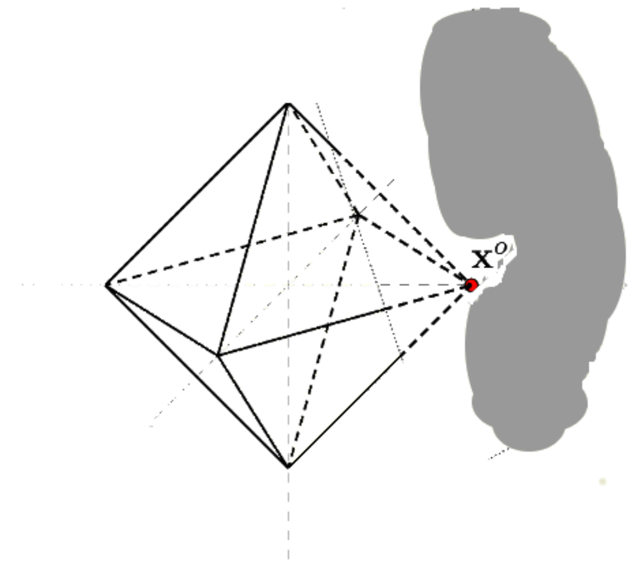
or

$$\min\left\{\|x\|_1 : \|Ax-b\|_2^2 \le \sigma\right\}$$

Example of sparse optimization $\min\{\|x\|_1 : \mathbf{h}(\mathbf{x}) \leq \mathbf{b}\}$

Basis pursuit: find least 1-norm point on a **nonlinear set**

Tends to return a sparse point (sometimes, the sparsest)



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$$\min\left\{\left\|\left(\mathbf{h}(\mathbf{x}) - b\right)^+\right\|_2^2 : \|x\|_1 \leq \tau\right\}$$

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$$\min\left\{\|x\|_1 + \frac{\mu}{2}\left\|\left(\mathbf{h}(\mathbf{x})x - b\right)^+\right\|_2^2\right\}$$

or

$$\min\left\{\|x\|_1 : \left\|\left(\mathbf{h}(\mathbf{x})x - b\right)^+\right\|_2^2 \leq \sigma\right\}$$

Lagrangian Relaxation Example

Real-life optimization problems

$$
\texttt{(primal)} \quad \begin{cases} \min & \sum_{j \in J} \mathcal{C}^j(p^j) \\ & \text{for } j \in J\text{: } p^j \in \mathcal{P}^j \\ & \sum_{j \in J} g^j(p^j) = \mathrm{Dem} \end{cases}
$$

Lagrangian Relaxation Example

Real-life optimization problems

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\min_x \quad f(x) := \quad f_0(x) \quad + \sum_{j \in J} \quad f^j(x)
$$

$$
\min_x \quad -\langle x, \mathrm{Dem} \rangle \quad + \sum_{j \in J} \begin{cases} \max & -\mathcal{C}^j(p^j) + \left\langle x, g^j(p^j) \right\rangle \\ & p^j \in \mathcal{P}^j \end{cases}
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Lagrangian Relaxation Example

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Benders Decomposition Example

Similar situation, but now the uncoupling is done on a primal level

$$
\texttt{(primal)} \quad \left\{ \begin{array}{ll} \min & \displaystyle\sum_{j \in J} \mathcal{I}^j(\Delta p^j) + \mathcal{C}^j(p^j) \\ & \text{for } j \in J\text{: } p^j \in \mathcal{P}^j \\ & \Delta p \in D \end{array} \right. \qquad \Longleftrightarrow \quad \mathbf{p^j \leq \bar{p}^j + \Delta p^j}
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Computing $\partial f(x^k)$: how difficult is it?

1. $f(x) = |x|$, for $n = 1$
2. A linear Lasso function, $f(x) = \|x\|_1 + \frac{\mu}{2}\|Ax - b\|_2^2$
3. A nonlinear Lasso function, $h \in C^1$,
   $f(x) = \|x\|_1 + \frac{\mu}{2}\|\Big(h(x) - b\Big)^+\|_2^2$
4. One of the local subproblems in the Lagrangian example,
   $$f^j(x^k) := \begin{cases} \max & -\mathcal{C}^j(p^j) + \Big\langle x^k, g^j(p^j)\Big\rangle \\ & p^j \in \mathcal{P}^j \end{cases}$$
5. One of the local subproblems in the Benders example,
   $(\mathcal{I}^j(\Delta p^j) + \mathcal{V}^j(\Delta p^j) = f^j(x^{k,j}) = \min\Big\{\mathcal{C}^j(p^j) : p^j \le \bar{p}^j + x^{k,j}\Big\}$

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Indisponsible to calculate the proximal point

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$$\iff \in \partial f(p) + \frac{1}{t}(p - x)$$

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Without full knowledge of the subdifferential, the **implicit** inclusion cannot be solved!

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note: $p \in x - t\partial f(p)$ akin to a subgradient method

Proximal point algorithms (Accel. Nesterov, FISTA, AugLag)

$$x^{k+1} = \mathrm{prox}_{t_k}^{f}(x^k)$$

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Proximal point: calculus rules

- separable sum:

$$f(x,y) = (g(x), h(y)) \Longrightarrow$$
$$\mathrm{prox}_t^f(x) = \Big(\mathrm{prox}_t^g(x), \mathrm{prox}_t^h(y)\Big)$$

- scalar factor ($\alpha \neq 0$) and translation ($v \neq 0$):

$$f(x) = g(\alpha x + v) \Longrightarrow$$
$$\mathrm{prox}_t^f(x) = \frac{1}{\alpha}\Big(\mathrm{prox}_t^{\alpha^2 g}(\alpha x + v) - v\Big)$$

- “perspective" ($\alpha > 0$):

$$f(x) = \alpha g(\tfrac{1}{\alpha}x) \Longrightarrow \mathrm{prox}_t^f(x) = \alpha\,\mathrm{prox}_t^{g/\alpha}(\tfrac{x}{\alpha})$$

Proximal point: special functions

- + linear term ($v \neq 0$):

  $$f(x) = g(x) + \langle v, x \rangle \Longrightarrow \mathrm{prox}_t^f(x) = \mathrm{prox}_t^g(x - v)$$

- + convex quadratic term ($t > 0$):

  $$f(x) = g(x) + \frac{1}{2t}\|x - v\|^2 \Longrightarrow$$

  $$\mathrm{prox}_t^f(x) = \mathrm{prox}_t^{\lambda g}(\lambda x + (1-\lambda)v) \text{ for } \lambda = \frac{t}{t+1}$$

- composition with linear term such that $A^\top A = \frac{1}{\alpha} I$, ($\alpha \neq 0$):

  $$f(x) = g(Ax + v) \Longrightarrow$$

  $$\mathrm{prox}_t^f(x) = (I - \alpha A^\top A)x + \alpha A^\top \left[\mathrm{prox}_t^{g/\alpha}(Ax + v) - v\right]$$

Proximal point algorithm: convergence

If $\arg\min f \neq \emptyset$ then

$$f(x^k) - f(\bar{x}) \leq \frac{\|x^0 - \bar{x}\|^2}{2\sum_{i=1}^{k} t_i}$$

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$\Longrightarrow$ convergence if $\sum t_i \to +\infty$

$\Longrightarrow$ rate $1/k$ if $\{t_k\}$ bounded away from zero

Proximal point algorithm: acceleration

$$x^{k+1} = \mathrm{prox}^{f}_{t_k}\left(x^k + \boldsymbol{\theta_{k+1}(\frac{1}{\theta_k} - 1)(x^k - x^{k-1})}\right)$$

for

$$\frac{\theta_{k+1}^2}{t_{k+1}} = (1 - \theta_{k+1})\frac{\theta_k^2}{t_k}$$

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When do bundle method prove most useful?

In situations

– when the objective function is not available explicitly

and/or

– when we do not have access to the full subdifferential

and/or

– when calculations need to be done with high precision

Bundling to approximate the prox

WANT: $$p = \operatorname{prox}_t^f(x) \iff p = \arg\min f(y) + \frac{1}{2t}\|y-x\|_2^2$$
$$\iff 0 \in \partial f(p) + \frac{1}{t}(p-x)$$
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$\mathbf{M}$ is a model of f for which we do have full knowledge of the subdifferential: the **implicit** inclusion can be solved!

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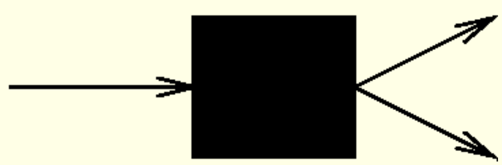
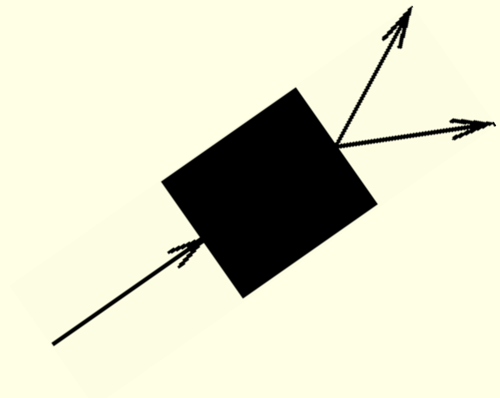


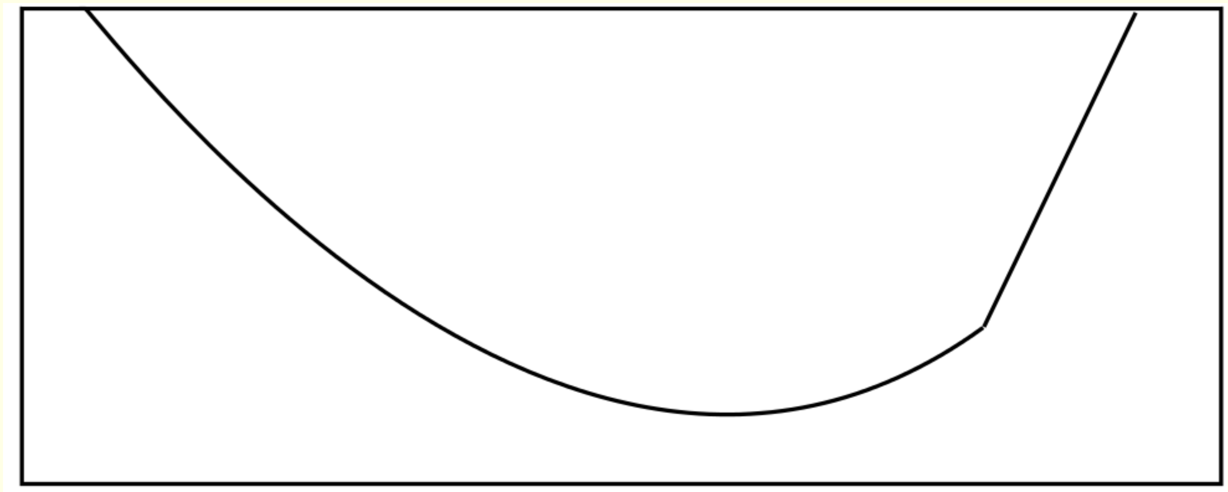
How is the model built?

Model built with the black box



A quick overview of Convex Analysis

An example of a convex nonsmooth function



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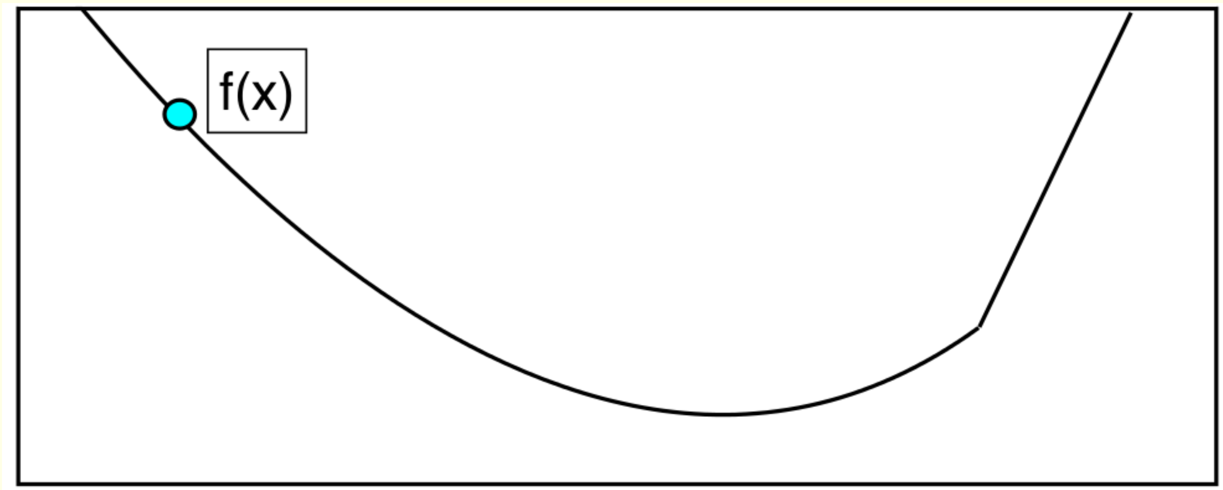

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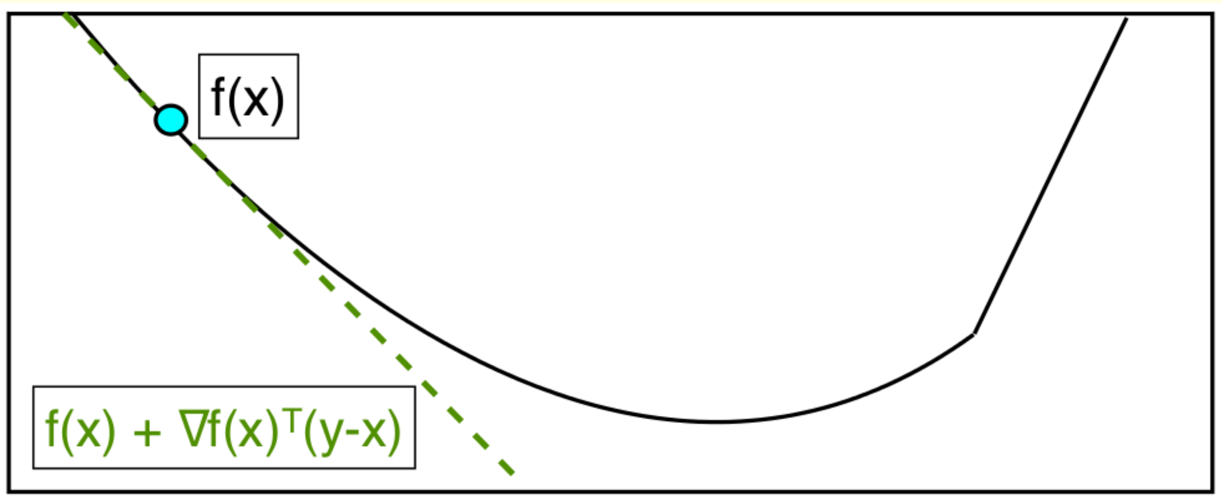

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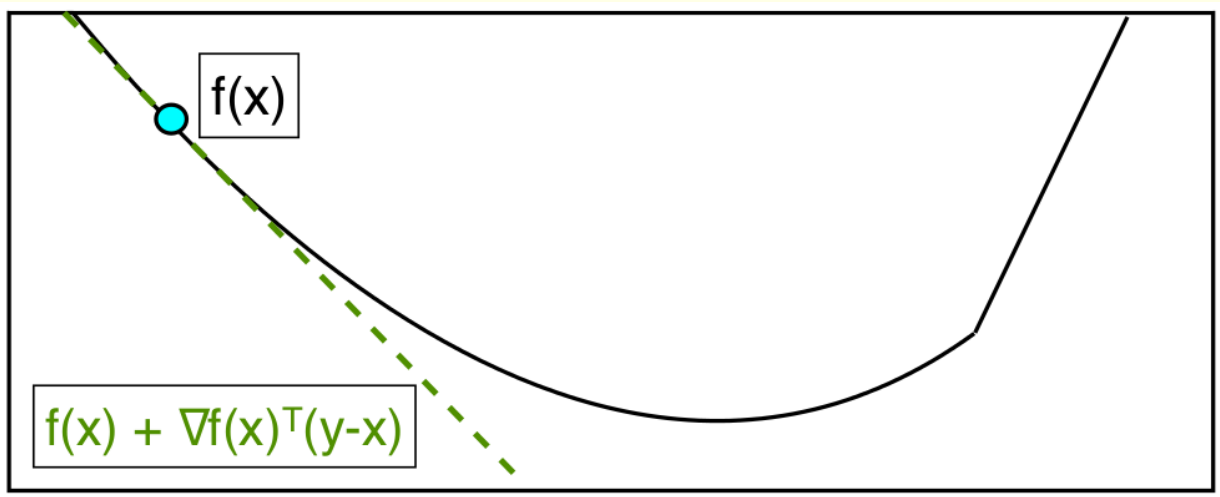

$$\{\nabla f(x)\} \quad = \quad \{\text{slope of the linearization supporting } f\text{, tangent at } x\}$$

By convexity,

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle \text{ for all } y$$

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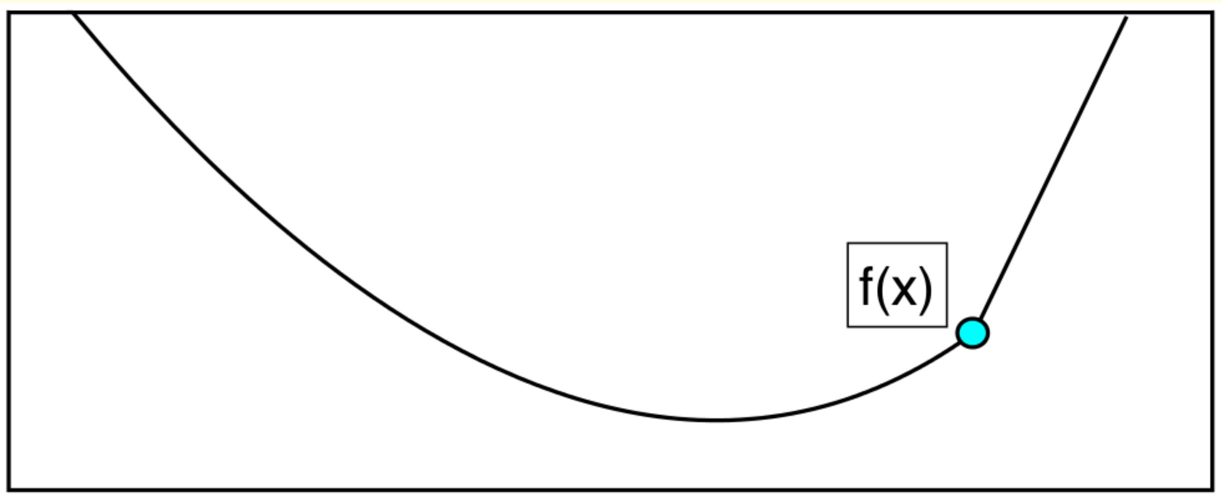

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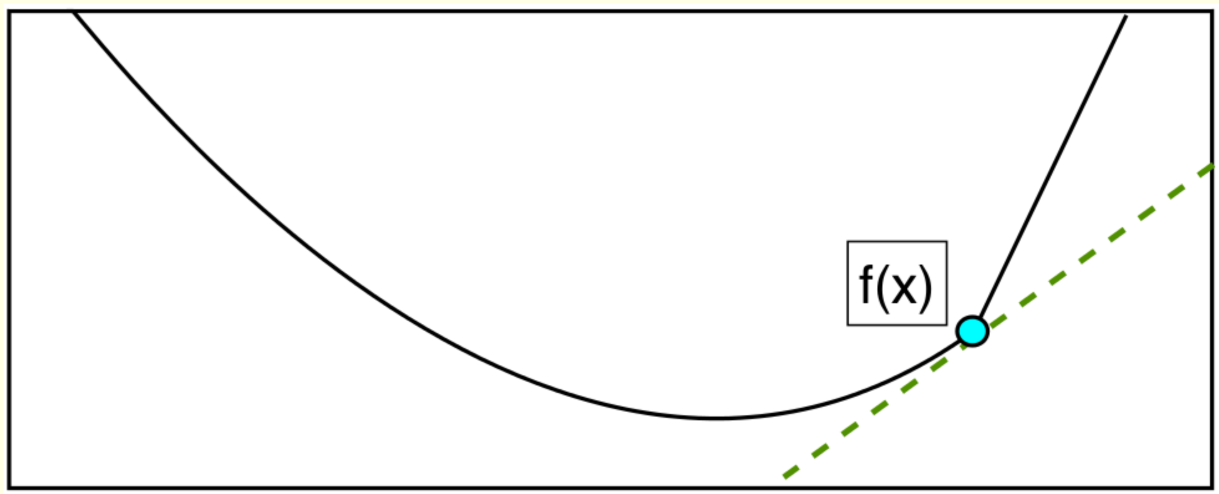

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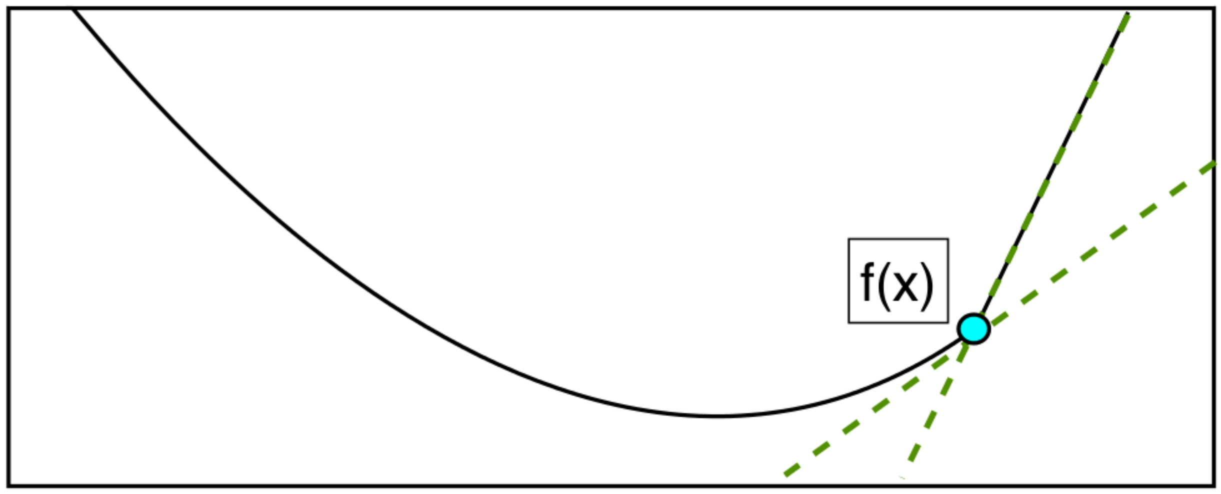

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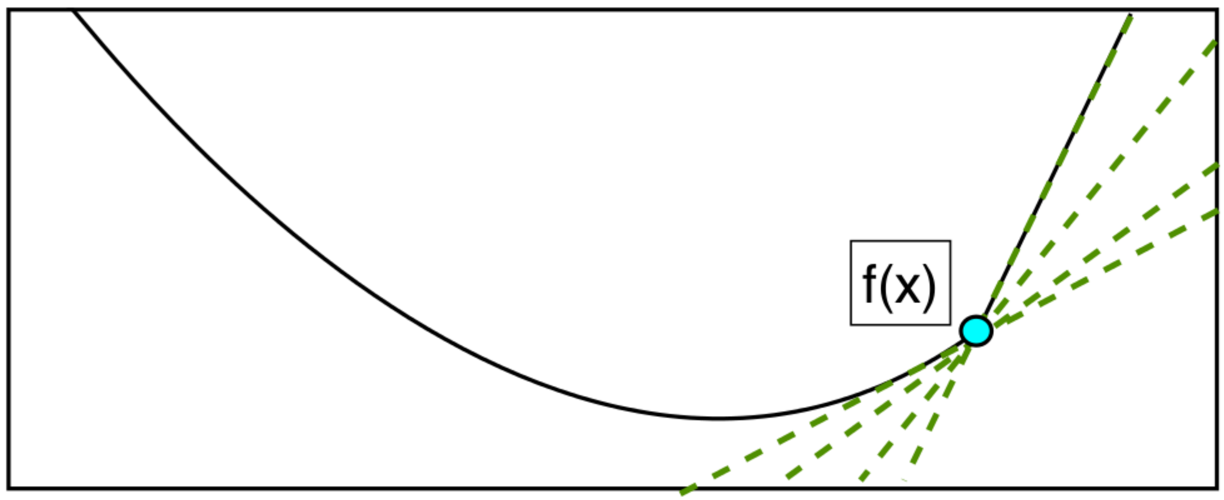

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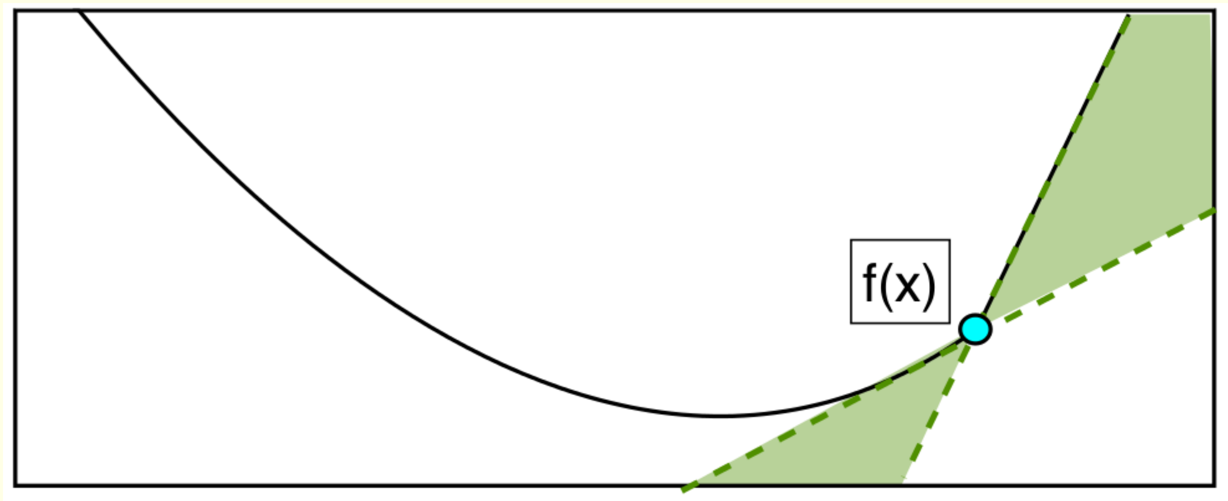
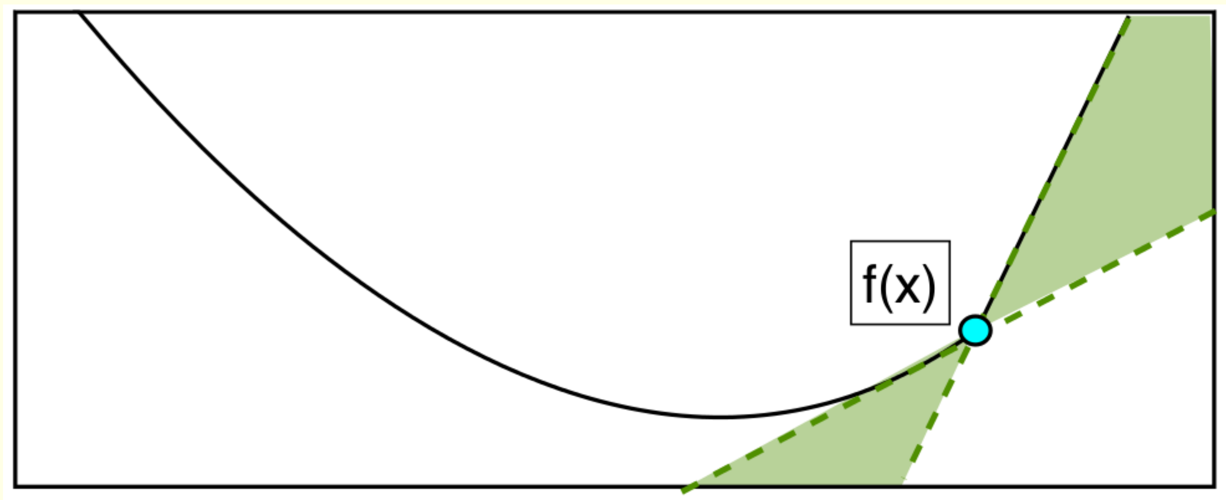


$$\partial f(x) \quad = \quad \{g \in \mathbb{R}^n : f(y) \geq f(x) + \langle g, y - x \rangle \text{ for all } y\}$$

A quick overview of Convex Analysis

An example of a convex nonsmooth function



$$\begin{aligned}\partial f(x) &= \{g \in \mathbb{R}^n : f(y) \geq f(x) + \langle g, y - x \rangle \text{ for all } y\} \\ &= \{\text{slopes of linearizations supporting } f, \text{ tangent at } x\}\end{aligned}$$

What can be done with the oracle output?

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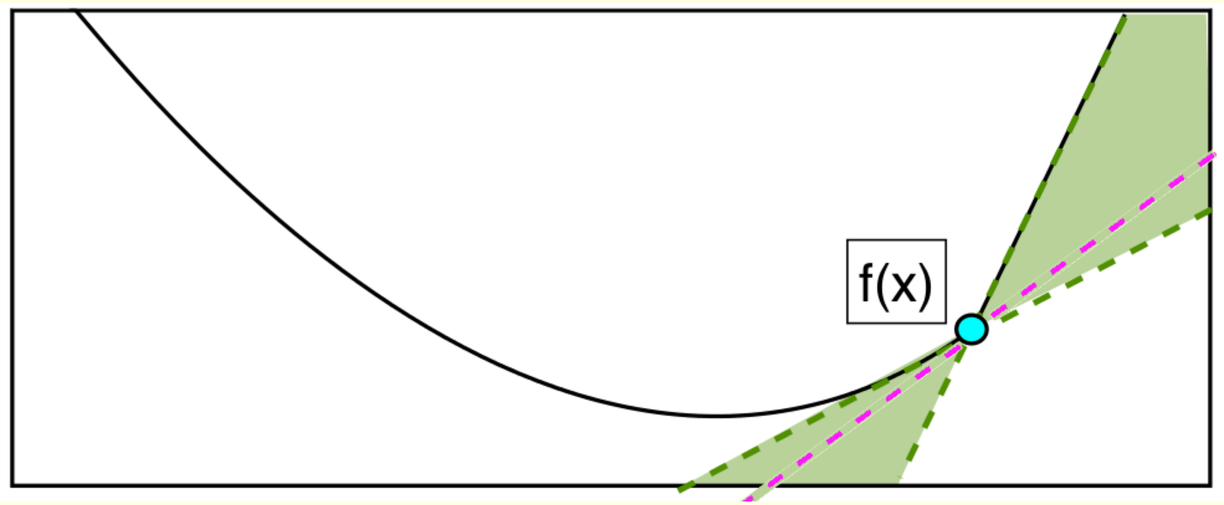

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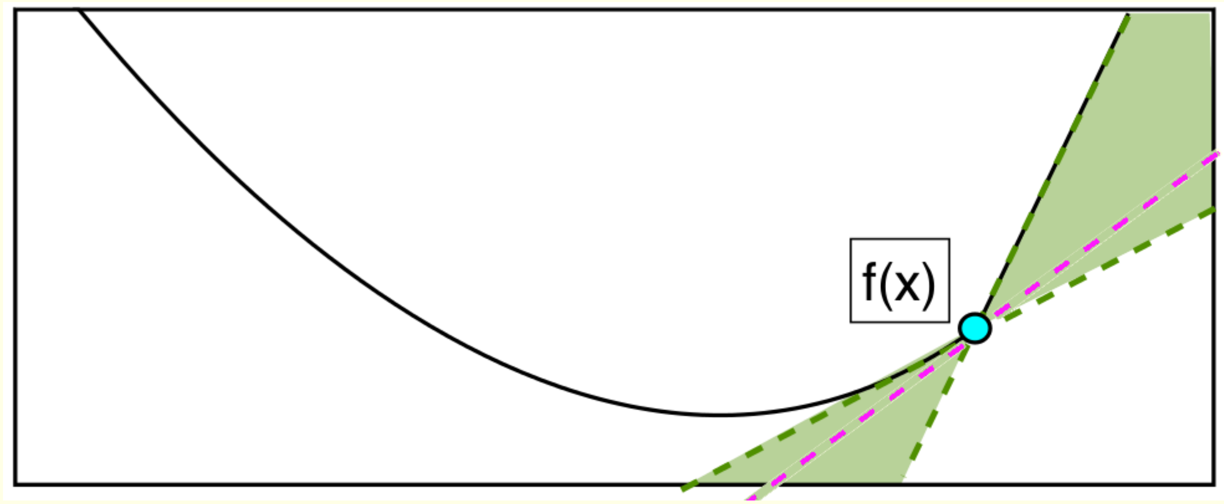

$$
\begin{aligned}
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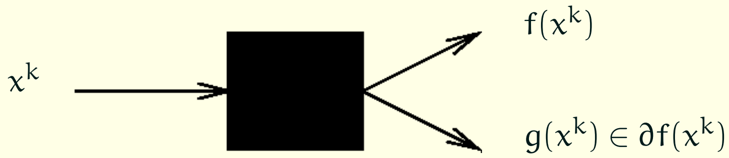
&= \{\text{slopes of linearizations supporting } f\text{, tangent at } x\}
\end{aligned}
$$

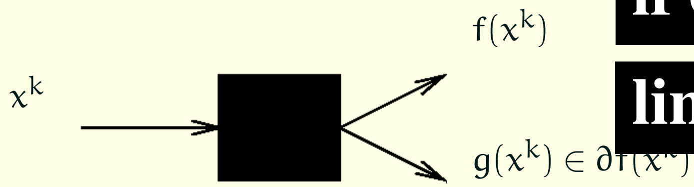
1 oracle call



=

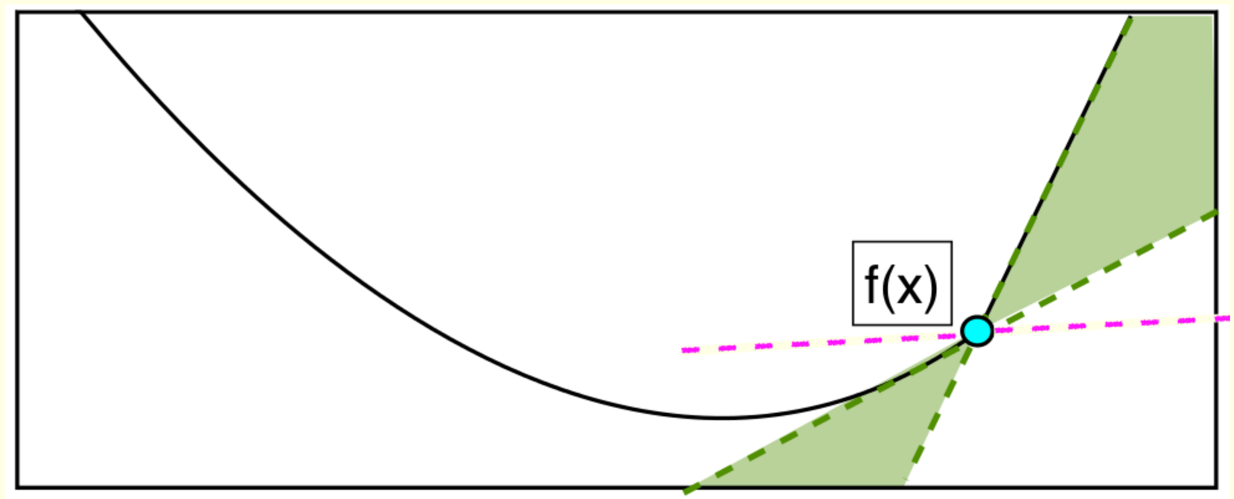
1 linearization

BEWARE:



if oracle output is not accurate,

linearization can be wrong!



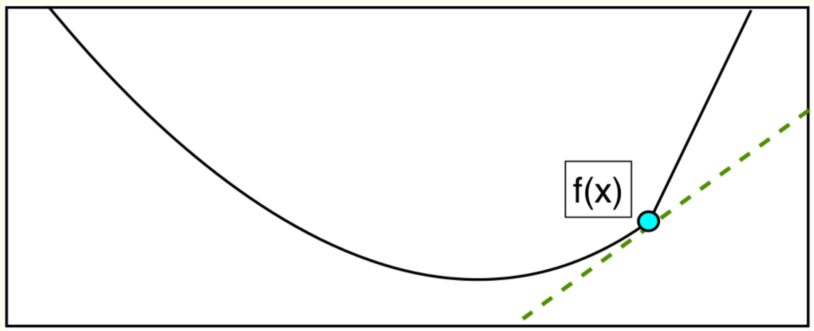
wrong $g(x^k)$ gives bad linearization at x^k

$$\partial f(x) \;=\; \{g \in \mathbb{R}^n : f(y) \geq f(x) + \langle g, y - x\rangle \text{ for all } y\}$$

(similarly if wrong $f(x^k)$, more on this later)

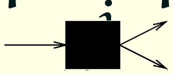
How is the oracle information used?

Putting together linearizations



creates a cutting-plane **model M** for f

$$f^i = f(x^i)$$



$$g^i = g(x^i) \qquad \Longrightarrow \qquad f^i + \left\langle g^i, x - x^i \right\rangle$$

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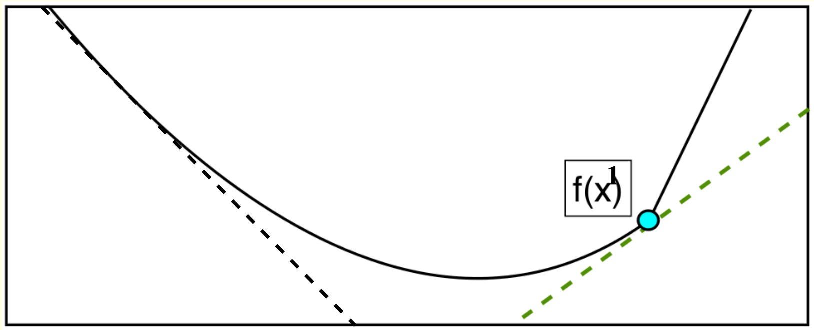

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$$f^i = f(x^i)$$

$$g^i = g(x^i)$$

$$\Longrightarrow \mathbf{M}(y) = \max_i \left\{ f^i + \left\langle g^i, x - x^i \right\rangle \right\}$$

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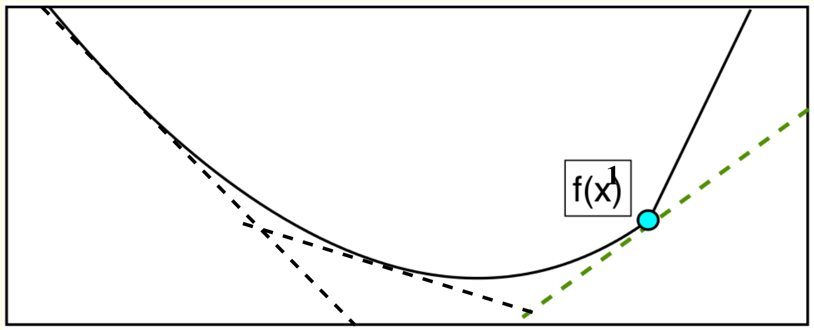
Putting together linearizations



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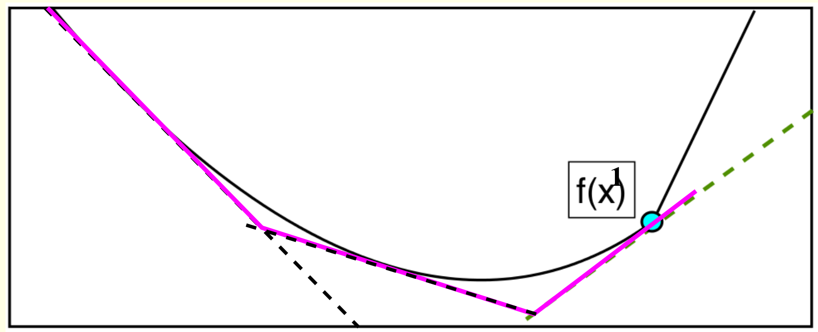

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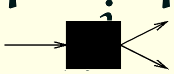


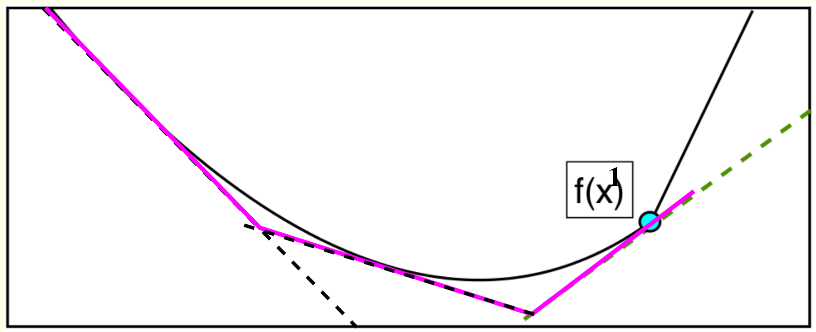
$g^i = g(x^i)$

$$\Longrightarrow \mathbf{M}(y) = \max_i \left\{ f^i + \left\langle g^i, y - x^i \right\rangle \right\}$$

(just one type of model, many others are possible)

How is the oracle information used?

Putting together linearizations



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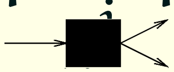

$$g^i = g(x^i)$$

$$\Longrightarrow \mathbf{M}_k(y) = \max_{i \le k} \left\{ f^i + \left\langle g^i, y - x^i \right\rangle \right\}$$

(just one type of model, many others are possible)

Infinite bundling yields prox_t^f

$$\text{WANT: } p = \operatorname{prox}_t^f(x) \iff p = \arg\min f(y) + \frac{1}{2t}\|y - x\|_2^2$$

$$\text{HAVE: } q^k = \operatorname{prox}_{t_k}^{M_k}(x) \iff q^k = \arg\min M_k(y) + \frac{1}{2t_k}\|y - x^k\|_2^2$$

$$\iff 0 = G^k + \frac{1}{t_k}(q^k - x^k)$$

for $G^k \in \partial M_k(q^k)$

Theorem [CL93] Suppose the models satisfy

- $M_k(y) \le f(y)$ for all k and y
- $M_{k+1}(y) \ge f(q^k) + \left\langle g(q^k), y - x^k \right\rangle$
- $M_{k+1}(y) \ge M_k(q^k) + \left\langle G^k, y - x^k \right\rangle$

If $0 < t_{\min} \le t_{k+1} \le t_k$, then

$$\lim_{k\to\infty} q^k = p \quad \text{and} \quad \lim_{k\to\infty} M_k(q^k) = f(p)$$

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Models for the half-and-half function

STRUCTURE	$f(x)$	
none	$\sqrt{x^\top A x} + x^\top B x$	
sum	$f_1(x) + f_2(x)$	$f_1(x) = \sqrt{x^\top A x}$ $f_2(x) = x^\top B x$ f_2 is smooth
compo sition	$(h \circ c)(x)$	$c(x) = (x, x^\top B x) \in \mathbb{R}^{n+1}$ c $h(C) = \sqrt{C_{1:n}^\top A C_{1:n}} + C_{n+1}$ h

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NSO pitfalls

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Stopping test in smooth optimization

Algorithms for unconstrained smooth optimization use as optimality certificate Fermat's rule

$$0 = \nabla f(\bar{x})$$

and generate a minimizing sequence:

$$\{x^k\} \to \bar{x} \text{ such that } \nabla f(x^k) \to 0.$$

If $f \in C^1$, then $\nabla f(\bar{x}) = 0$

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If $f \in C^1$, then $\nabla f(\bar{x}) = 0$ things are less straightforward if f is nonsmooth…

What happens with the stopping test in NSO?

Algorithms for unconstrained NSO use as optimality certificate the inclusion

$$0 \in \partial f(\bar{x})$$

- As a set-valued mapping $\partial f(x)$ is osc:

$$\left(x^k, g(x^k) \in \partial f(x^k)\right) : \begin{cases} x^k \to \bar{x} \\ g(x^k) \to \bar{g} \end{cases} \Longrightarrow \bar{g} \in \partial f(\bar{x})$$

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- As a set-valued mapping, $\partial f(x)$ is **not** isc:
Given $\bar{g} \in \partial f(\bar{x})$

$$\not\exists \left(x^k, g(x^k) \in \partial f(x^k)\right) : \begin{cases} x^k \to \bar{x} \\ g(x^k) \to \bar{g} \end{cases}$$

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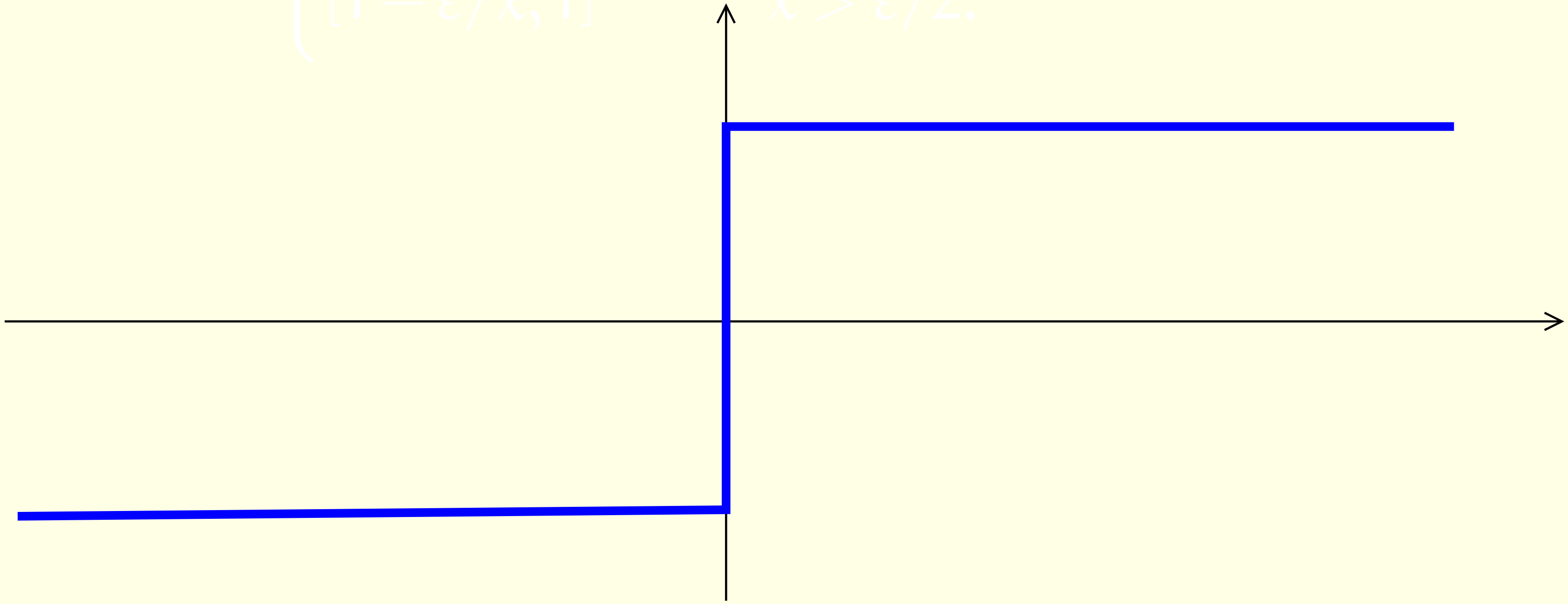
The subdifferential

For the absolute value function, $f(x) = |x|$

$$\partial f(x) = \begin{cases} -1 & x < 0 \\ [-1, 1] & x = 0 \\ 1 & x > 0 \end{cases}$$



What happens with the stopping test in NSO?

We need to design a sound stopping test that does not rely on the straightforward extension of Fermat's rule.

What happens with the stopping test in NSO?

We need to design a sound stopping test that does not rely on the straightforward extension of Fermat's rule. We use instead

$$\bar{g} \in \partial_{\bar{\varepsilon}} f(\bar{x}) \qquad \text{for } \|\bar{g}\| \text{ and } \bar{\varepsilon} \text{ small}$$

where the ε-subdifferential contains the slopes of linearizations supporting f **up to** ε, tangent at x:

$$\partial_\varepsilon f(x) = \{g \in \mathbb{R}^n : f(y) \geq f(x) + \langle g, y - x\rangle - \varepsilon \text{ for all } y\}$$

The ε-subdifferential

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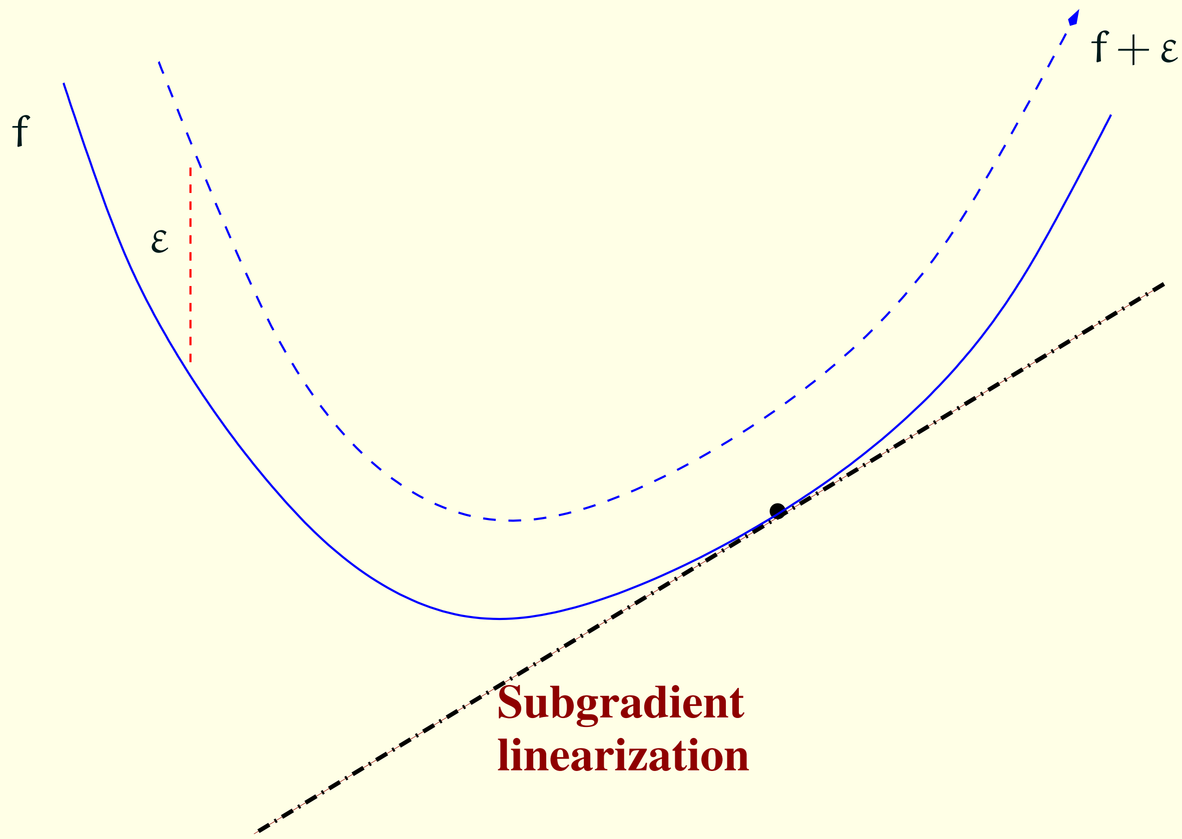
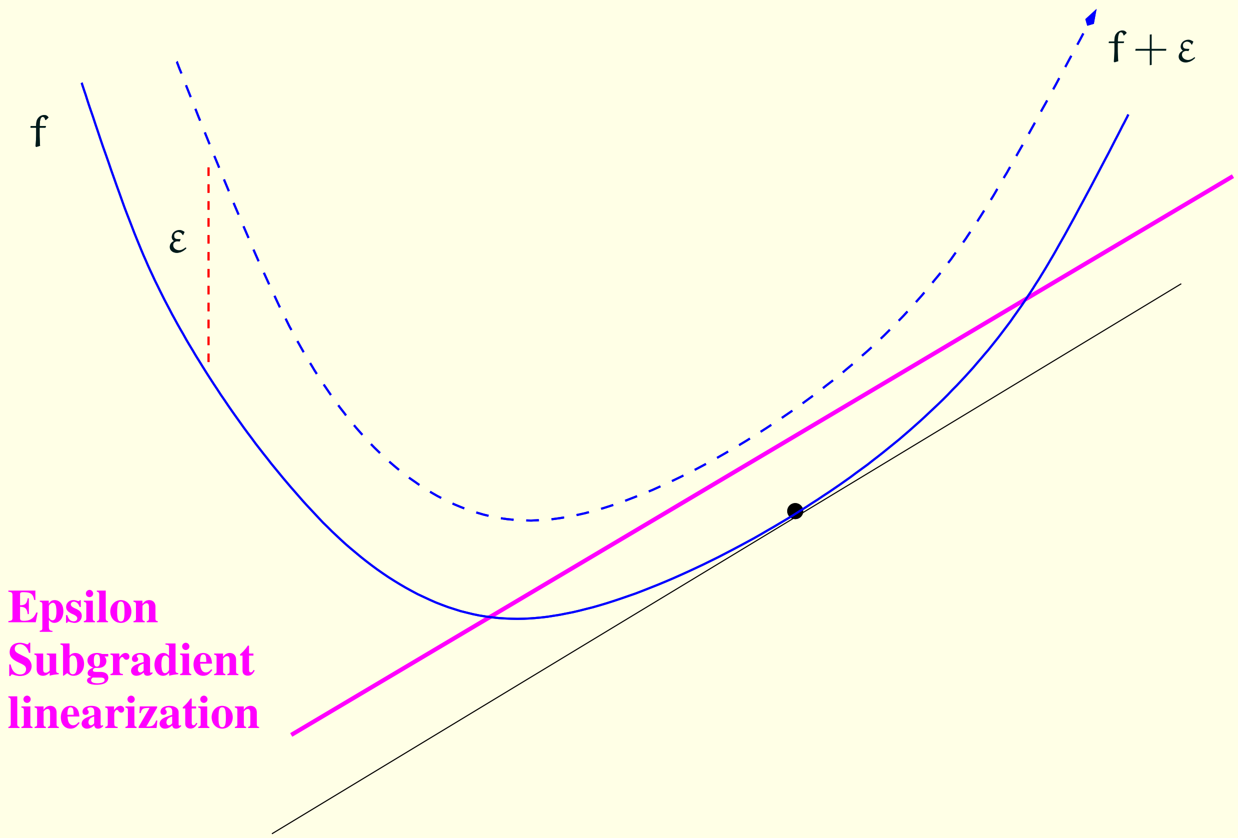


The ε-subdifferential

$$\partial_\varepsilon f(x) = \{g \in \mathbb{R}^n : f(y) \geq f(x) + \langle g, y - x \rangle \boxed{-\varepsilon} \text{ for all } y\}$$



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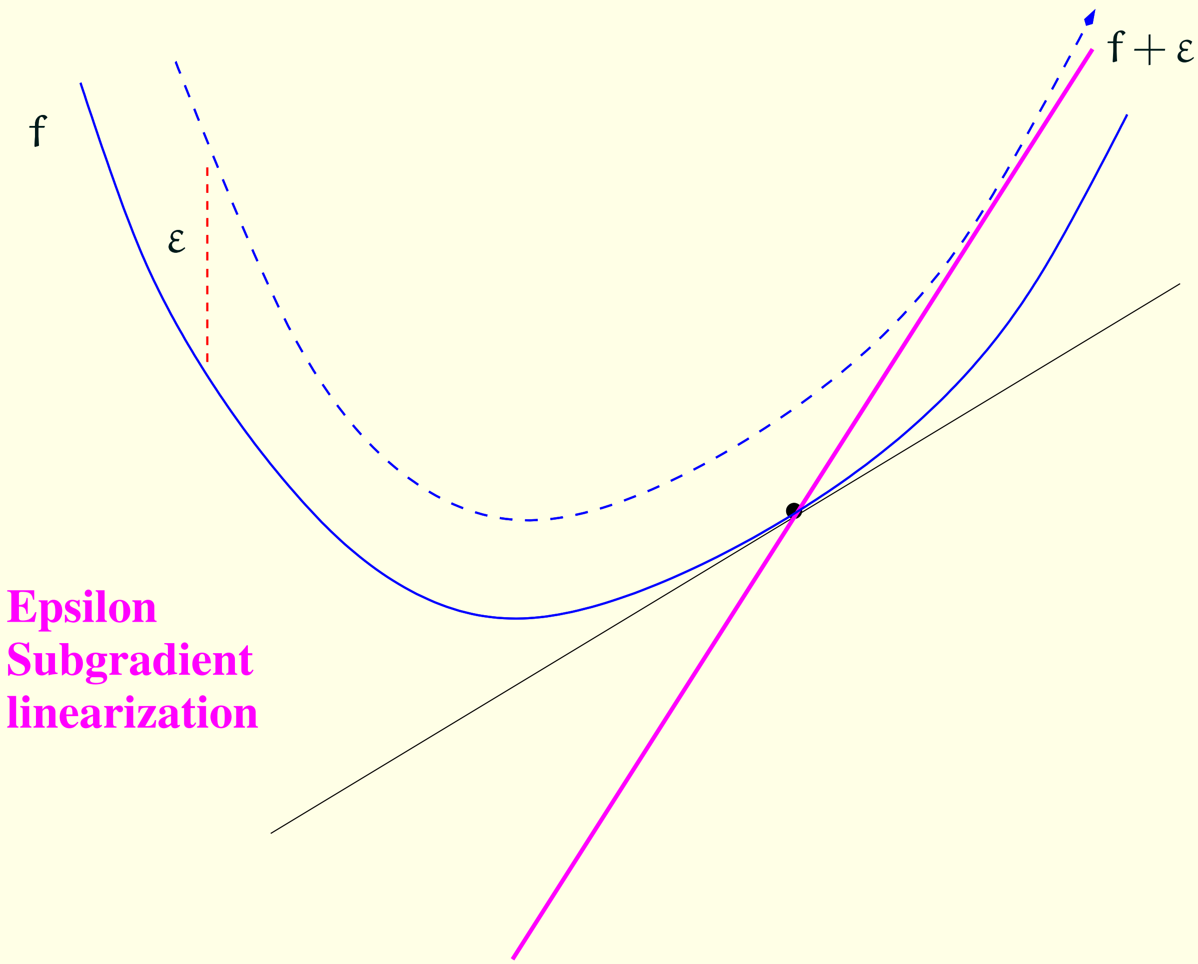

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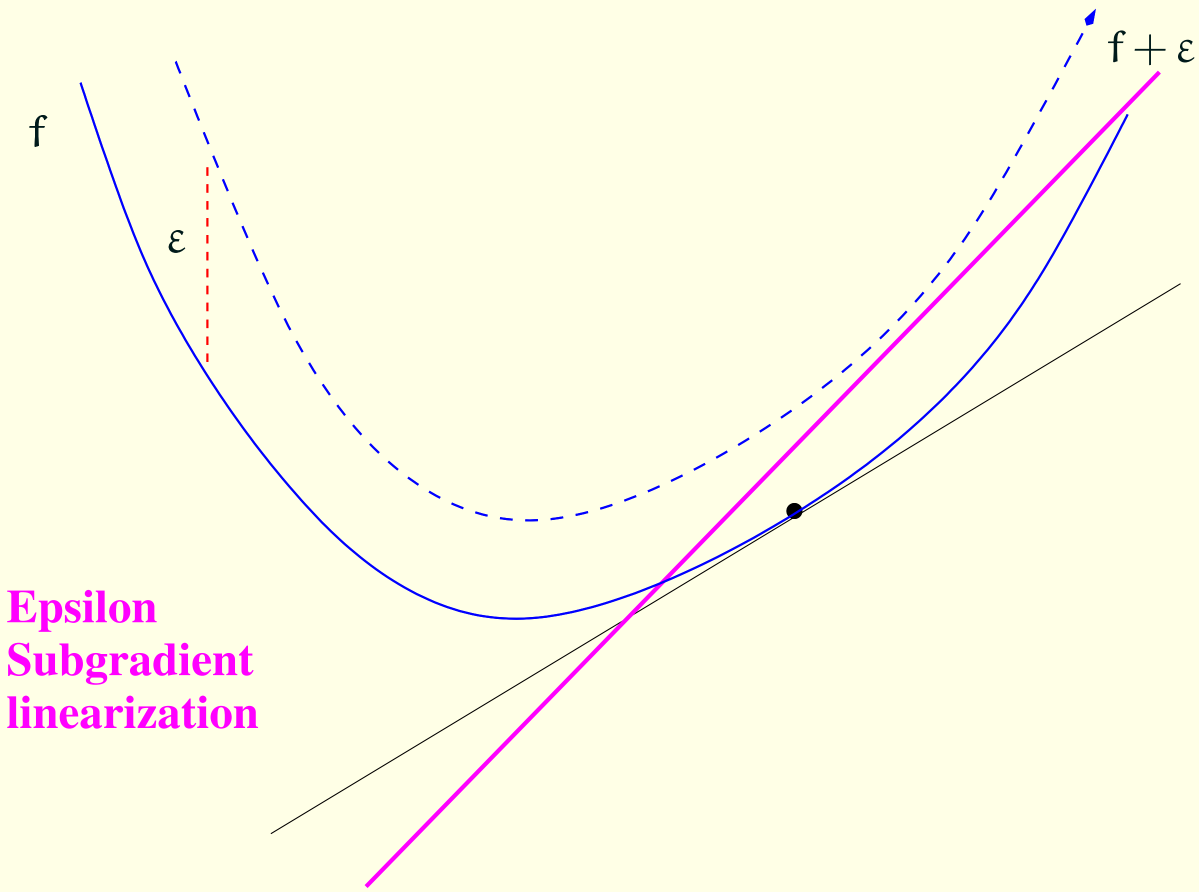

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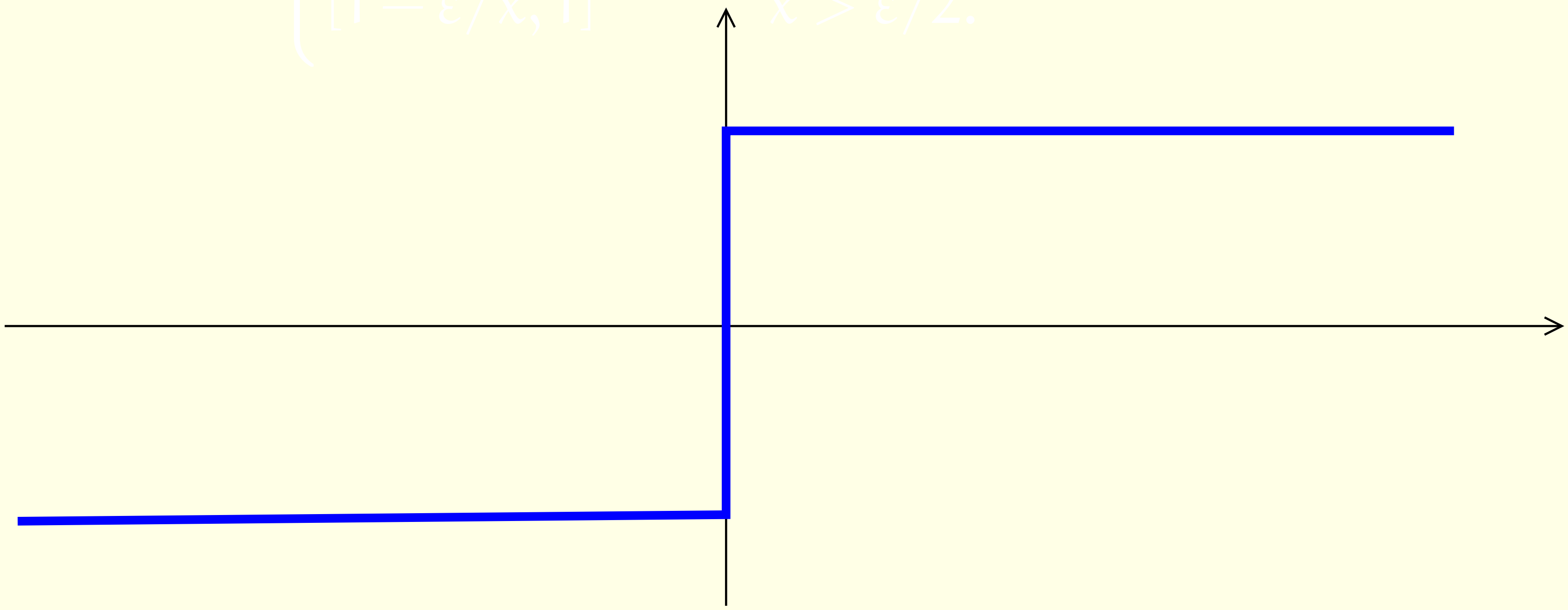
For the absolute value function, $f(x) = |x|$

$$\partial f(x) = \begin{cases} -1 & x < 0 \\ [-1, 1] & x = 0 \\ 1 & x > 0 \end{cases}$$

$$\partial_\varepsilon f(x) = \begin{cases} [-1, -1 - \varepsilon/x] & x < -\varepsilon/2, \\ [-1, 1] & -\varepsilon/2 \leq x1 \leq \varepsilon1/2, \\ [1 - \varepsilon/x, 1] & x > \varepsilon/2. \end{cases}$$



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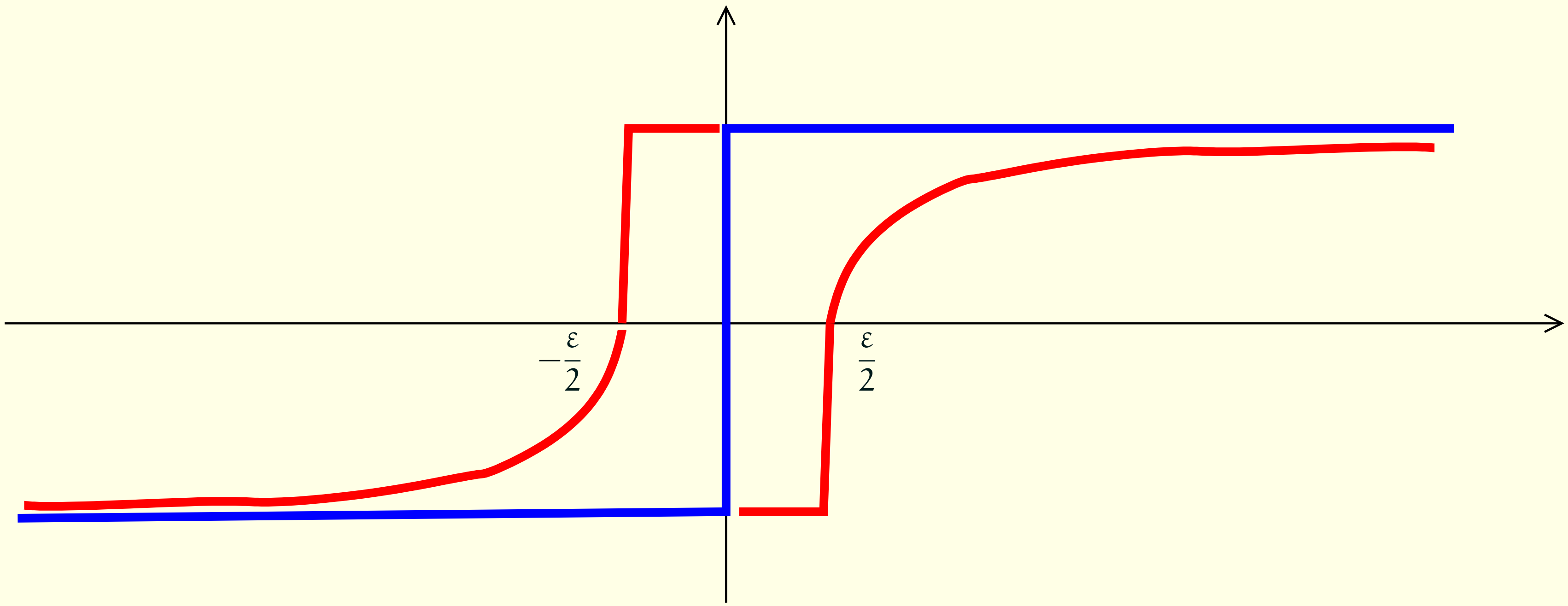

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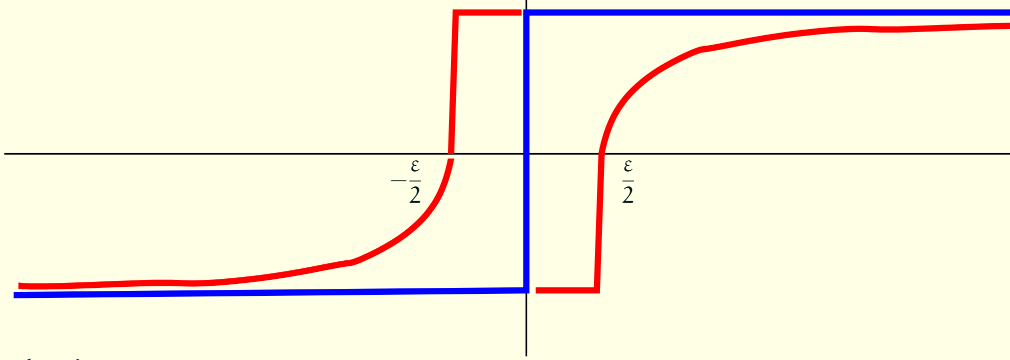


- As a set-valued mapping $\partial_\varepsilon f(x)$ is osc:

$$\left(\varepsilon^k, x^k, G(x^k) \in \partial_{\varepsilon^k} f(x^k)\right) : \begin{cases} \varepsilon^k \longrightarrow \varepsilon \\ x^k \longrightarrow \bar{x} \\ G(x^k) \longrightarrow \bar{g} \end{cases} \Longrightarrow \bar{g} \in \partial_{\bar{\varepsilon}} f(\bar{x})$$

- As a set-valued mapping, $\partial_\varepsilon f(x)$ is isc: Given $\bar{g} \in \partial_{\bar{\varepsilon}} f(\bar{x})$

$$\exists \left(\varepsilon^k, x^k, G(x^k) \in \partial_{\varepsilon^k} f(x^k)\right) : \begin{cases} \varepsilon^k \longrightarrow \bar{\varepsilon} \\ x^k \longrightarrow \bar{x} \\ G(x^k) \longrightarrow \bar{g} \end{cases}$$

The ε-subdifferential and bundle methods

Generate iterates so that for a **subsequence** $\{\hat{x}^k\}$

- As a set-valued mapping $\partial_\varepsilon f(x)$ is osc:

$$\left(\varepsilon^k, \hat{x}^k, G(\hat{x}^k) \in \partial_{\varepsilon^k} f(\hat{x}^k)\right) : \begin{cases} \varepsilon^k \to \bar{\varepsilon} \\ x^k \to \bar{x} \\ G(\hat{x}^k) \to \bar{g} \end{cases} \Longrightarrow \bar{g} \in \partial_{\bar{\varepsilon}} f(\bar{x})$$

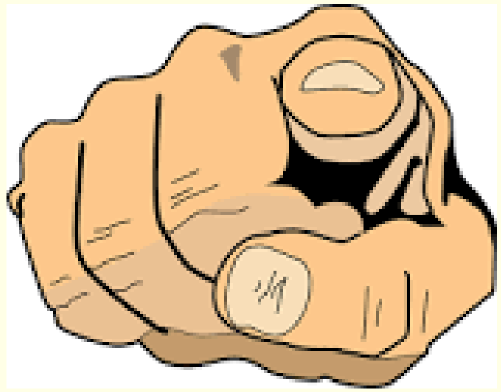
with $\bar{\varepsilon} = 0$ and $\bar{g} = 0$

- As a set-valued mapping, $\partial_\varepsilon f(x)$ is isc:Given $\bar{g} \in \partial_{\bar{\varepsilon}} f(\bar{x})$:

$$\exists\left(\varepsilon^k, \hat{x}^k, G(\hat{x}^k) \in \partial_{\varepsilon^k} f(\hat{x}^k)\right) : \begin{cases} \varepsilon^k \to \bar{\varepsilon} \\ x^k \to \bar{x} \\ G(x^k) \to \bar{g} \end{cases}$$

The ε-subdifferential and bundle methods

You told us



we were going to use subgradient information provided by an oracle or a black box, and now you want to use ε-subgradients!

The transportation formula

How to express subgradients at x^i as ε-subgradients at $\hat{x}^k$?

$$g^i \in \partial f(x^i) \quad \text{if and only if, for all } y \in \mathbb{R}^n$$

$$f(y) \;\geq\; f(x^i) + \left\langle g^i, y - x^i \right\rangle$$

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$$\begin{aligned}
f(y) &\geq f(x^i) + \left\langle g^i, y - x^i \right\rangle \\
&= f(x^i) + \left\langle g^i, y - x \right\rangle \pm f(\hat{x}^k) \\
&= f(\hat{x}^k) + g^{i\top}(y - x) - \left(f(\hat{x}^k) - f(x^i) \right) \\
&= f(\hat{x}^k) + g^{i\top}(y - x \pm \hat{x}^k) - \left(f(\hat{x}^k) - f(x^i) \right) \\
&= f(\hat{x}^k) + g^{i\top}(y - \hat{x}^k) - \left(f(\hat{x}^k) - f(x^i) - \left\langle g^i, \hat{x}^k - x^i \right\rangle \right) \\
&= f(\hat{x}^k) + g^{i\top}(y - \hat{x}^k) - e^i(\hat{x}^k)
\end{aligned}$$

$$\Longrightarrow g^i \in \partial_{e^i(\hat{x}^k)} f(\hat{x}^k)$$

$$e^i(\hat{x}^k) := f(\hat{x}^k) - f(x^i) - \left\langle g^i, \hat{x}^k - x^i \right\rangle \geq 0$$

The transportation formula

How to express subgradients at x^i as ε-subgradients at $\hat{x}^k$?

$$g^i \in \partial f(x^i) \quad \text{if and only if, for all } y \in \mathbb{R}^n$$

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f(y) &\geq f(x^i) + \left\langle g^i, y - x^i \right\rangle \\
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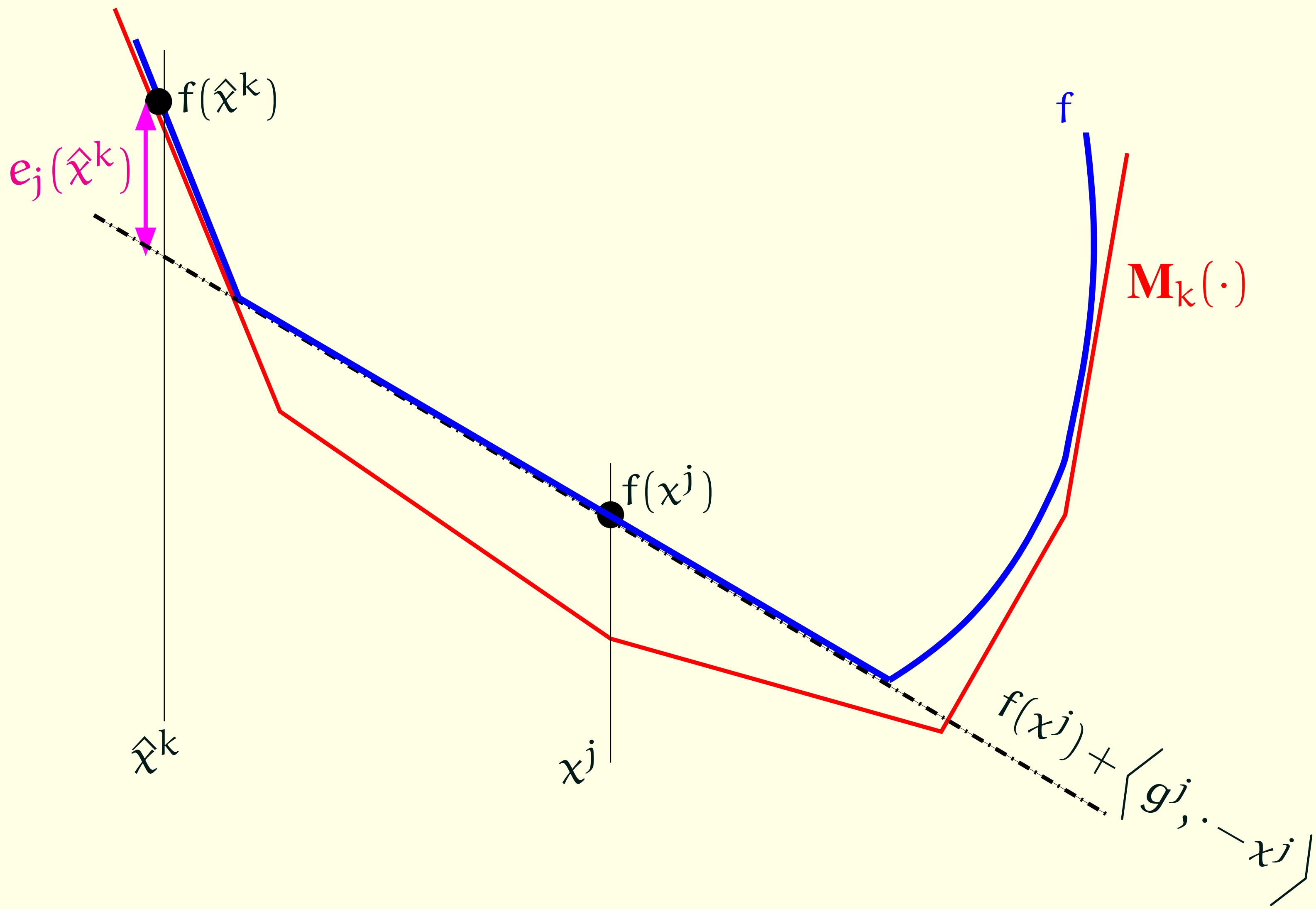
Linearization errors



The ε-subdifferential and bundle methods

We collect the black-box

$x^i, i = 1, 2, \ldots, k$, so that at iteration k we can define a **bundle** of information, centered at a special iterate $\hat{x}^k \in \{x^i\}$

$$\mathcal{B}^k := \begin{pmatrix} e^i(\hat{x}^k) = f(\hat{x}^k) - f(x^i) - \left\langle g^i, \hat{x}^k - x^i \right\rangle \\ g^i \in \partial_{e^i(\hat{x}^k)} f(\hat{x}^k) \end{pmatrix}$$

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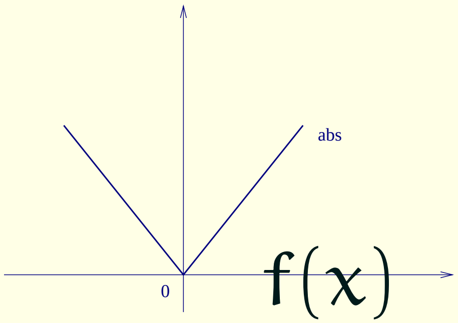
A suitable convex combination

$$\varepsilon^k := \sum_{i \in \mathcal{B}^k} \alpha^i e^i(\hat{x}^k) \text{ and } G^k := \sum_{i \in \mathcal{B}^k} \alpha^i g^i$$

will eventually satisfy the optimality condition!

Why special NSO methods?

Smooth optimization techniques **do not work**



$$\begin{aligned} f(x) &= |x| \\ |\nabla f(x^k)| &= 1,\ \forall x^k \neq 0 \quad \partial f(0) = [-1, 1] \end{aligned}$$

Smooth stopping test **fails**:

$|\nabla f(x^k)| \leq$TOL $\qquad (\leftrightarrow |g(x^k)| \leq$TOL$)$

Why special NSO methods?

Smooth optimization techniques **do not work**

Smooth approximations of derivatives by finite differences **fail**

For $f : \mathbb{R}^3 \to \mathbb{R}$ defined by $f(x) = \max(x_1, x_2, x_3)$

$\partial f(0) = ?$

Forward finite difference $\frac{f(x+\Delta x)-f(x)}{\Delta x}$

Central finite difference $\frac{f(x+\Delta x)-f(x-\Delta)}{2\Delta x}$

Why special NSO methods?

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Smooth approximations of derivatives by finite differences **fail**

For $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ defined by $f(x) = \max(x_1, x_2, x_3)$

$\partial f(0) = ?$

Forward finite difference $\frac{f(x+\Delta x) - f(x)}{\Delta x} = (\mathbf{1}, \mathbf{1}, \mathbf{1})$

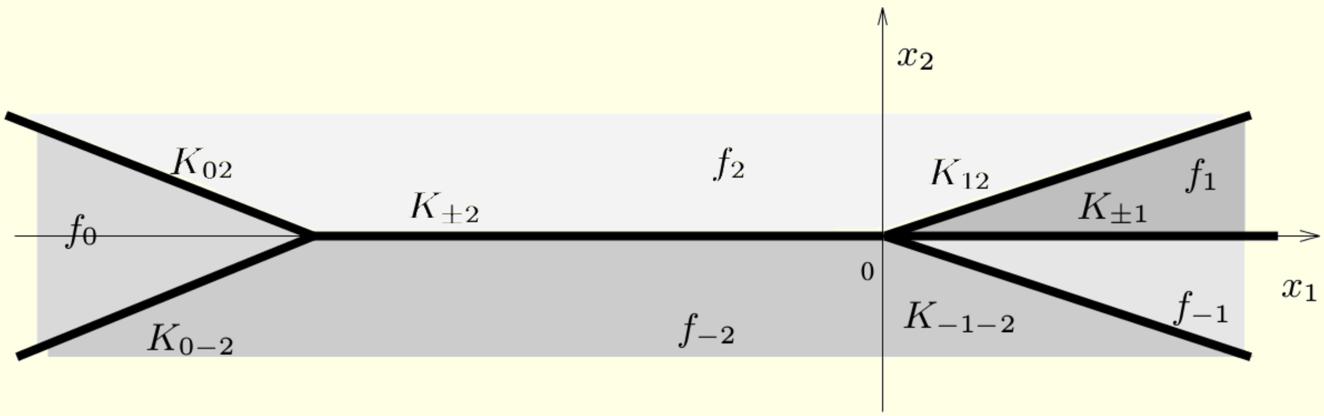
Central finite difference $\frac{f(x+\Delta x) - f(x-\Delta)}{2\Delta x} = (\frac{\mathbf{1}}{\mathbf{2}}, \frac{\mathbf{1}}{\mathbf{2}}, \frac{\mathbf{1}}{\mathbf{2}}$

none of them in the subdifferential!

Why special NSO methods?

Smooth optimization techniques **do not work**

Linesearches get trapped in kinks and **fail**



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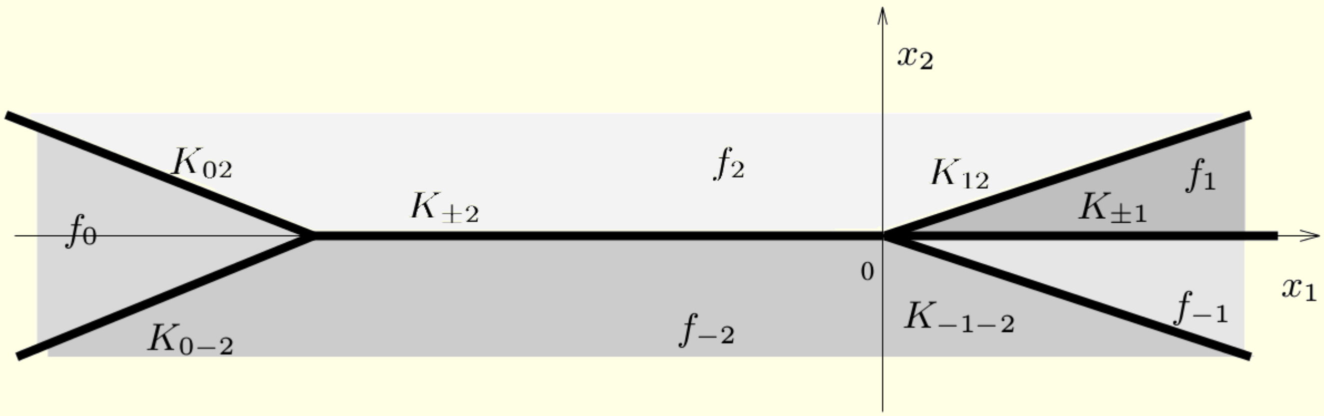
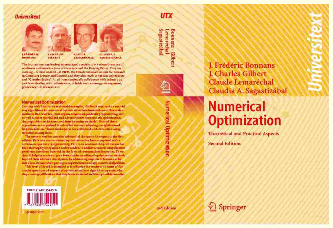


Example 9.1 "Instability of steepest descent"



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$-g(x^k)$ may **not** provide descent

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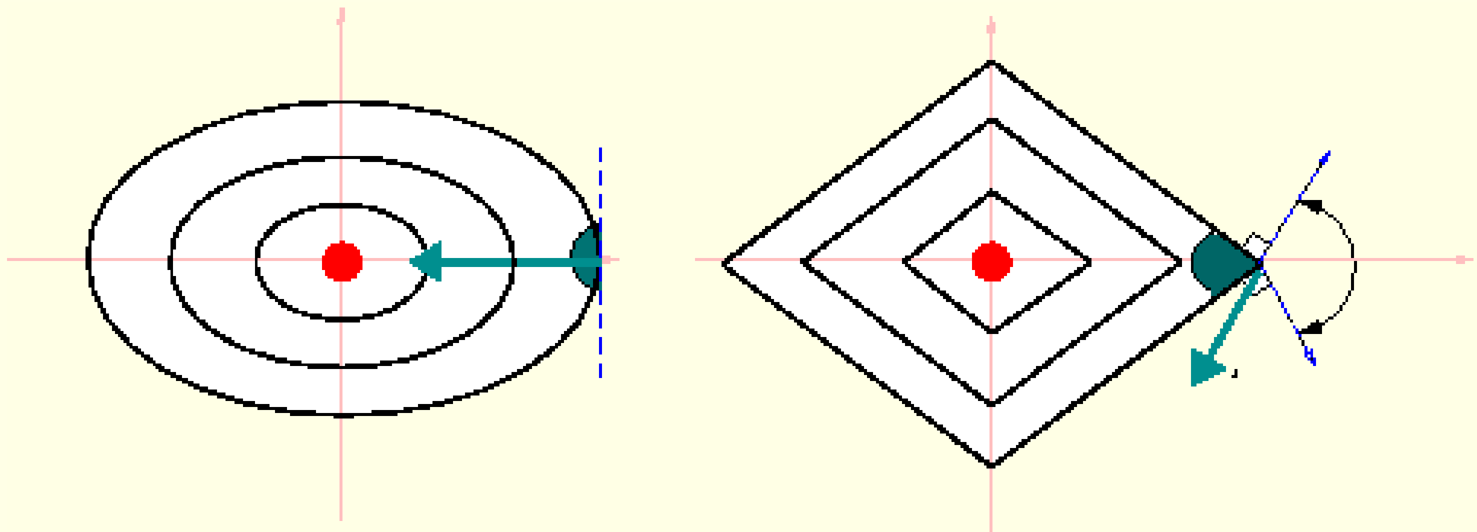


Why special NSO methods?

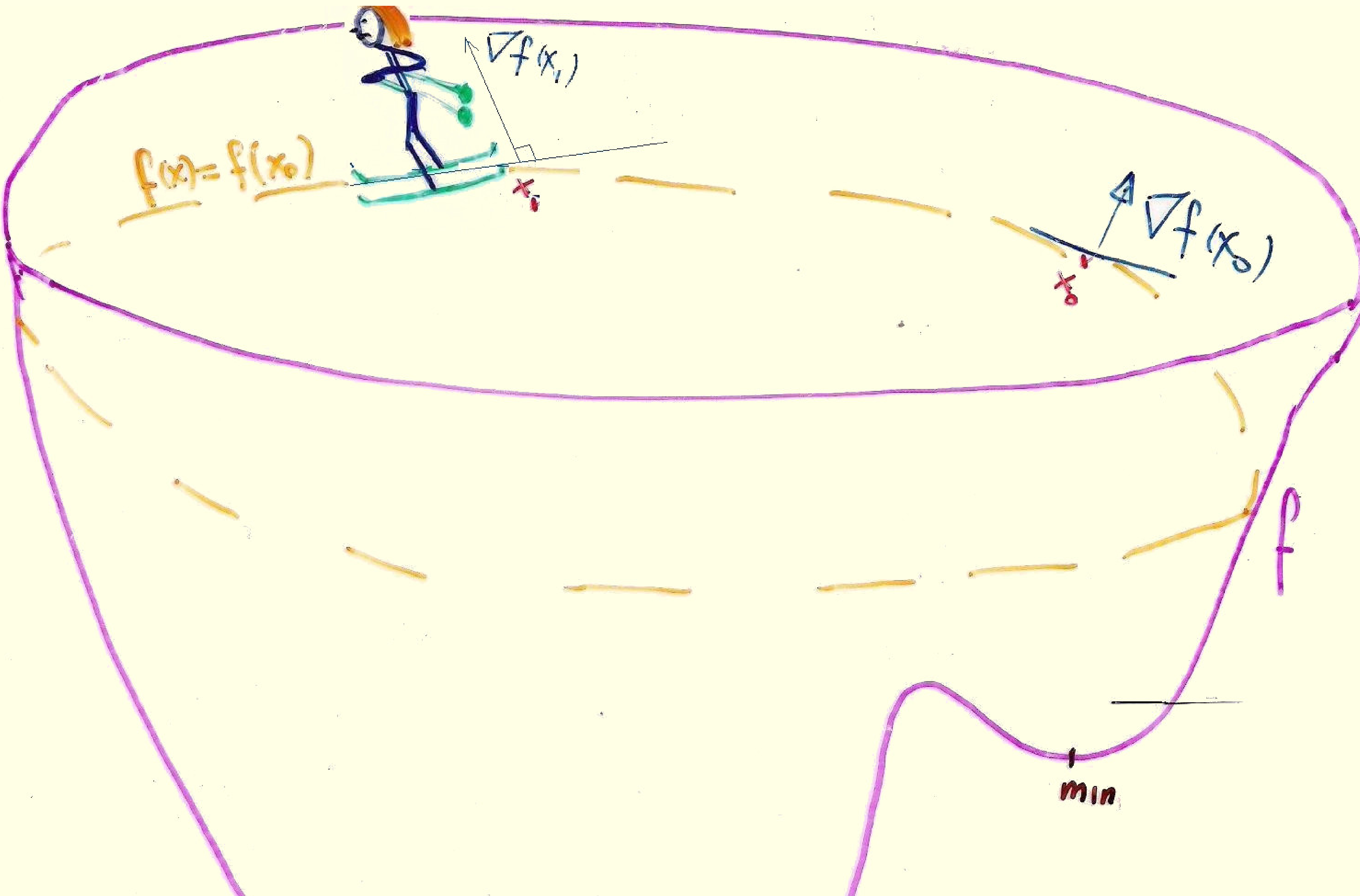
Smooth optimization techniques **do not work**

Smooth stopping test **fails**

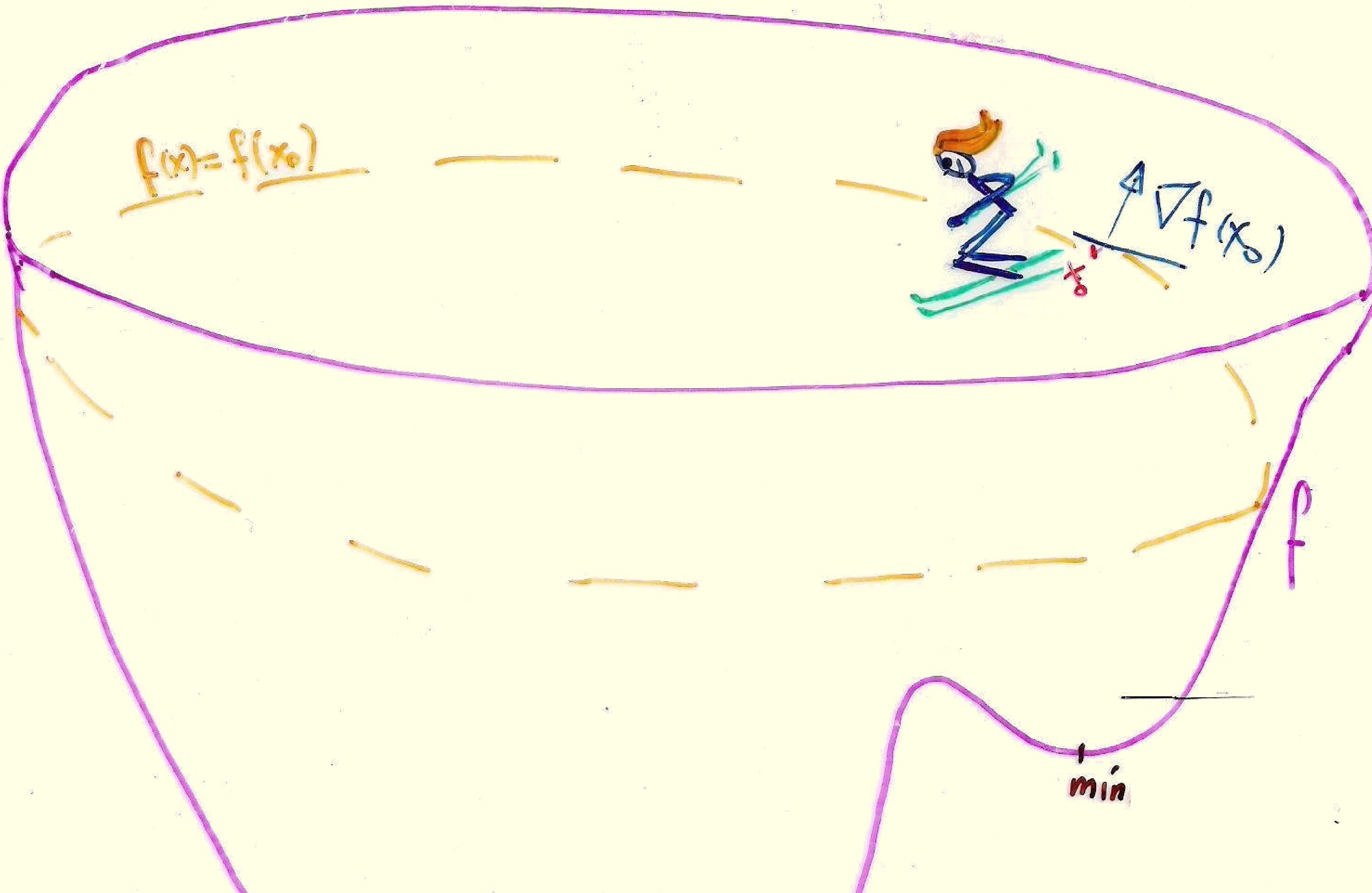
Finite difference approximations **fail**

Linesearches get trapped in kinks and **fail**

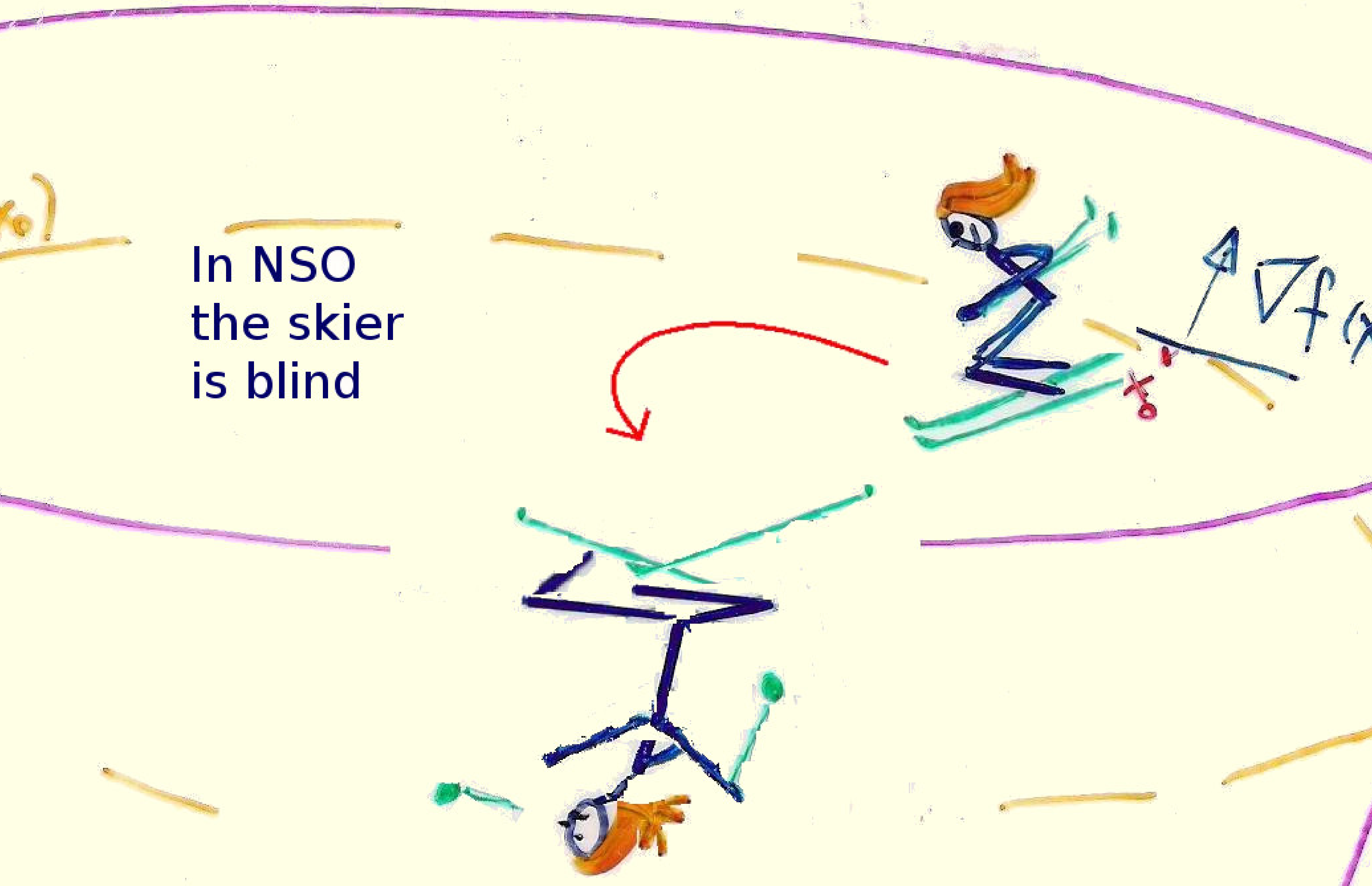
Direction opposite to a subgradient may **increase** the functional values



$\nabla f(x_1)$
$f(x) = f(x_0)$
x_1
$\nabla f(x_0)$
x_0
f
min



f(x) = f(x_0)
∇f(x_0)
x_0
f
min


In NSO
the skier
is blind
x_0

Bundle Methods

$$\text{WANT: } p = \text{prox}_t^f(x) \iff p = \arg\min f(y) + \frac{1}{2t}\|y - x\|_2^2$$

$$\text{HAVE: } q^k = \text{prox}_{t_k}^{M_k}(x) \iff q^k = \arg\min M_k(y) + \frac{1}{2t_k}\|y - x^k\|_2^2$$

$$\iff 0 = G^k + \frac{1}{t_k}(q^k - x^k)$$

$$\text{for } G^k \in \partial M_k(q^k)$$

$$\iff G^k \in \partial_{\varepsilon_k} f(x)$$

$$\text{for } \varepsilon_k = f(x) - M_k(q^k) - t_k\|G^k\|_2^2$$

Bundle Methods

$$\begin{aligned}
\text{WANT: } p = \operatorname{prox}_t^f(x) \quad &\Longleftrightarrow \quad p = \arg\min f(y) + \tfrac{1}{2t}\|y - x\|_2^2 \\
\text{HAVE: } q^k = \operatorname{prox}_{t_k}^{M_k}(x) \quad &\Longleftrightarrow \quad q^k = \arg\min M_k(y) + \tfrac{1}{2t_k}\|y - x^k\|_2^2 \\
&\Longleftrightarrow \quad 0 = G^k + \tfrac{1}{t_k}(q^k - x^k) \\
&\qquad\qquad \text{for } G^k \in \partial M_k(q^k) \\
&\Longleftrightarrow \quad G^k \in \partial_{\varepsilon_k} f(x) \\
&\qquad\qquad \text{for } \varepsilon_k = f(x) - M_k(q^k) - t_k\|G^k\|_2^2
\end{aligned}$$

Two subsequences

- Iterates giving sufficiently good approximal points
- Iterates just helping the optimization process

Bundle Methods

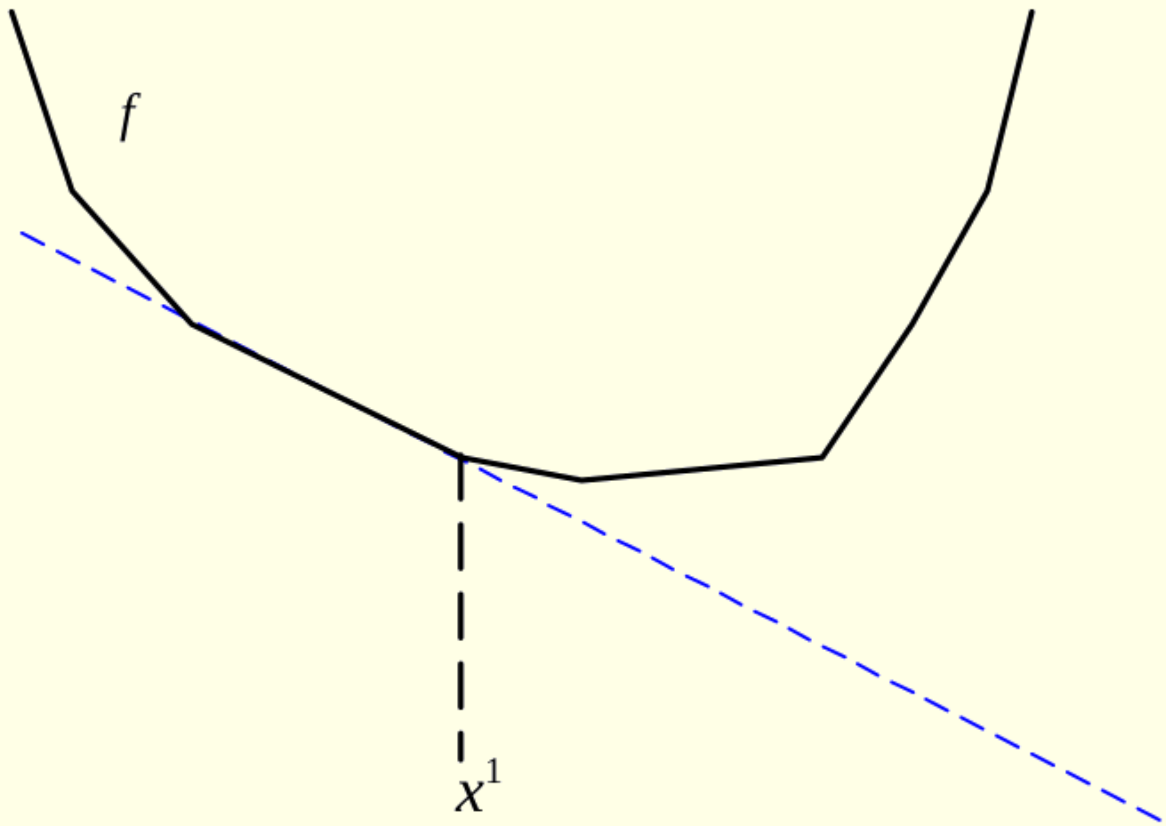
HAVE: $q^k = \mathrm{prox}_{t_k}^{M_k}(x) \;=\; x^k + t_k G^k \qquad\qquad G^k \in \partial_{\varepsilon_k} f(x)$

for $\varepsilon_k = f(x) - M_k(q^k) - t_k \|G^k\|_2^2$

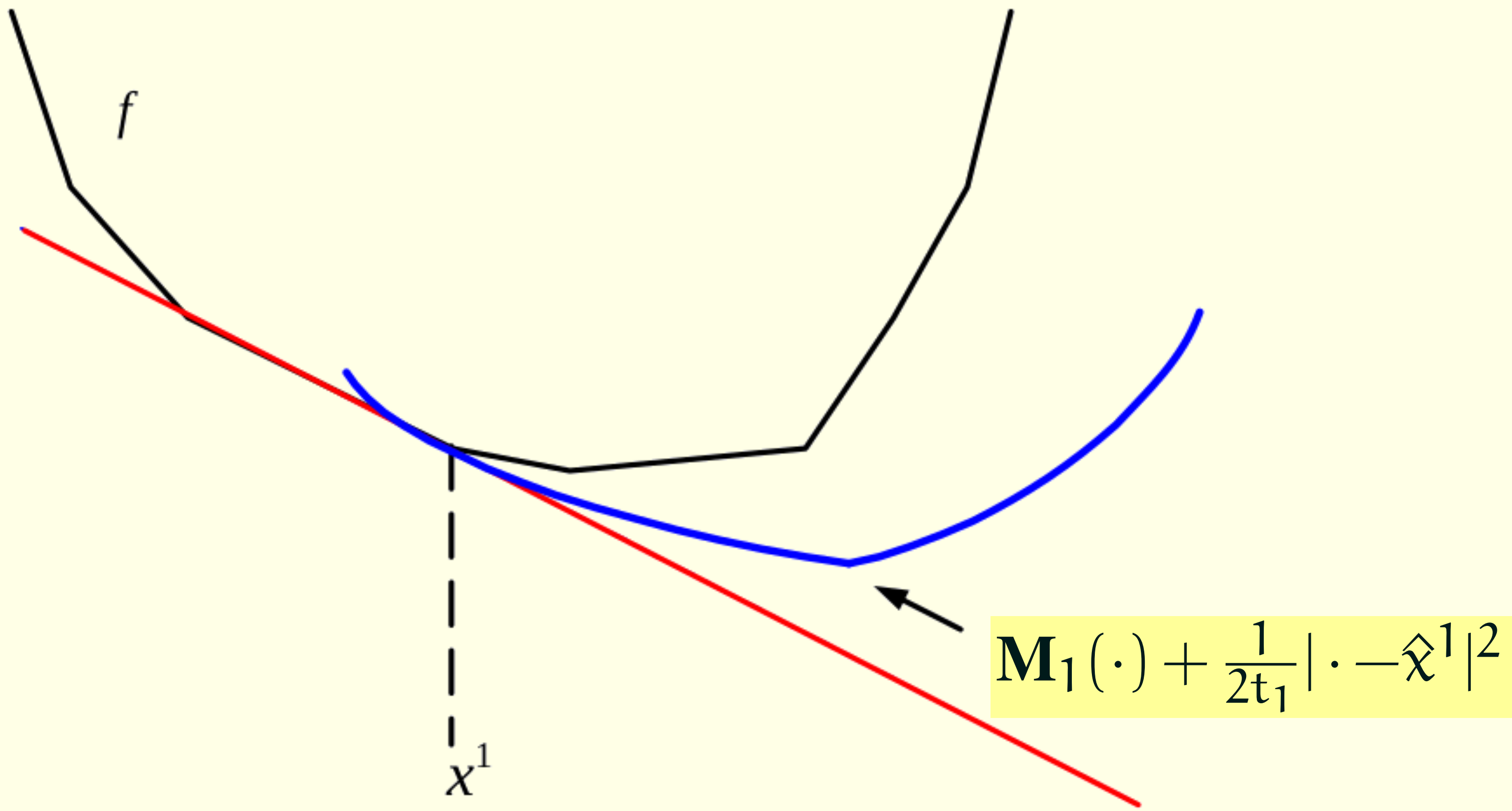
Two subsequences

- Iterates giving sufficiently good approximal points
  moving towards minimum
  in a manner that makes $\delta_k := \varepsilon_k + t_k \|G^k\|_2^2 \to 0$
  (serious)
- Iterates just helping the optimization process
  CL93 eventually applies **(null)**

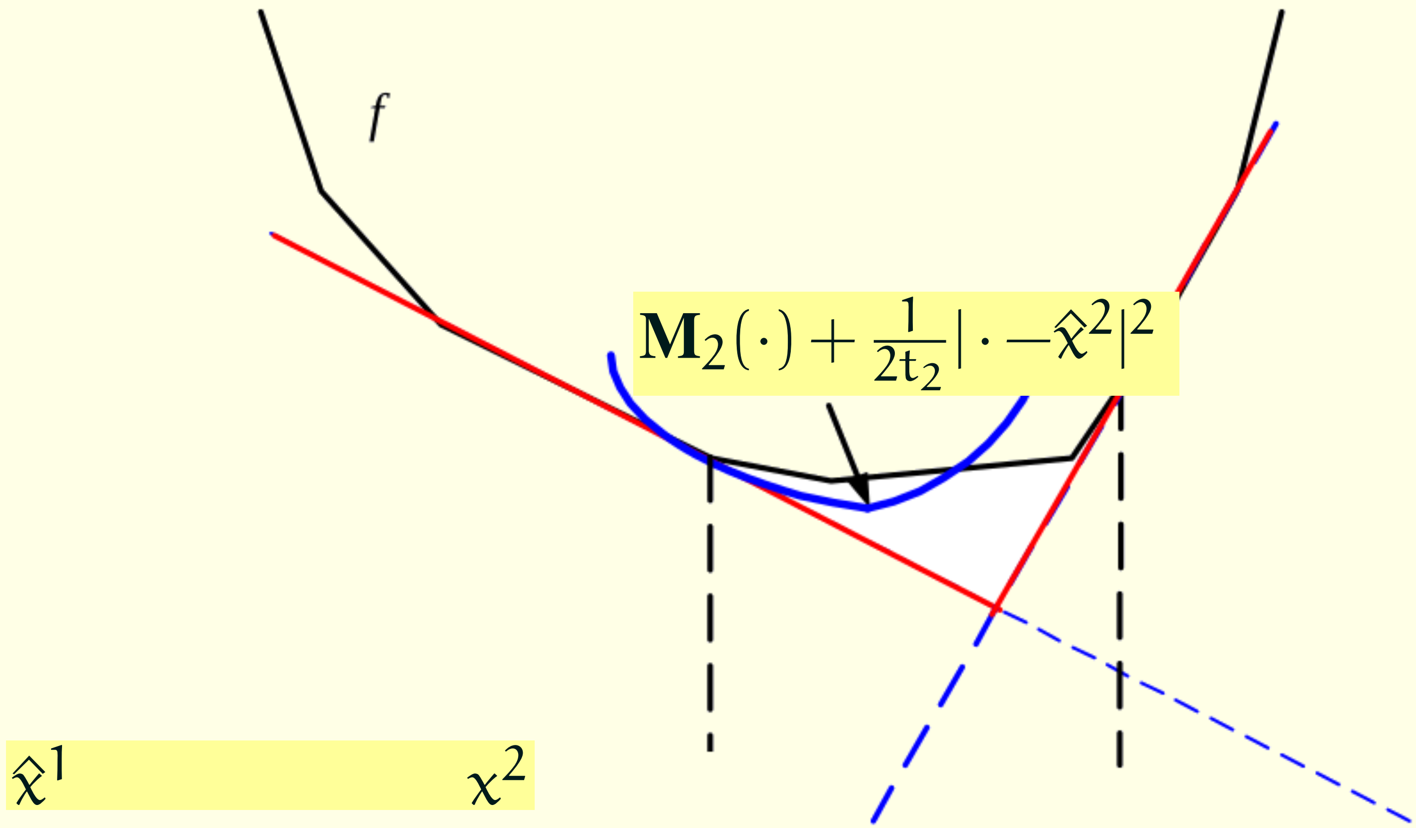
Bundle Methods



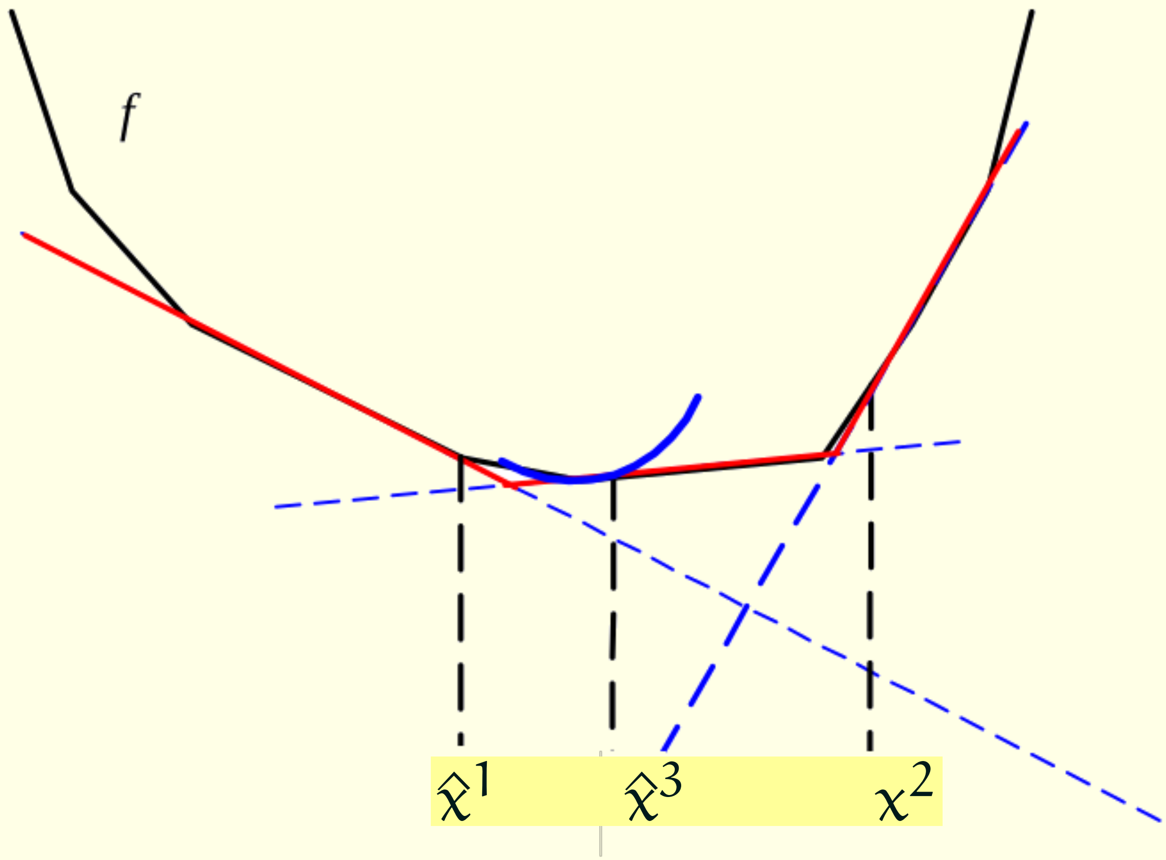
Bundle Methods



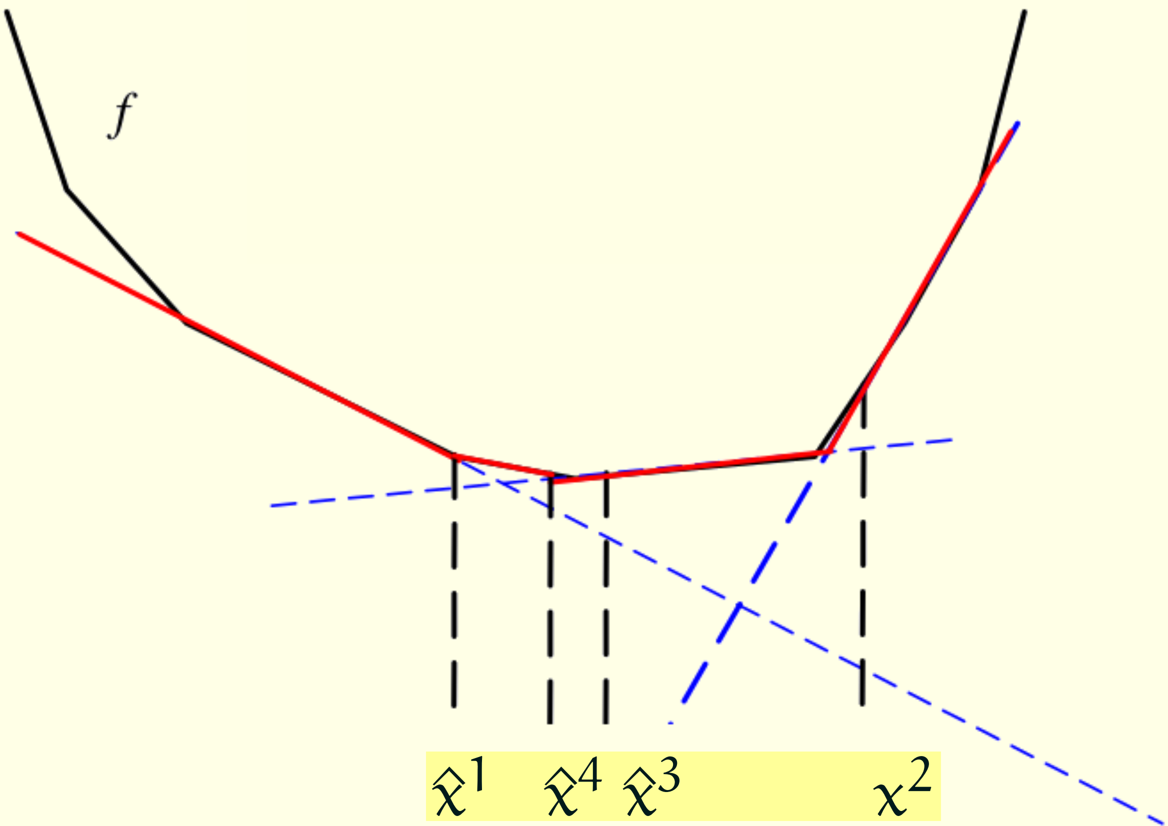
Bundle Methods



Bundle Methods



Bundle Methods



Bundle Methods

0 Choose x^1, set $k = 1$, and let $\hat{x}^1 = x^1$.

1 Compute $x^{k+1} = \arg\min \mathbf{M}_k(x) + \frac{1}{2t_k}|x - \hat{x}^k|^2$

2 If $\delta_{\mathbf{k}} := f(\hat{x}^k) - \mathbf{M}_k(x^{k+1}) \leq \mathtt{tol}$ STOP

3 Call the oracle at x^{k+1}. If

$f(x^{k+1}) \leq f(\hat{x}^k) - m\delta_k$, set $\hat{x}^{k+1} = x^{k+1}$ •

(Serious Step) Otherwise, maintain $\hat{x}^{k+1} = \hat{x}^k$
(Null Step)

4 Define $\mathbf{M}_{k+1}$, t_{k+1}, make $k = k + 1$, and loop to 1.

Bundle Methods: selection mechanism

$$\mathbf{M}_{k+1}(\cdot) = \max\left(\mathbf{M}_k(\cdot), f^k + \left\langle g^k, \cdot - x^k \right\rangle\right),$$

now the choice of the new model is more flexible:

$$x^{k+1} \in \arg\min \mathbf{M}_k(x) + \frac{1}{2t_k}|x - \hat{x}^k|^2$$

with $\mathbf{M}_k(x) = \max_{i \leq k}\{f^i + \left\langle g^i, x - x^i \right\rangle\}$ is equivalent to a QP:

$$\begin{cases} \min_{r \in \mathbb{R}, x \in \mathbb{R}^n} & r + \frac{1}{2t_k}|x - \hat{x}^k|^2 \\ \text{s.t.} & r \geq f^i + \left\langle g^i, x - x^i \right\rangle \text{ for } i \leq k \end{cases}$$

A posteriori, the solution remains the same if …

Bundle Methods: selection mechanism

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A posteriori, the solution remains the same if all, or

...

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A posteriori, the solution remains the same if all, or active, or . . .

Bundle Methods: selection mechanism

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A posteriori, the solution remains the same if all, or active, or the **optimal convex combination**

Bundle Methods: selection mechanism

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A posteriori, the solution remains the same if all, or active, or the optimal convex combination are kept

Bundle Methods: next model options

$$\mathbf{M}_{k+1}(\cdot) = \max\left(\mathbf{M}_k(\cdot), f^k + \left\langle g^k, \cdot - x^k \right\rangle\right)$$

or

$$\mathbf{M}_{k+1}(\cdot) = \max\left(\max_{active}, f^k + \left\langle g^k, \cdot - x^k \right\rangle\right)$$

or

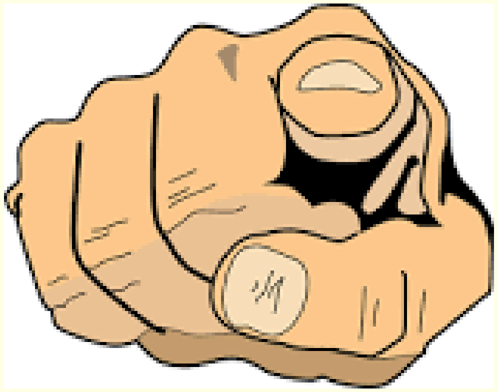
$$\mathbf{M}_{k+1}(\cdot) = \max\left(aggregate, f^k + \left\langle g^k, \cdot - x^k \right\rangle\right)$$

Same QP solution if all, or active, or the optimal convex combination

aggregate=full Bundle Compression: QP with only 2 constraints (but slows down the overall process)

The cutting-plane model

You told us

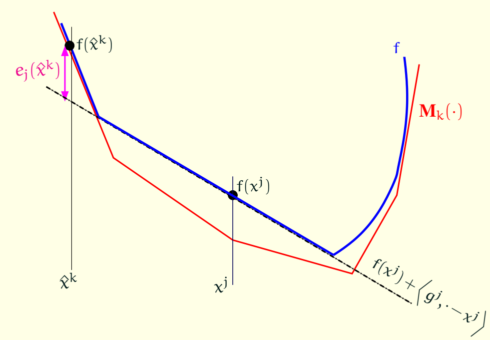


we were going to use a bundle $\mathcal{B}_k$ composed by linearization errors and ε-subgradients at $\hat{x}^k$, but the model uses f^i and $g^i \in \partial f(x^i)$

Rewriting the cutting-plane model

The transportation formula centers the ith linearization in the serious iterate

$$\begin{aligned} f(y) &\geq f(x^i) + \left\langle g^i, y - x^i \right\rangle \\ &= f(\hat{x}^k) + \left\langle g^i, y - \hat{x}^k \right\rangle - e^i(\hat{x}^k) \end{aligned}$$



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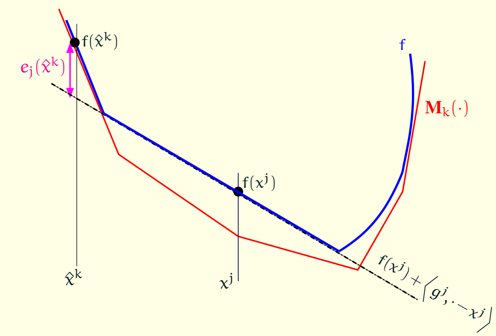

this translates into the model as follows

$$\begin{aligned} \mathbf{M}_k(y) &= \max\left\{ f(x^i) + \left\langle g^i, y - x^i \right\rangle \quad : i \in \mathcal{B}_k \right\} \\ &= \max\left\{ f(\hat{x}^k) + \left\langle g^i, y - \hat{x}^k \right\rangle - e^i(\hat{x}^k) \quad : i \in \mathcal{B}_k \right\} \\ &= f(\hat{x}^k) + \max\left\{ \left\langle g^i, y - \hat{x}^k \right\rangle - e^i(\hat{x}^k) \quad : i \in \mathcal{B}_k \right\} \end{aligned}$$

Bundle Method

0 Choose x^1, set $k = 1$, and let $\hat{x}^1 = x^1$.

1 Compute $x^{k+1} = \arg\min \mathbf{M}_k(x) + \frac{1}{2t_k}|x - \hat{x}^k|^2$

2 If $\delta_k := f(\hat{x}^k) - \mathbf{M}_k(x^{k+1}) \leq \mathtt{tol}$ STOP

3 Call the oracle at x^{k+1}. If

$f(x^{k+1}) \leq f(\hat{x}^k) - m\delta_k$, set $\hat{x}^{k+1} = x^{k+1}$

Otherwise, maintain $\hat{x}^{k+1} = \hat{x}^k$

4 Define $\mathbf{M}_{k+1}$, t_{k+1}, make $k = k + 1$, and loop to 1.

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(Serious Step) $\mathbf{k \in K_S}$

Otherwise, maintain $\hat{x}^{k+1} = \hat{x}^k$

(Null Step) $k \in K_N$

4 Define $\mathbf{M}_{k+1}$, t_{k+1}, make $k = k + 1$, and loop to 1.

Bundle Method

When $k \rightarrow \infty$, the algorithm generates two subsequences. Convergence analysis addresses the mutually exclusive situations

- either the SS subsequence is infinite

  $\mathbf{K}_\infty := \{\mathbf{k} \in \mathbf{K}_S\}$

- or there is a last SS, followed by infinitely many null steps

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Bundle Method

When $k \to \infty$, the algorithm generates two subsequences. Convergence analysis addresses the mutually exclusive situations

- either the SS subsequence is infinite

  $\mathbf{K}_\infty := \{\mathbf{k} \in \mathbf{K}_\mathbf{S}\}$ **(limit point minimizes f)**

- or there is a last SS, followed by infinitely many null steps

  $\mathbf{K}_\infty := \{\mathbf{k} \in \mathbf{K}_\mathbf{N} : \mathbf{k} \geq \textbf{last SS}\}$

  (last SS minimizes f and null$\to$ last SS)

Equivalent QPs

1. Given t_k, the stepsize parameter of the proximal bundle method, with QP subproblem given by

$$(PB)_k \quad \min \mathbf{M}_k(x) + \frac{1}{2t_k}|x - \hat{x}^k|^2$$

2. Given Δ_k, the radius parameter of the trust-region bundle method, with QP subproblem given by

$$(TRB)_k \quad \begin{cases} \min & \mathbf{M}_k(x) \\ \text{s.t.} & |x - \hat{x}^k|^2 \leq \Delta_k \end{cases}$$

3. Given ℓ_k, the level parameter of the level bundle method,

with QP subproblem given by

$$(\mathrm{LB})_k \quad \begin{cases} \min & \frac{1}{2}|x-\hat{x}^k|^2 \\ \text{s.t.} & \mathbf{M}_k(x) \le \ell_k \end{cases}$$

Show that

1. given t_k, there exists Δ_k such that if x^{k+1} solves $(\mathrm{PB})_k$, then x^{k+1} solves $(\mathrm{TRB})_k$.
2. given Δ_k, there exists ℓ_k such that if x^{k+1} solves $(\mathrm{TRB})_k$, then x^{k+1} solves $(\mathrm{LB})_k$.
3. given
   ell_k, there exists t_k such that if x^{k+1} solves $(\mathrm{LB})_k$, then x^{k+1} solves $(\mathrm{PB})_k$.

Theorem $\mathbf{K}_\infty := \{\mathbf{k} \in \mathbf{K}_S\}$

Suppose the bundle method loops forever and there are infinitely many serious steps. Either the solution set of $\min f$ is empty and $f(\hat{x}^k) \searrow -\infty$ or the following holds

(i) $\lim\limits_{k\in K_S} \delta_k = 0$ and $\lim\limits_{k\in K_S} \varepsilon_k = 0$.

(ii) If the stepsizes are chosen so that $\sum\limits_{k\in K_S} t_k = +\infty$ then $\{\hat{x}^k\}$ is a minimizing sequence.

(iii) If, in addition, $t_k \le t^{up}$ for all $k \in K_S$, then the subsequence $\{\hat{x}^k\}$ is bounded. In this case, any limit point x^∞ minimizes f and the whole sequence converges to x^∞

Theorem $\mathbf{K}_\infty := \left\{\mathbf{k} \in \mathbf{K_N} \geq \hat{\mathbf{k}}\right\}$

Suppose the bundle method loops forever and there are infinitely many null steps after a last serious one, denoted by $\hat{x}$ and generated at iteration $\hat{k}$. Suppose stepsizes are chosen so that

$$t_{lo} \leq t_{k+1} \leq t_k \quad \text{for all } k \in K_\infty$$

The following holds

1. The sequence $\{x^{k+1}\}$ is bounded
2. $\lim_{k \in K_\infty} \mathbf{M}_k(x^{k+1}) = f(\hat{x})$
3. $\hat{x}$ minimizes f
4. $\lim_{k \in K_\infty} x^{k+1} = \hat{x}$

Model requirements

1. $\mathbf{M}_k \leq f$

2. If k was declared a null step

    a) $\mathbf{M}_{k+1}(x) \geq f^{k+1} + \left\langle g^{k+1}, x - x^{k+1} \right\rangle$

    b) $\mathbf{M}_{k+1}(x) \geq A_k(x) = \mathbf{M}_k(x^{k+1}) + \left\langle G^k, x - x^{k+1} \right\rangle$

Model requirements

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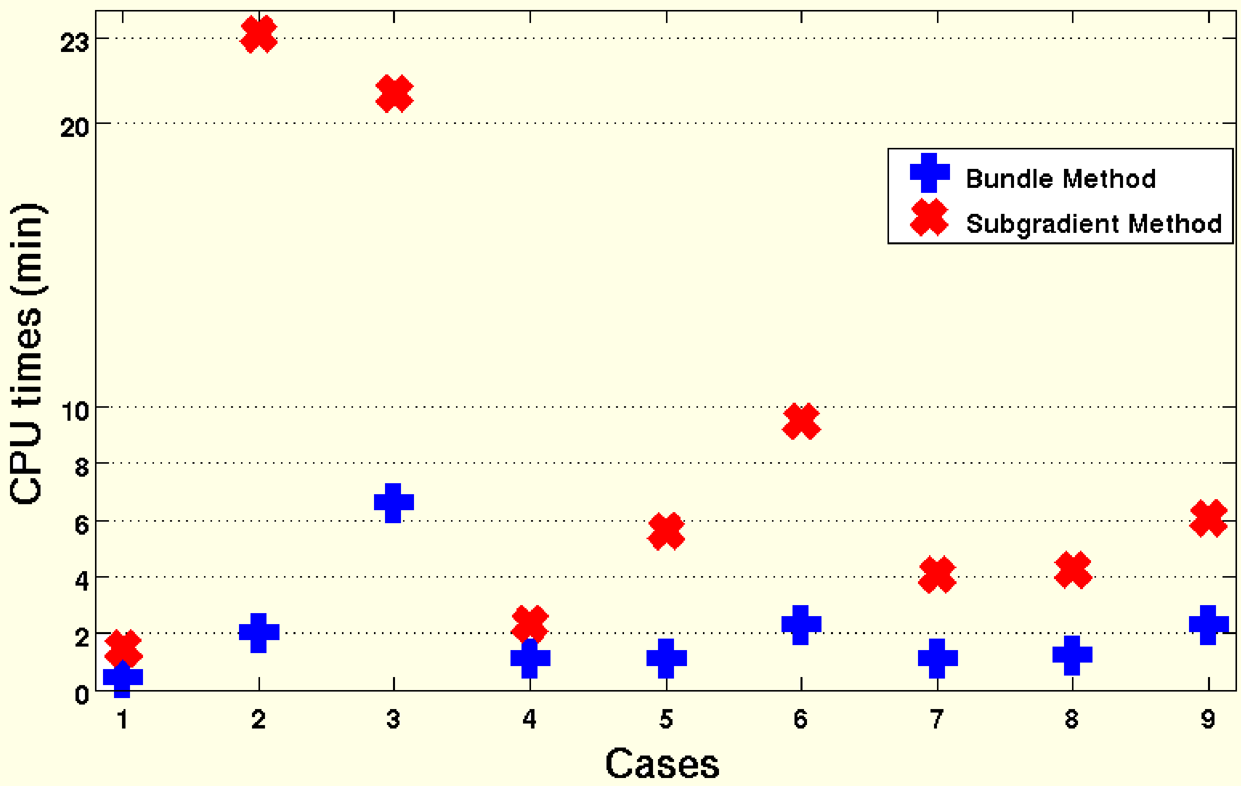
Any model satisfying these conditions

that is used in the QP

maintains the convergence results

Comparing the methods: bundle and SG

Typical performance on a battery of Unit Commitment problems

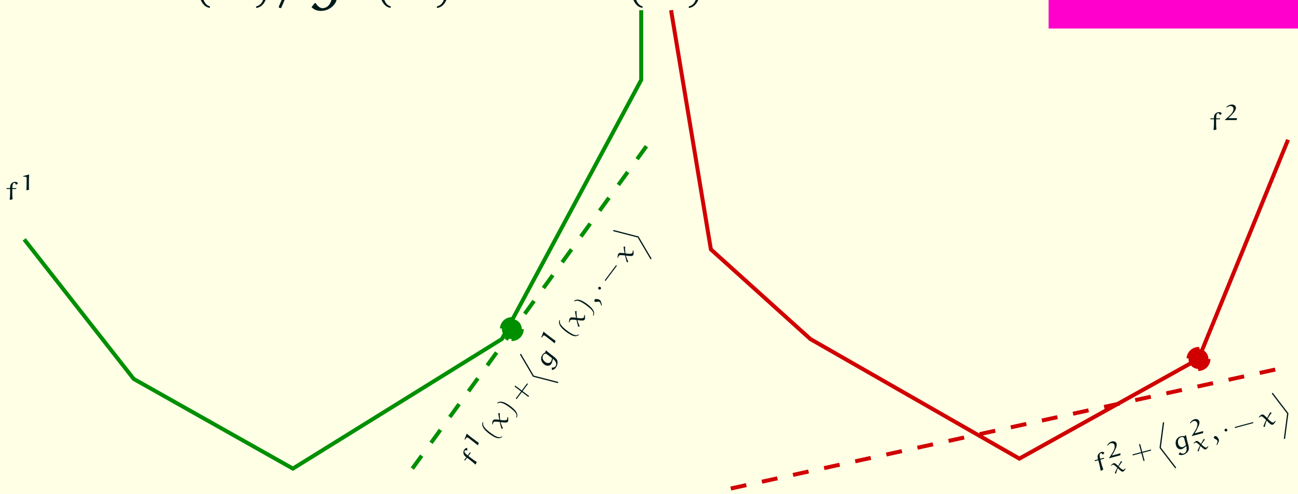


Bundle Methods with on-demand accuracy

the new generation

Oracle types: exact and upper

- $f^1(x)/g^1(x) \in \partial f^1(x)$ is **easy**: **exact $f^1(x)/g^1(x)$**
- $f^2(x)/g^2(x) \in \partial f^2(x)$ is **difficult:** **inexact f^2_x/g^2_x**



Oracle f^2_x/g^2_x NOT of lower type

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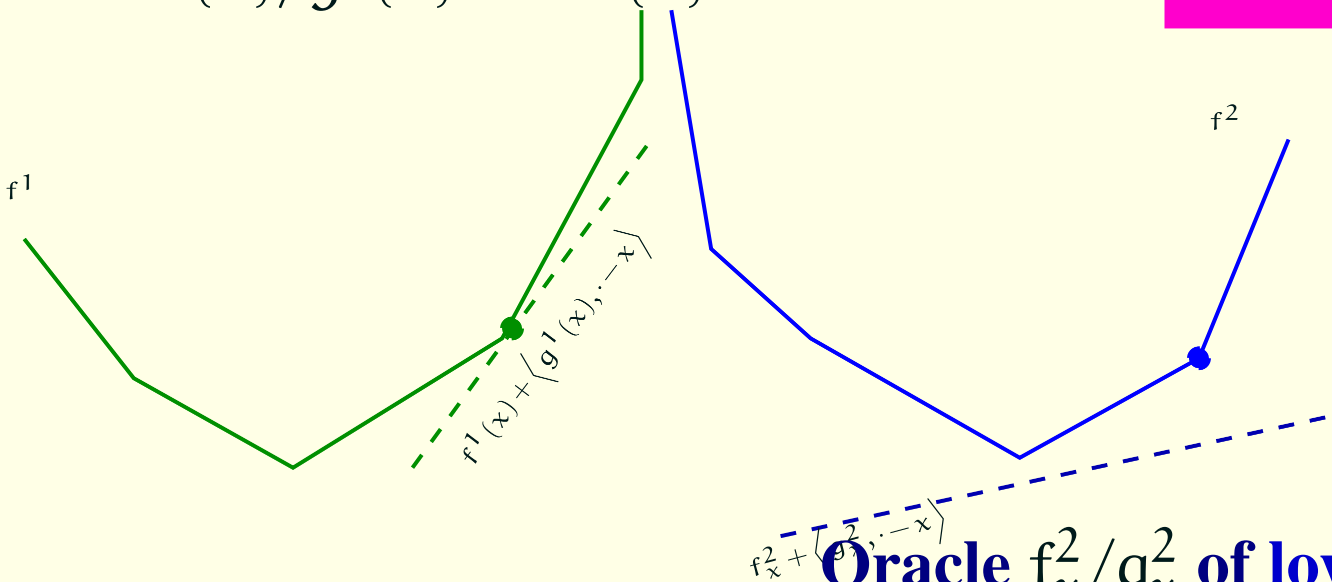
- $f^2(x)/g^2(x) \in \partial f^2(x)$ is **less difficult:** **inexact f^2_x/g^2_x**



Oracle f^2_x/g^2_x of lower type

For the EM problem $f^j(x) = \max\{-\mathcal{C}^j(q^j) + \left\langle x, g^j(q^j)\right\rangle : q^j \in \mathcal{P}^j\}$

By computing f_{x^k} and g_{x^k} satisfying

$$f_{x^k} = f(x^k) - \eta^k \quad \text{and} \quad g_{x^k} \in \partial_{\eta^k} f(x^k)$$

we can build

- A lower oracle
- An asymptotically exact oracle

$$\eta^k \to 0 \quad \text{as} \quad k \to \infty$$

- A partly asymptotically exact oracle

$$\eta^k \to 0 \quad \text{as} \quad K_s \ni k \to \infty$$

- An on-demand accuracy oracle

$$\eta^k \leq \bar{\eta}^k \quad \text{when} \quad f_{x^k} \leq f_{\hat{x}^k} - m\delta_k$$

BM with lower inexact oracles

- $\mathbf{M}_k(x) = \max\{f_{x^i} + \left\langle g_{x^i}, x - x^i \right\rangle : i \in \boldsymbol{\mathcal{B}}_k\}$
- $\delta^k = \varepsilon_k + t_k|G^k|^2$
- SS test: $f_{x^{k+1}} \leq \hat{f}^k - m\delta^k$
- $\hat{f}^k := \max\left\{f_{\hat{x}^k}, \max\left(\mathbf{M}_j(\hat{x}^k), j \geq \hat{k}\right)\right\}$

+ Oracle inaccuracy is locally bounded:
$\forall R \geq 0 \exists \eta(R) \geq 0 : |x| \leq R \Longrightarrow \eta \leq \eta(R)$ convergence as before, up to the accuracy on SS

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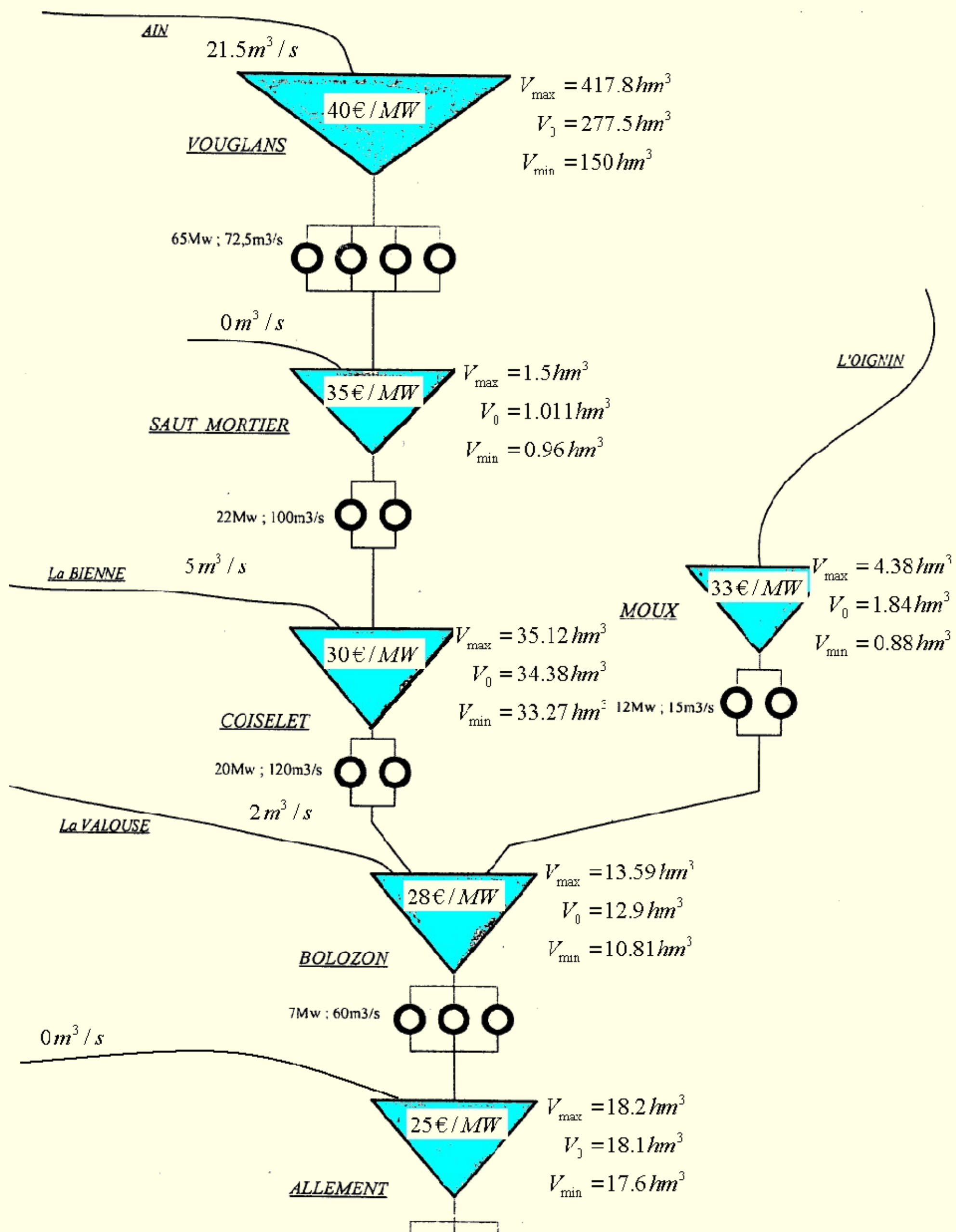
General comments

Bundle methods are

- robust (do not oscillate, as CP methods do)
- reliable (have a stopping test, unlike SG methods)
- can deal with inaccuracy in a reasonable manner

Extending bundle methods

Constrained NSO problems: an example



Optimal management of the hydrovalley

$$\begin{cases} \max & \lambda^\top \mathbb{E}_\eta\Big(\rho(u)\Big) \\ \text{s.t.} & (x,u) \in \mathcal{P} \\ & \mathbb{P}_\eta\Big(Au + a_{\min} \leq M\eta \leq Au + a_{\max}\Big) \geq p \end{cases}$$

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Is this a convex program? YES: the function

$$u \mapsto \log\Big(\mathbb{P}_\eta\Big(Au + a_{\min} \le M\eta \le Au + a_{\max}\Big)\Big) \qquad \text{is convex.}$$

We need to solve $\begin{cases} \min & f(u) \\ \text{s.t.} & (x,u) \in \boldsymbol{\mathcal{P}} \\ & c(u) \le 0 \end{cases}$ for linear f and with

$$c(u) := \log\Big(\mathbb{P}_\eta\Big(Au + a_{\min} \le M\eta \le Au + a_{\max}\Big)\Big) - \log p$$

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$$c(u) := \log\left(\mathbb{P}_\eta\left(Au + a_{\min} \le M\eta \le Au + a_{\max}\right)\right) - \log p$$

difficult to compute!

Need to solve the constrained problem

$$(P) \qquad \left\{ \begin{array}{ll} \min & f(u) \\ \text{s.t.} & (x,u) \in \mathcal{P} \\ & c(u) \leq 0 \end{array} \right.$$

for linear f and with inexact evaluation of c and its gradient, via a black box with controllable inaccuracy (bounded by a given tolerance ε, with confidence level 99%, noting that evaluation errors can be positive or negative)

Handling constraints in NSO

For nonsmooth constrained problems

$$\min f(u) \quad \text{s.t.} \quad c(u) \leq 0$$

use the Improvement Function

$$\max_u \{f(u) - f(\hat{u}), c(u)\}$$

(changes with each serious point $\hat{u}$ and supposes exact f/c values available) [SagSol SiOPT, 2005 and KarasRibSagSol MPB, 2009]

Improvement function

Let $(\bar{x}, \bar{u})$ be a solution to (P). The function

$$H_{\bar{u}}(u) := \max_{(x,u)\in\mathcal{P}} \{f(u) - f(\bar{u}), c(u)\}$$

has perfect theoretical properties:

If Slater condition ($\exists\,(x,u) \in \mathcal{P}$ s.t. $c(u) < 0$) holds, then

$$\bar{u} \text{ solves } \min_{(x,u)\in\mathcal{P}} f(u) \quad \text{s.t.} \quad c(u) \le 0 \qquad \textbf{(P)}$$

$$\Updownarrow$$

$$\min_{(x,u)\in\mathcal{P}} H_{\bar{u}}(u) = H_{\bar{u}}(\bar{u}) = 0$$

$$\Updownarrow$$

$$0 \in \partial H(\bar{u}) \text{ for } H(\cdot) := H_{\bar{u}}(\cdot)$$

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Without Slater condition

$$\bar{u} \text{ solves } \min_{(x,u)\in\mathcal{P}} f(u) \quad \text{s.t.} \quad c(u) \leq 0 \qquad \textbf{(P)}$$

$$\Downarrow \quad \textbf{BUT} \not\Uparrow$$

$$\min_{(x,u)\in\mathcal{P}} H_{\bar{u}}(u) = H_{\bar{u}}(\bar{u}) = 0$$

$$\Downarrow \quad \text{and also} \Uparrow$$

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$\Uparrow$: **when $c(\bar{u}) \le 0$ $\bar{u}$ solves (P), otherwise it minimizes infeasibility over $\mathcal{P}$**

$$\min_{(x,u)\in\mathcal{P}} H_{\bar{u}}(u) = H_{\bar{u}}(\bar{u}) = 0$$

$$\Updownarrow$$

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Handling nonconvex problems

- Nonconvex proximal point mapping [PR96]

$$p_R f(x) := \operatorname{argmin}_{y \in \mathbb{R}^N} \left\{ f(y) + \frac{R}{2}|y - x|^2 \right\}$$

x is the <u>prox-center</u> and $R > R_x$ is the <u>prox-parameter</u>

Theorem If f is convex

- $p_R f$ is well defined **for any** $R > 0$.
- $p_R f$ is single valued and loc. Lip.
- $p = p_R f(x) \iff R(x - p) \in \partial f(p)$
- x^* minimizes $f \iff x^* = p_R f(x^*)$ for any $R > 0$.
- $x_{k+1} = p_R f(x_k)$ converges to a minimizer x^*.

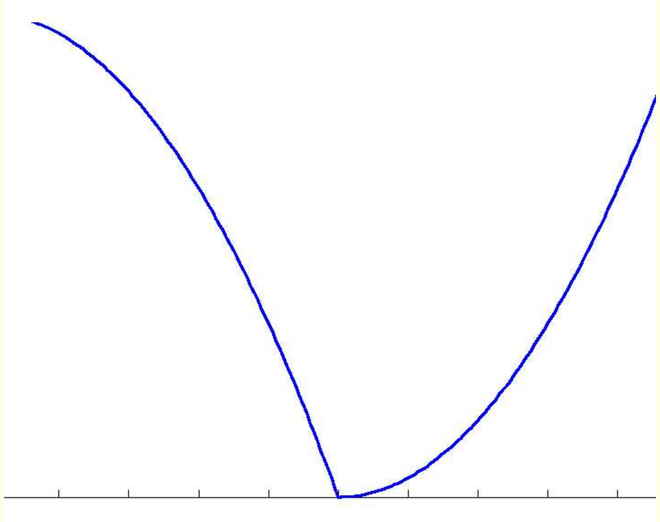
What is f is nonconvex?

Nonconvex difficulties

Proximal Bundle Methods are the most robust and reliable (oracle) methods for convex minimization. Their success relies heavily on convexity. If f is convex:

- $x_{k+1} = p_R f(x_k)$ converges to a minimizer x^*.
- $\check{f}_k$ lies **entirely** below f.

May no longer be true for nonconvex f



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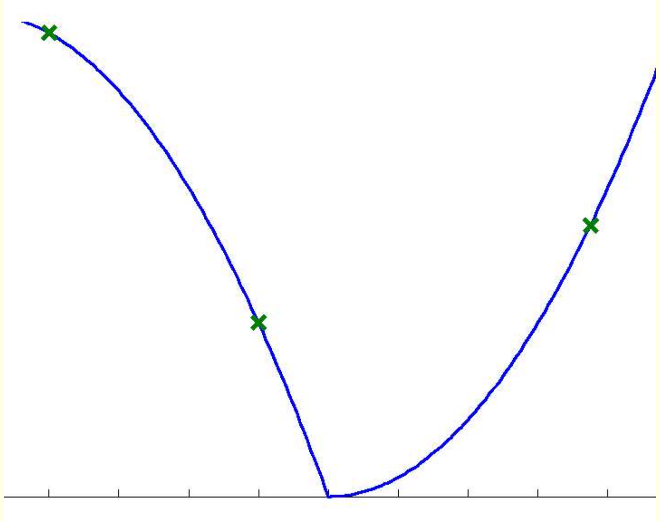

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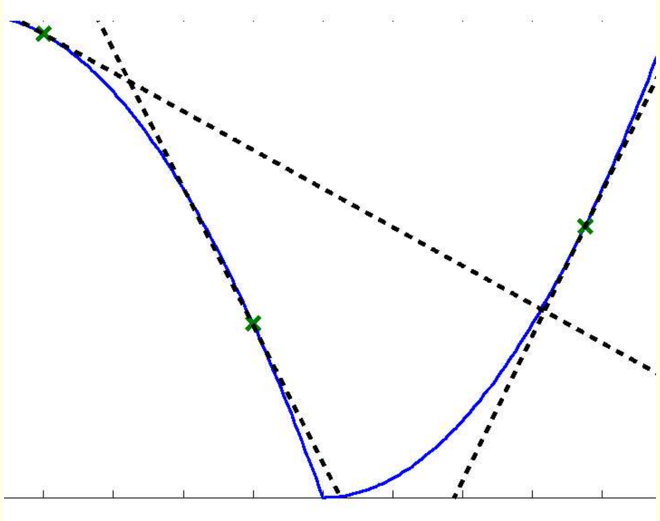

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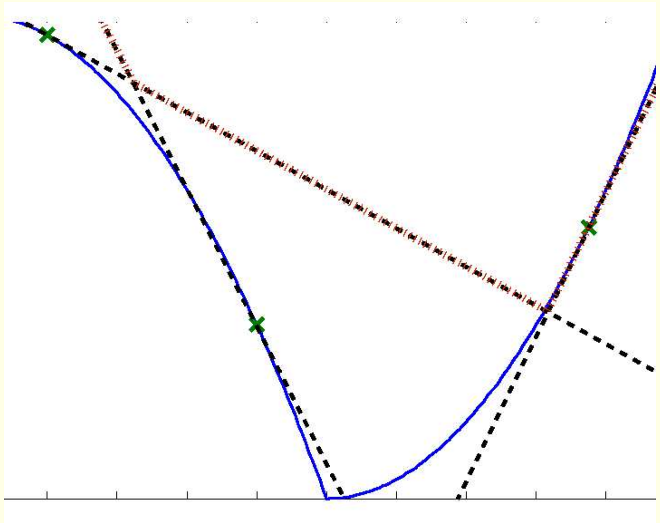

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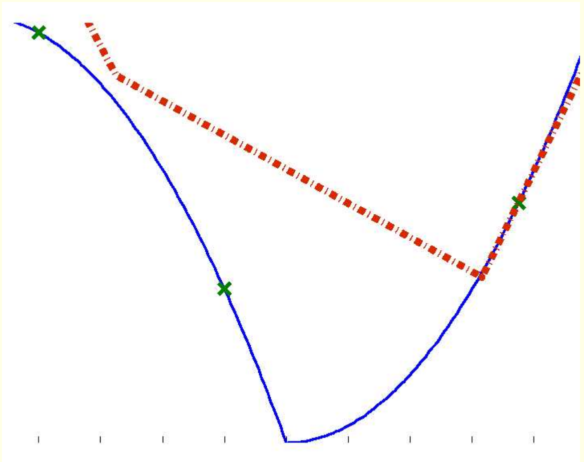


How this difficulty has been addressed?

Take each plane in the model: $f_i + \langle g_i, \cdot - y_i \rangle$ and rewrite it, centered at x_k:

$$\begin{array}{lcl} f(x_k) - & \left[f(x_k) - \left(f_i + \langle g_i, x_k - y_i \rangle \right) \right] & + \langle g_i, \cdot - x_k \rangle \\ f(x_k) - & e^f_{k,i} & + \langle g_i, \cdot - x_k \rangle \end{array}$$

$$\Rightarrow \check{f}_k(y) = \max \left\{ f(x_k) - e^f_{k,i} + \langle g_i, y - x_k \rangle \right\}$$

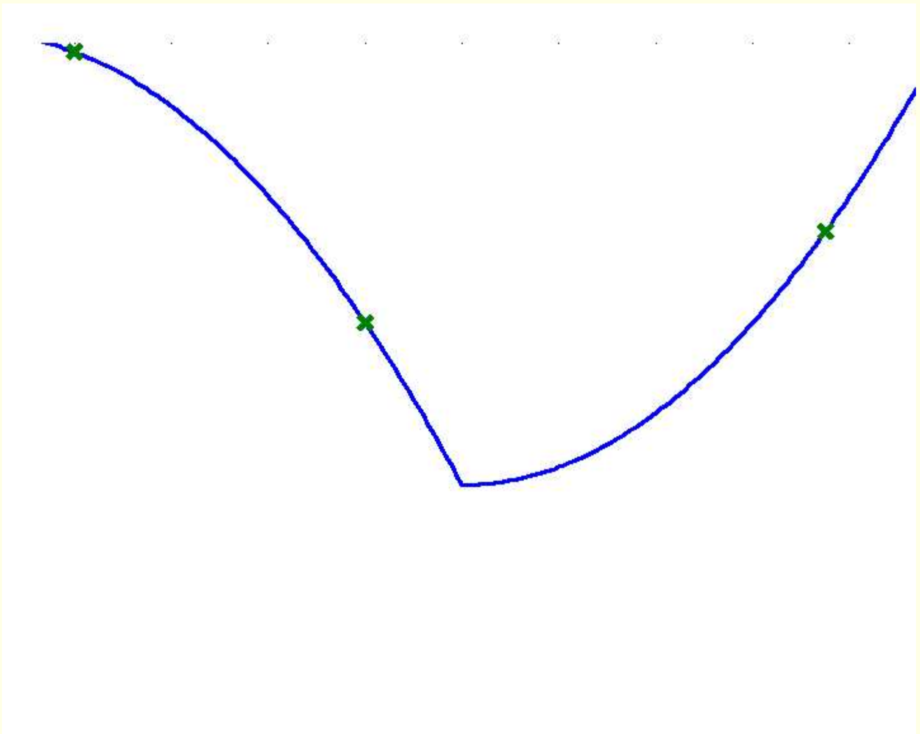
Good: $e^f_{k,i}$ positive $\Rightarrow$ convergence **Good**: If f convex $\Rightarrow e^f_{k,i}$ positive. **BAD**: If f nonconvex, $e^f_{k,i}$ may be **negative**

Nonconvex bundle methods

fix negative linearization errors, replacing $\check{f}_k$ by:

$$\check{f}_k^{\mathbf{FIX}}(y) = \max\left\{ f(x_k) - |\mathbf{e}_{\mathbf{k,i}}^{\mathbf{f}}| + \langle g_i, y - x_k \rangle \right\}$$

[Mif77, Lem80, Kiw85, Luk98]



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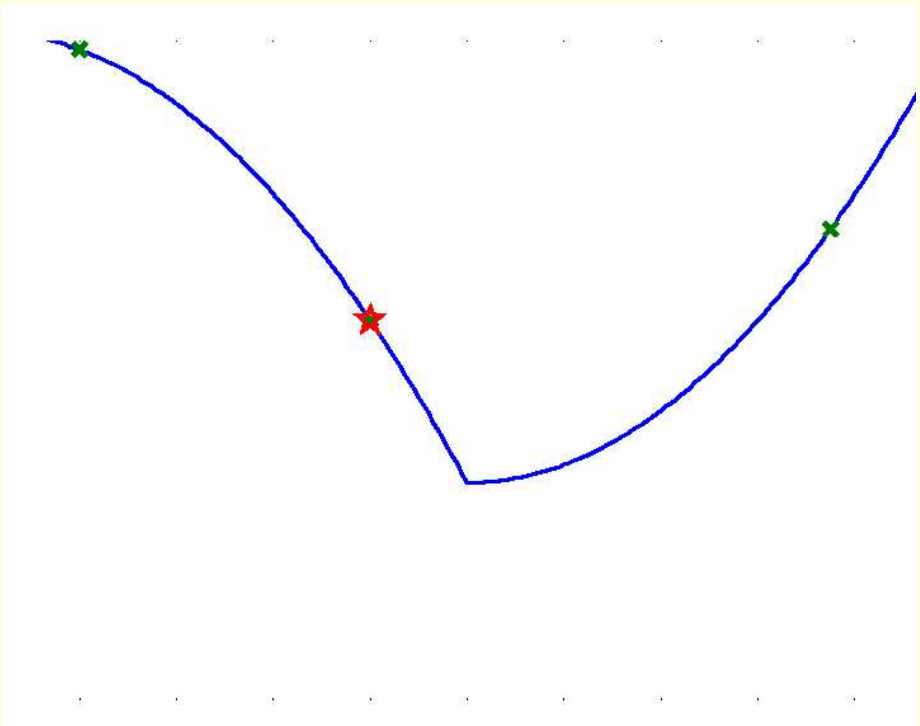

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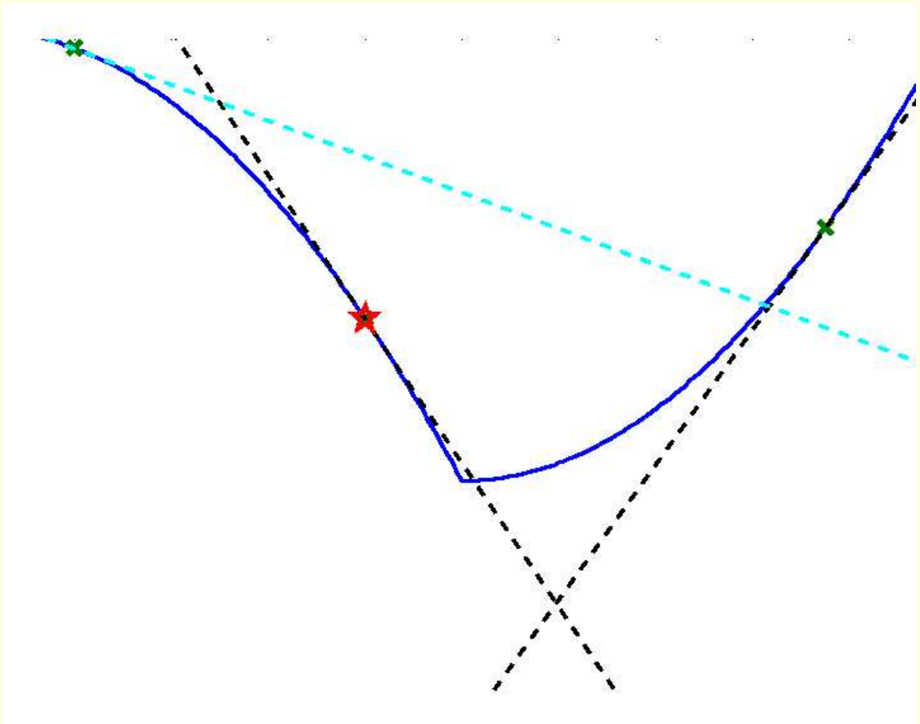

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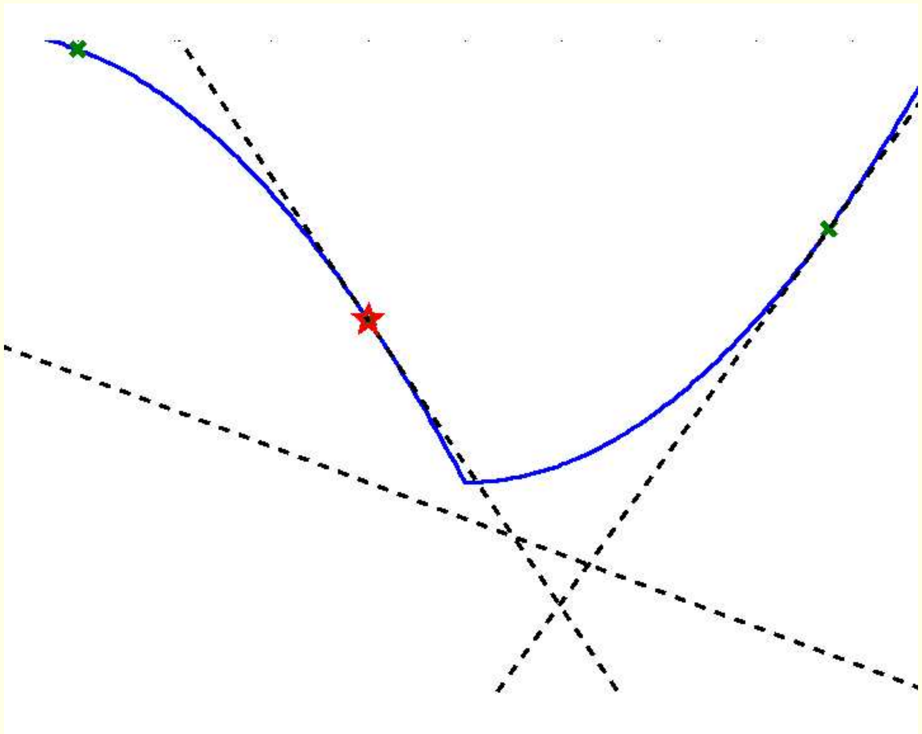
$$\check{f}_k^{\mathbf{FIX}}(y) = \max\left\{ f(x_k) - |\mathbf{e}_{\mathbf{k,i}}^{\mathbf{f}}| + \langle g_i, y - x_k \rangle \right\}$$

[Mif77, Lem80, Kiw85, Luk98]



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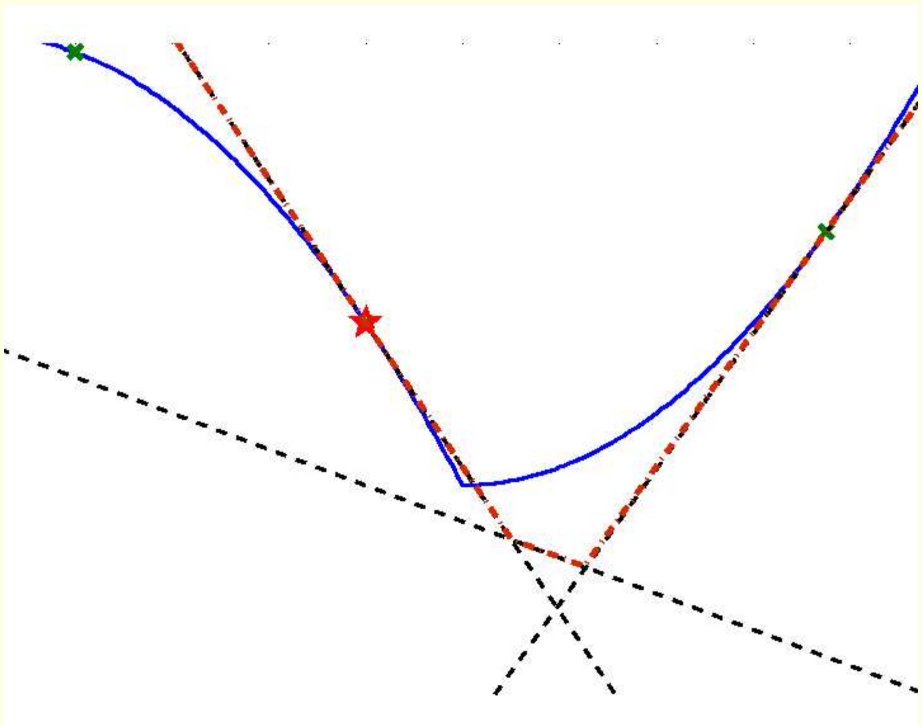

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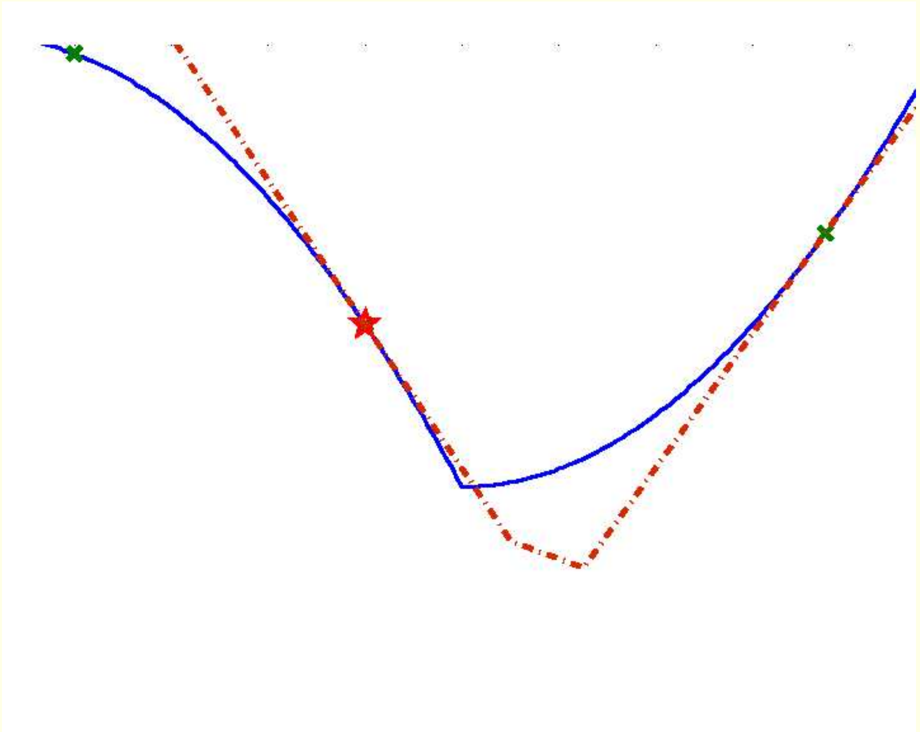


A new method

A different approach (ours) is based on the following trick

Take $\eta, \mu > 0 : R = \eta + \mu$ and note

$$
\begin{aligned}
p_R f(x_k) &= \min_w \Big\{ f(w) + R \tfrac{1}{2}|w - x_k|^2 \Big\} \\
&= \min_w \Big\{ f(w) + (\eta + \mu) \tfrac{1}{2}|w - x_k|^2 \Big\} \\
&= \min_w \Big\{ f(w) + \eta \tfrac{1}{2}|w - x_k|^2 + \mu \tfrac{1}{2}|w - x_k|^2 \Big\} \\
&= \min_w \Big\{ F_\eta(w) + \mu \tfrac{1}{2}|w - x_k|^2 \Big\} \\
&= p_\mu(F_\eta) \ (x_k)
\end{aligned}
$$

$$\Rightarrow p_R f = p_\mu(F_\eta)$$

Redistributed Proximal Bundle Method

At ℓ^{th}-iteration, for $k = k(\ell)$, given R_k, x_k and a bundle
$\mathcal{B} = \{y_i, f_i, g_i\,, i \in I_\ell\}$

0. Split R_k into η_ℓ and μ_ℓ.

1. Model F_{η_ℓ} $\quad \check{F}_{\eta_\ell,\ell}(y) = \max_{i\in\mathcal{B}}\{F_{\eta_\ell\, i} + \langle g_{\eta_\ell\, i}, y - y_i\rangle\}$

2. Minimize **the penalized model**
$y_{\ell+1} = \arg\min\{\check{F}_{\eta_\ell,\ell}(y) + \frac{\mu_\ell}{2}|y - x_k|^2\}$

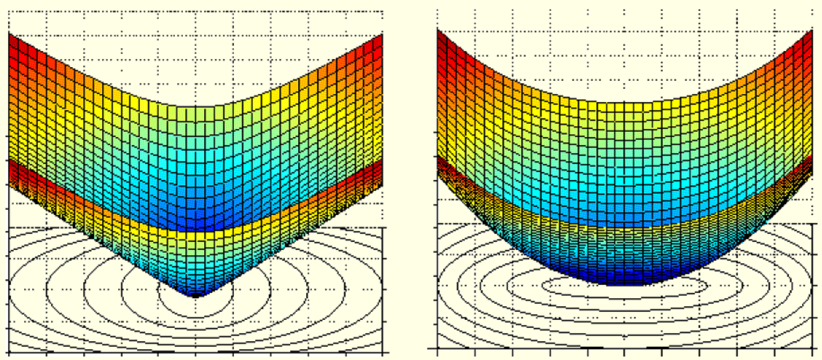
3. Descent test If $y_{\ell+1}$ good: $x_{k+1} \leftarrow y_{\ell+1}$, define R_{k+1} **serious step**

If $y_{\ell+1}$ bad: **null step**

4. Update bundle $\quad \mathcal{B} \leftarrow \mathcal{B} \cup \{y_{\ell+1}, f_{\ell+1}, g_{\ell+1}\}$

$\mathcal{VU}$ quasi-Newton bundle

For $x \in \mathbb{R}^n$, given matrices $A \succeq 0$, $B \succ 0$, $f(x) = \sqrt{x^\top A x} + x^\top B x$ has a unique minimizer at $\bar{x} = 0$. On $\mathcal{N}(A)$ the function is not differentiable, and the first term vanishes: $f|_{\mathcal{N}(A)}$ looks smooth.



$\mathcal{R}(A)$ $\mathcal{N}(A)$

$\mathcal{V}$ $\mathcal{U}$

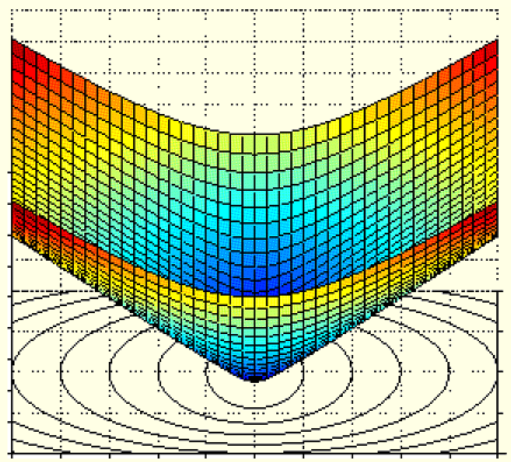
parallel to $\partial f(\bar{x})$ $\mathcal{U}$ perpendicular to $\mathcal{V}$

$\mathcal{V}$ is parallel to $\mathcal{N}(A)$, the “ridge" of nonsmoothness

$\mathcal{VU}$-Algorithm:

(Mifflin&Sagastizábal, MathProg 05) Recall that

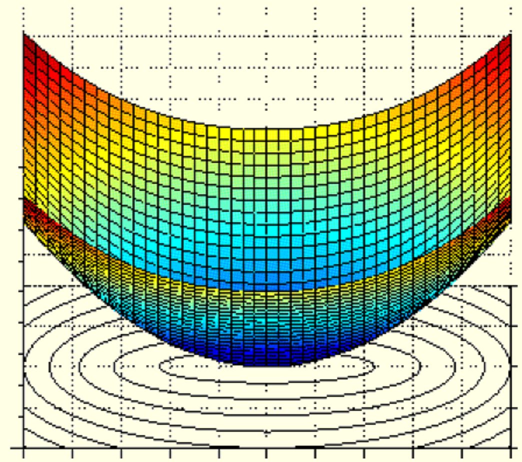
$f|_{\mathcal{V}\|\mathcal{N}(A)}$ is nice: **the key is the two QP-solves**



$\mathcal{R}(A)$

$\mathcal{V}$

2 bundle QPs



$\mathcal{N}(A)$

$\mathcal{U}$

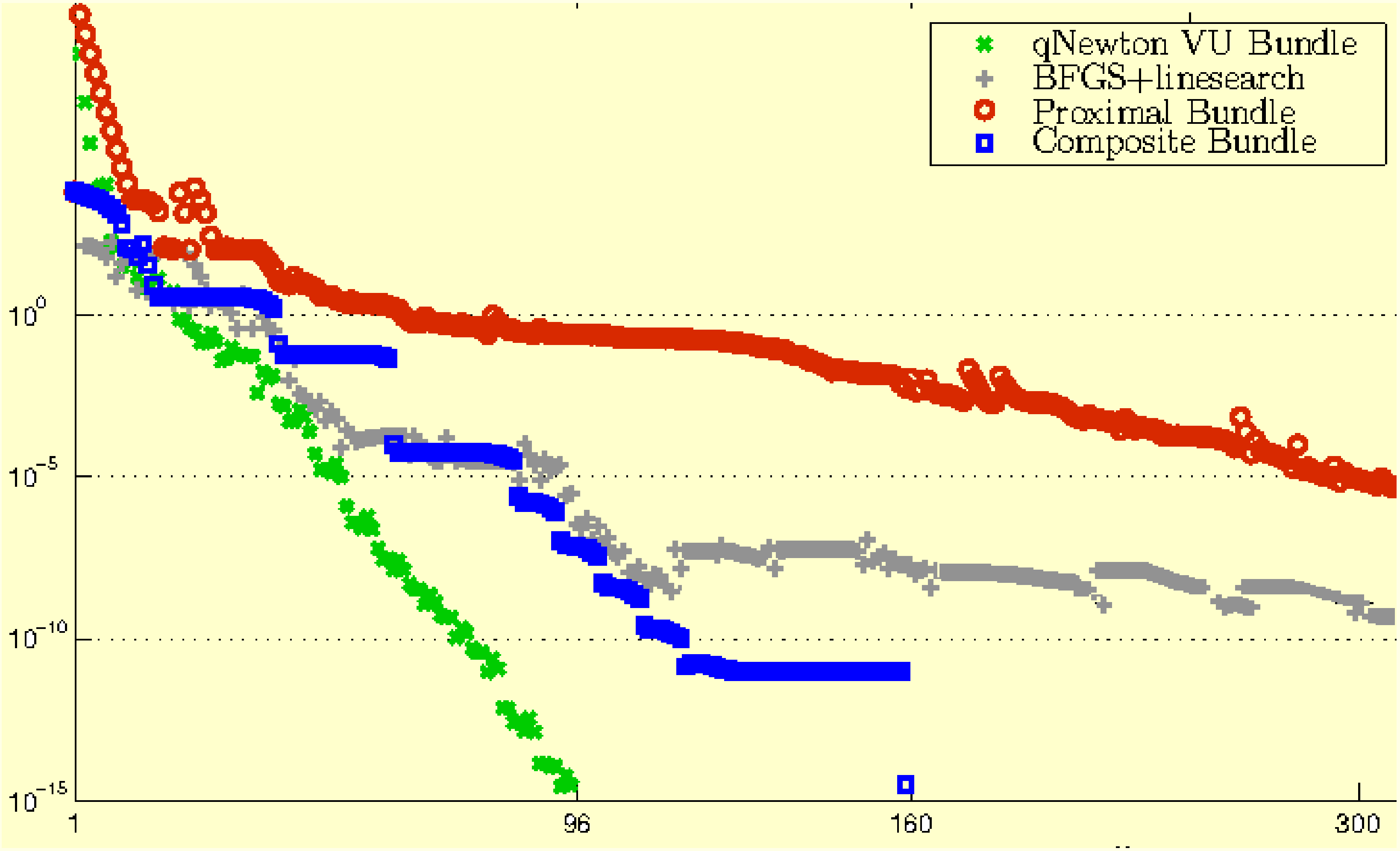
Newton-move

Two successive bundle QPs identify the “ridge” of nonsmoothness

Solve a 2nd QP to create an approximation of $\mathcal{V}$ based on $\partial \check{f}(\hat{p}^k)$

$\mathcal{VU}$-Algorithm:

superlinear "serious" subsequence (Mifflin&Sag, MathProg 05)



To learn more

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Any doubts or questions?

Just e-mail me