Using random models in derivative free optimization

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Derivative free optimization

> Unconstrained optimization problem

 $\min_{x \in \Omega} f(x)$

- Function f is computed by a black box, no derivative information is available.
- Numerical noise is often present, but we do not account for it in this talk!

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- > $f \in C^1$ or C^2 and is deterministic.
- > May be expensive to compute.

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Black box function evaluation

 $x = (x_1, x_2, x_3, \dots, x_n)$

 $v = f(x_1, \dots, x_n)$

All we can do is "sample" the function values at some sample points



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different DFO methods

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Outline

- Review with illustrations of existing methods as motivation for using models.
- Polynomial interpolation models and motivation for models based on random sample sets.
- Structure recovery using random sample sets and compressed sensing in DFO.
- > Algorithms using random models and conditions on these models.
- Convergence theory for TR framework based on random models.

Algorithms

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The simplex changes shape during the algorithm to adapt to curvature. But the shape can deteriorate and NM gets stuck

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Nelder Mead on Rosenbrock

Surprisingly good, but essentially a heuristic



















Fixed pattern, never deteriorates: theoretically convergent, but slow

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Compass Search on Rosenbrock

Very slow because of badly aligned axis directions



Random directions on Rosenbrock

Polyak, Yuditski, Nesterov, Lan, Nemirovski, Audet & Dennis, etc Better progress, but very sensitive to step size choices



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Model based trust region methods



Model based trust region methods



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Model based trust region methods



Powell, Conn, S. Toint, Vicente, Wild, etc.

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Model Based trust region methods



Exploits curvature, flexible efficient steps, uses second order models.

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Second order model based TR method on Rosenbrock



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Moral:

 > Building and using models is a good idea.
 > Randomness may offer speed up.
 > Can we combine randomization and models successfully and what would we gain?

Polynomial models

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Linear Interpolation

Any linear polynomial m(x) can be expressed as

$$m(x) = \alpha_0 + \sum_{k=1}^n \alpha_k x_k$$

Given an interpolation set $Y = \{y^0, \ldots, y^n\}$ the interpolation conditions are

$$m(y^i) = \alpha_0 + \sum_{k=1}^n \alpha_k y^i_k = f(y^i) \quad \forall i = 0, \dots, n$$

We have a system of linear equations

$$M(Y)\alpha = f(Y) \qquad M(Y) = \begin{bmatrix} 1 & y_1^0 & y_2^0 & \cdots & y_n^0 \\ 1 & y_1^1 & y_2^1 & \cdots & y_n^1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_1^n & y_2^n & \cdots & y_n^n \end{bmatrix}$$

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Good vs. bad linear Interpolation

If
$$M(Y) = \begin{bmatrix} 1 & y_1^0 & y_2^0 & \cdots & y_n^0 \\ 1 & y_1^1 & y_2^1 & \cdots & y_n^1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_1^n & y_2^n & \cdots & y_n^n \end{bmatrix}$$
 is nonsingular

then linear model exists for any f(x)

Better conditioned M => better models

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Examples of sample sets for linear interpolation

Badly poised set



Finite difference sample set





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Polynomial Interpolation

Given a polynomial basis $\phi = (\phi_1(x), \dots, \phi_q(x))$ any polynomial m(x) is expressed as

$$m(x) = \sum_{k=1}^{q} \alpha_k \phi_k(x)$$

Given an interpolation set $Y = \{y^1, \ldots, y^p\}$ the interpolation conditions are

$$m(y^i) = \sum_{k=1}^q \alpha_k \phi_k(y^i) = f(y^i) \quad \forall i = 1, \dots, p.$$

The coefficient matrix of the system is:

$$M(\phi, Y) = \begin{bmatrix} \phi_1(y^1) & \phi_2(y^1) & \cdots & \phi_q(y^1) \\ \phi_1(y^2) & \phi_2(y^2) & \cdots & \phi_q(y^2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(y^p) & \phi_2(y^p) & \cdots & \phi_q(y^p) \end{bmatrix} \qquad (p = q).$$

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Specifically for quadratic interpolation

Specifically for $\bar{\phi} = \{1, x_1, \cdots, x_n, \frac{1}{2}x_1^2, x_1x_2, \cdots, \frac{1}{2}x_n^2\}$

$$M(\bar{\phi}, Y) = M = \begin{bmatrix} 1 & y_1^1 & \cdots & y_n^1 & \frac{1}{2}(y_1^1)^2 & y_1^1 y_2^1 & \cdots & \frac{1}{2}(y_n^1)^2 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & y_1^p & \cdots & y_n^p & \frac{1}{2}(y_1^p)^2 & y_1^p y_2^p & \cdots & \frac{1}{2}(y_n^p)^2 \end{bmatrix}$$

Interpolation model:

find α : $M\alpha = f(Y)$ $m(x) = \sum_{i=1}^{q} \alpha_i \bar{\phi}_i(x) = \frac{1}{2} x^\top H x + g^\top x + \kappa$ $\bullet g = (\alpha_2, \dots, \alpha_{n+1})$ $\bullet H_{ij} = \alpha_{n+(i-1)*n+j+1}$

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Sample sets and models for f(x)=cos(x)+sin(y)









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Sample sets and models for f(x)=cos(x)+sin(y)



Sample sets and models for f(x)=cos(x)+sin(y)

0.4 0.6

0.6 0.2

0.8

0.2

0



Example that shows that we need to maintain the quality of the sample set $f(x) = \begin{cases} x_1^2 + \alpha(x_2^2 + (10 - x_1)x_2) & \text{if } x_1 < 10; \\ x_1^2 + \alpha x_2^2 & \text{if } x_1 \ge 10, \end{cases}$







Observations:

- > Building and maintaining good models is needed.
- But it requires computational and implementation effort and many function evaluations.
- Random sample sets usually produce good models, the only effort required is computing the function values.
- This can be done in parallel and random sample sets can produce good models with fewer points.

How?

"sparse" black box optimization



Sparse linear Interpolation

Given an interpolation set $Y = \{y^0, \ldots, y^p\}$ find

$$m(x) = \alpha_0 + \sum_{k=1}^n \alpha_k x_k$$

with sparse coefficient vector α such that

$$m(y^i) = \alpha_0 + \sum_{k=1}^n \alpha_k y^i_k = f(y^i) \quad \forall i = 0, \dots, p$$

Sparse linear Interpolation

We have an (underdetermined) system of linear equations with a sparse solution

$$M(Y)\alpha = f(Y) \qquad M(Y) = \begin{bmatrix} 1 & y_1^0 & y_2^0 & \cdots & y_n^0 \\ 1 & y_1^1 & y_2^1 & \cdots & y_n^1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_1^p & y_2^p & \cdots & y_n^p \end{bmatrix}$$

Can we find correct sparse α using less than n+1 sample points in Y?

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Using celebrated compressed sensing results (Candes&Tao, Donoho, etc)

By solving $\min \|\alpha\|_{1} : M(Y)\alpha = f(Y)$ Whenever $M(Y) = \begin{bmatrix} 1 & y_{1}^{0} & y_{2}^{0} & \cdots & y_{n}^{0} \\ 1 & y_{1}^{1} & y_{2}^{1} & \cdots & y_{n}^{1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_{1}^{p} & y_{2}^{p} & \cdots & y_{n}^{p} \end{bmatrix}$ has RIP

Using celebrated compressed sensing results and random matrix theory

(Candes&Tao, Donoho, Rauhut, etc)

Does
$$M(Y) = \begin{bmatrix} 1 & y_1^0 & y_2^0 & \cdots & y_n^0 \\ 1 & y_1^1 & y_2^1 & \cdots & y_n^1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_1^p & y_2^p & \cdots & y_n^p \end{bmatrix}$$

have **RIP**?

Yes, with high prob., when Y is random and $p=O(|S|\log n)$

Note: O(|S|log n)<<n

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Quadratic interpolation models

$$M(\bar{\phi}, Y) = M = \begin{bmatrix} 1 & y_1^1 & \cdots & y_n^1 & \frac{1}{2}(y_1^1)^2 & y_1^1 y_2^1 & \cdots & \frac{1}{2}(y_n^1)^2 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & y_1^p & \cdots & y_n^p & \frac{1}{2}(y_1^p)^2 & y_1^p y_2^p & \cdots & \frac{1}{2}(y_n^p)^2 \end{bmatrix}$$

Need p=(n+1)(n+2)/2 sample points!!!

Interpolation model:

find
$$\alpha$$
: $M\alpha = f(Y)$
• $\kappa = \alpha_1$
 $m(x) = \sum_{i=1}^{q} \alpha_i \bar{\phi}_i(x) = \frac{1}{2} x^\top H x + g^\top x + \kappa$
• $g = (\alpha_2, \dots, \alpha_{n+1})$
• $H_{ij} = \alpha_{n+(i-1)*n+j+1}$
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Example of a model with sparse Hessian Colson, Toint

$$\min f(x) = \sum_{i}^{n} ((x_i^2 - x_n^2)^2 - 4x_i)$$

$$\nabla_{ij}^2 f(x) = 0, \ \forall i \neq j, j \neq n$$

α has only 2n+n nonzeros

Can we recover the sparse α using less than O(n) points?

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Sparse quadratic interpolation models Mo Μ, $M(\bar{\phi}, Y) = M = \begin{bmatrix} 1 & y_1^1 & \cdots & y_n^1 & \frac{1}{2}(y_1^1)^2 & y_1^1 y_2^1 & \cdots & \frac{1}{2}(y_n^1)^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & y_1^p & \cdots & y_n^p & \frac{1}{2}(y_1^p)^2 & y_1^p y_2^p & \cdots & \frac{1}{2}(y_n^p)^2 \end{bmatrix}$ Recover sparse α $m(x) = \frac{1}{2}x^{\top}Hx + g^{\top}x + \kappa$ min $\|\alpha_Q\|_1$ α s.t. $M_L \alpha_L + M_Q \alpha_Q = f(Y)$ • $\alpha_L \to (k,g)$ • $\alpha_Q \to H$

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$M(\bar{\phi}, Y) = M = \begin{bmatrix} 1 & y_1^1 & \cdots & y_n^1 & \frac{1}{2}(y_1^1)^2 & y_1^1y_2^1 & \cdots & \frac{1}{2}(y_n^1)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & y_1^p & \cdots & y_n^p & \frac{1}{2}(y_1^p)^2 & y_1^py_2^p & \cdots & \frac{1}{2}(y_n^p)^2 \end{bmatrix}$



Actually we need RIP for M_Q and some other property on M_L

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Yes, with high probability, when Y is random and $p=O((n+s)(\log n)^4)$

Note: *p*=*O*((*n*+*s*)(*log n*)⁴)<<n² (sometimes)

For more detailed analysis see Afonso Bandeira's talk ISMP 2012 Tue 15:15 - 16:45, room: H 3503

Model-based method on 2-dimensional Rosenbrock function lifted into 10 dimensional space

Consider $f(x_1, x_2, \dots, x_{10})$ =Rosenbrock(x_1, x_2)

To build full quadratic interpolation we need 66 points. We test two methods:

- 1. Deterministic model-based TR method: builds a model using whatever points it has on hand up to 66 in the neighborhood of the current iterate, using MFN Hessian models (standard reliable good approach).
- 2. Random model based TR method: builds sparse models using 31 randomly sampled points.

Deterministic MFN model based method



Random sparse model based method



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Comparison of sparse vs MFN models (no randomness) within TR on CUTER problems



Algorithms based on random models

- We now forget about sample sets and how we build the models.
- We focus on properties of the models that are essential for convergence.
- Ensure that those properties are satisfied by models we just discussed.

What do we need from a deterministic model for convergence?

We need Taylor-like behavior of first-order models

A model is called κ -fully-linear in $B(x, \Delta)$, for $\kappa = (\kappa_{ef}, \kappa_{eg})$ if $\|\nabla f(x+s) - \nabla m(x+s)\| \leq \kappa_{eg} \Delta, \quad \forall s \in B(0; \Delta),$ $|f(x+s) - m(x+s)| \leq \kappa_{ef} \Delta^2, \quad \forall s \in B(0; \Delta),$

What do we need from a model to explore the curvature?

We may want Taylor-like behavior of second-order models

A model is called κ -fully-quadratic in $B(x, \Delta)$ for $\kappa = (\kappa_{ef}, \kappa_{eg}, \kappa_{eh})$ if

$$\|\nabla^2 f(x+s) - \nabla^2 m(x+s)\| \leq \kappa_{eh} \Delta, \quad \forall s \in B(0; \Delta),$$

$$\begin{aligned} \|\nabla f(x+s) - \nabla m(x+s)\| &\leq \kappa_{eg} \,\Delta^2, \quad \forall s \in B(0;\Delta), \\ |f(x+s) - m(x+s)| &\leq \kappa_{ef} \,\Delta^3, \quad \forall s \in B(0;\Delta), \end{aligned}$$

What do we need from a random model for convergence?

We need likely Taylor-like behavior of first-order models

A random model is called (κ, δ) -fully-linear in $B(x, \Delta)$ if

 $\|\nabla f(x+s) - \nabla m(x+s)\| \le \kappa_{eg} \Delta, \quad \forall s \in B(0; \Delta),$

 $|f(x+s) - m(x+s)| \leq \kappa_{ef} \Delta^2, \quad \forall s \in B(0; \Delta),$

with probability at least $1 - \delta$.

What do we need from a random model to explore curvature?

We need likely Taylor-like behavior of second order models

A random model is called (κ, δ) -fully-quadratic in $B(x, \Delta)$ if $\|\nabla^2 f(x+s) - \nabla^2 m(x+s)\| \leq \kappa_{eh} \Delta, \quad \forall s \in B(0; \Delta),$ $\|\nabla f(x+s) - \nabla m(x+s)\| \leq \kappa_{eg} \Delta^2, \quad \forall s \in B(0; \Delta),$ $|f(x+s) - m(x+s)| \leq \kappa_{ef} \Delta^3, \quad \forall s \in B(0; \Delta),$ with probability at least $1 - \delta$.

What random models have such properties?

- > Linear interpolation and regression models based on random sample sets of n+1 points are (κ , δ)-fully-linear.
- > Quadratic interpolation and regression models based on random sample sets of (n+1)(n+1)/2 points are (κ, δ) -fully-quadratic.
- > Sparse linear interpolation and reg. models based on smaller random sample sets are (κ , δ)-fully-linear.
- > Sparse quadratic interpolation and reg. models based on smaller random sample sets are (κ , δ)-fully-quadratic.
- > Taylor models based on finite difference derivative evaluations with asynchronous faulty parallel function evaluations are (κ , δ)-FL or FQ.
- > Gradient sampling models? Other examples?

Basic Trust Region Algorithm

Model selection

Pick a random model $m_k(x)$ which is κ -fully-linear in $B(x_k, \Delta_k)$ w.p. $1-\delta$.

Compute potential step

Compute a point x^+ which minimizes (reduces) m(x) in $B(x_k, \Delta_k)$. Compute $f(x^+)$ and check if f is reduced comparably to m by x^+ .

Successful step

If yes and if the radius Δ_k is not too big compared to $\nabla m_k(x_k)$ then we take the step and increase Δ_k by a constant factor.

Unsuccessful step

Otherwise, decrease Δ_k by the constant factor and repeat the iteration.

Convergence results for the basic TR framework

If models are fully linear with prob. $1-\delta > 0.5$ then with probability *one* $\lim ||\nabla f(x_k)|| = 0$

If models are fully quadratic w. p. $1-\delta > 0.5$ then with probability *one liminf max* {|| $\nabla f(x_k)$ ||, $\lambda_{min}(\nabla^2 f(x_k))$ }=0

For *lim* result δ need to decrease occasionally

For details see Afonso Bandeira's talk on Tue 15:15 - 16:45, room: H 3503

Intuition behind the analysis shown through line search ideas

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When m(x) is linear ~ line search instead of Δ_k use $\alpha_k || \nabla m_k(x_k) ||$

Model selection step

Pick a random model $m_k(x) = f(x_k) + g_k^{\top}(x - x_k)$ κ -fully-linear in $B(x_k, \alpha_k ||g_k||)$ w.p. $1 - \delta$.

Compute Step

 $x^+ = x_k - \alpha_k g_k$. Check if f is sufficiently reduced an x^+ .

Successful step

If yes accept x^+ as the new iterate. Increase α_k by a constant factor if not too large.

Unsuccessful step

Otherwise decrease α_k by the constant factor. Repeat the iteration.

Random directions vs. random fully linear model gradients



Key observation for line search convergence

If m_k is κ -fully linear and ∇f is *L*-Lipschitz continuous then when α_k is small enough (i.e. $\alpha_k \leq (1-\theta)/(L/2+\kappa)$)

$$f(x^+) = f(x_k - \alpha_k g_k) \le f(x_k) - \frac{\alpha_k \theta}{\|g_k\|^2}$$

Successful step!

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Analysis of line search convergence

Assume m_k is always κ -fully linear

 $\alpha_k \ge C \; \forall k$

C is a constant depending on κ , θ , L, etc

and

if $\|\nabla f(x_k)\| \ge \epsilon$ then $\|g_k\| \ge \epsilon/2$

 $f(x_k) - f(x_{k+1}) \ge \frac{C\theta\epsilon^2}{4}$

Convergence!!

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Analysis of line search convergence

Assume m_k is above κ -fully linear w.p. $\geq 1-\delta$



and if $\|
abla f(x_k)\| \geq \epsilon$ then $\|g_k\| \geq \epsilon/2$ w.p. $\geq 1-\delta$

success

 $f(x_k) - f(x_{k+1}) \ge \frac{\alpha_k \theta \epsilon^2}{4}$ w.p. $\ge 1-\delta$ $\alpha_{k+1} = \gamma \alpha_k$

no success

 $\alpha_{k+1} = \gamma^{-1} \alpha_k$

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w.p. $\leq \delta$

Analysis via martingales

Analyze two stochastic processes: X_k and Y_k :

$$X_{k+1} = \begin{cases} \min\{C, \gamma X_k\} & \text{w.p. } 1 - \delta \\ \gamma^{-1} X_k & \text{w.p. } \delta \end{cases}$$

$$Y_{k+1} = \begin{cases} Y_k + X_k \theta \epsilon^2 / 4 & \text{w.p. } 1 - \delta \\ Y_k & \text{w.p. } \delta \end{cases}$$

We observe that

 $\alpha_k \ge X_k$ $f(x_0) - f(x_k) \ge Y_k$

If random models are independent of the past, then X_k and Y_k are random walks, otherwise they are submartingales if $\delta \le 1/2$.
Analysis via martingales

Analyze two stochastic processes: X_k and Y_k :

$$X_{k+1} = \begin{cases} \min\{C, \gamma X_k\} & \text{w.p. } 1 - \delta \\ \gamma^{-1} X_k & \text{w.p. } \delta \end{cases}$$

$$Y_{k+1} = \begin{cases} Y_k + X_k \theta \epsilon^2 / 4 & \text{w.p. } 1 - \delta \\ Y_k & \text{w.p. } \delta \end{cases}$$

We observe that

 $\alpha_k \ge X_k$ $f(x_0) - f(x_k) \ge Y_k$

 X_k does not converge to 0 w.p. 1 => algorithm converges Expectations of Y_k and X_k will facilitate convergence rates.

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Behavior of X_k for γ =2, C=1 and δ =0.45



 X_k

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k

Future work

- Convergence rates theory based on random models.
- > Extend algorithmic random model frameworks.
- > Extending to new types of models.
- > Recovering different types of function structure.
- > Efficient implementations.

Thank you!

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Analysis of line search convergence

If m_k is κ -fully linear

$$\|g_k - \nabla f(x_k)\| \le \kappa \Delta_k = \kappa \alpha_k \|g_k\|$$

If ∇f is *L*-Lipschitz continuous and $\alpha_k \leq (1-\theta)/(L/2+\kappa)$

$$f(x_k - \alpha_k * g_k) \le f(x_k) - \alpha_k \theta \|g_k\|^2$$

If $\|\nabla f(x_k)\| \ge \epsilon$ then $\|g_k\| \ge \epsilon/2$ and

$$f(x_k) - f(x_{k+1}) \ge \frac{\alpha_k \theta \epsilon^2}{4}$$

Hence only so many line search steps are needed to get a small gradient

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Analysis of line search convergence

If m_k is κ -fully linear

$$\|g_k - \nabla f(x_k)\| \le \kappa \Delta_k = \kappa \alpha_k \|g_k\|$$

If ∇f is *L*-Lipschitz continuous and $\alpha_k \leq (1-\theta)/(L/2+\kappa)$

$$f(x_k - \alpha_k * g_k) \le f(x_k) - \alpha_k \theta \|g_k\|^2$$

If $\|\nabla f(x_k)\| \ge \epsilon$ then $\|g_k\| \ge \epsilon/2$ and

$$f(x_k) - f(x_{k+1}) \ge \frac{\alpha_k \theta \epsilon^2}{4}$$

We assumed that $m_k(x)$ is κ -fully-linear every time.

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