CS-GY 9223 D: Lecture 5 Gradient Descent and Projected Gradient Descent

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PROJECT

- Choose your partner and email me by **next Wednesday**, 10/14.
- Topic and 1 page proposal due 11/04.
- · See project guidelines on course webpage for details.

RANDOMIZED ALGORITHMS RECAP

What techniques did we learn?

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prescoe geometry

NEW UNIT: CONTINUOUS OPTIMIZATION

Have some function $f: \mathbb{R}^d \to \mathbb{R}$. Want to find \mathbf{x}^* such that:

$$f(\underline{\underline{x}^*}) = \min_{\mathbf{x}} f(\mathbf{x}).$$

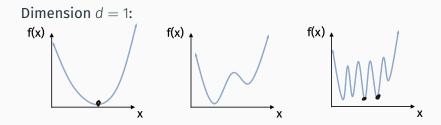
Or at least $\hat{\mathbf{x}}$ which is close to a minimum. E.g.

$$f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x}} f(\mathbf{x}) + \epsilon = f(\mathbf{x}) + \epsilon$$

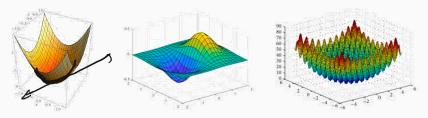
Often we have some additional constraints:

- x > 0.
- $\|\mathbf{x}\|_2 \le R$, $\|\mathbf{x}\|_1 \le R$.
- $\mathbf{a}^T \mathbf{x} > c$.

CONTINUOUS OPTIMIZATION



Dimension d = 2:



OPTIMIZATION IN MACHINE LEARNING

Continuouos optimization is the foundation of modern machine learning.

Supervised learning: Want to learn a model that maps inputs

- numerical data vectors
- · images, video
- text documents

to predictions

- numerical value (probability stock price increases)
- · label (is the image a cat? does the image contain a car?)
- decision (turn car left, rotate robotic arm)

MACHINE LEARNING MODEL

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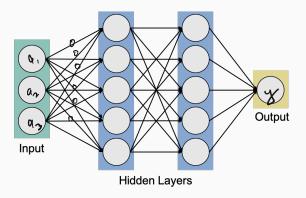
Let $\underline{M}_{\mathbf{x}}$ be a model with parameters $\mathbf{x} = \{x_1, \dots, x_k\}$, which takes as input a data vector \mathbf{a} and outputs a prediction.

Example:

$$M_{\mathbf{x}}(\mathbf{a}) = \text{sign}(\mathbf{\underline{a}}^{\mathsf{T}}\mathbf{\underline{x}})$$

MACHINE LEARNING MODEL

Example:



 $\mathbf{x} \in \mathbb{R}^{(\text{\# of connections})}$ is the parameter vector containing all the network weights.

SUPERVISED LEARNING

Classic approach in <u>supervised learning</u>: Find a model that works well on data that you already have the answer for (labels, values, classes, etc.).

- Model M_x parameterized by a vector of numbers x.
- Dataset $\underline{\mathbf{a}^{(1)}}, \dots, \underline{\mathbf{a}^{(n)}}$ with outputs $\underline{y^{(1)}}, \dots, \underline{y^{(n)}}$.

Want to find $\hat{\mathbf{x}}$ so that $\underline{\underline{\mathcal{M}}_{\hat{\mathbf{x}}}}(\mathbf{a}^{(i)}) \approx y^{(i)}$ for $i \in 1, \dots, n$.

How do we turn this into a function minimization problem?

LOSS FUNCTION

Loss function $L(M_x(a)y)$: Some measure of distance between prediction $M_x(a)$ and target output y. Increases if they are further apart.

- Squared (ℓ_2) loss: $|\underline{M}_{\mathbf{x}}(\mathbf{a}) \underline{y}|^2$
- Absolute deviation (ℓ_1) loss: $|M_x(a) y|$
- Hinge loss: $1 y \cdot M_x(a)$
- Cross-entropy loss (log loss).
- · Etc.

EMPIRICAL RISK MINIMIZATION

Empirical risk minimization:

$$\underline{f(\mathbf{x})} = \sum_{i=1}^{n} L\left(M_{\mathbf{x}}(\mathbf{a}^{(i)}), y^{(i)}\right)$$

Solve the optimization problem $\min_{\mathbf{x}} f(\mathbf{x})$.

EXAMPLE: LINEAR REGRESSION

- $M_{x}(a) = x^{T}a$. x contains the regression coefficients.
- $\cdot L(\underline{z},\underline{y}) = |z-y|^2.$

•
$$f(\mathbf{x}) = \sum_{i=1}^{n} |\mathbf{x}^{T} \mathbf{a}^{(i)} - y^{(i)}|^{2}$$

$$f(x) = ||Ax - y||_2^2$$

where **A** is a matrix with $\mathbf{a}^{(i)}$ as its i^{th} row and \mathbf{y} is a vector with $y^{(i)}$ as its i^{th} entry.

ALGORITHMS FOR CONTINUOUS OPTIMIZATION

The choice of algorithm to minimize f(x) will depend on:

- The form of f(x) (is it linear, is it quadratic, does it have finite sum structure, etc.)
- If there are any additional constraints imposed on ${\bf x}$. E.g.

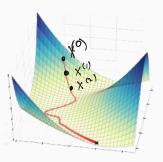
 $||x||_2 \le c$. Mowether Acceleded Gradient Descent What are some example algorithms for continuous optimization?

Optimization? Restor Programing.

Gradient Descent Coadinate Descent

GRADIENT DESCENT

Gradient descent: A greedy algorithm for minimizing functions of multiple variables that often works amazingly well.



CALCULUS REVIEW

For $i = 1, ..., \underline{d}$, let x_i be the i^{th} entry of x. Let $e^{(i)}$ be the i^{th} standard basis vector. $[0 \circ \circ \circ 1 \circ \circ 7] = e^{(i)}$

Partial derivative:

$$\underbrace{\frac{\partial f}{\partial x_i}}(x) = \lim_{t \to 0} \frac{f(x + te^{(i)}) - f(x)}{t}$$

Directional derivative:

$$D_{\mathbf{y}}f(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{v}) - f(\mathbf{x})}{t}$$

CALCULUS REVIEW

Gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \frac{\partial f}{\partial x_2}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix}$$

Directional derivative:

$$D_{\underline{v}f(\underline{x})} = \lim_{t \to 0} \frac{f(\underline{x} + \underline{v}) - f(\underline{x})}{t} = \nabla f(\underline{x})^{\mathsf{T}} \underline{v}.$$

$$\nabla f(\underline{x}) \cdot \underline{v}$$

$$\langle \nabla f(\underline{x}), \underline{v} \rangle$$

FIRST ORDER OPTIMIZATION

Given a function *f* to minimize, assume we have:

- Function oracle: Evaluate f(x) for any x.
- Gradient oracle: Evaluate $\nabla f(\mathbf{x})$ for any \mathbf{x} .

We view the implementation of these oracles as black-boxes, but they can often require a fair bit of computation.

EXAMPLE GRADIENT EVALUATION

Linear least-squares regression:

- Given $\mathbf{a}^{(1)}, \dots \mathbf{a}^{(n)} \in \mathbb{R}^d, v^{(1)}, \dots v^{(n)} \in \mathbb{R}$.
- · Want to minimize:

minimize:
$$f(\mathbf{x}) = \sum_{i=1}^{n} \left(\mathbf{x}^{\mathsf{T}} \mathbf{a}^{(i)} - \mathbf{y}^{(i)} \right)^{2} = \underbrace{\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{2}^{2}}_{2}.$$
time

$$\frac{\partial f}{\partial x_j} = \sum_{i=1}^{n} 2\left(\mathbf{x}^{\mathsf{T}} \mathbf{a}^{(i)} - \mathbf{y}^{(i)}\right) \cdot a_j^{(i)} = (2\mathbf{A}\mathbf{x} - \mathbf{y})^{\mathsf{T}} \alpha^{(j)}$$

$$(\mathbf{w}_{\mathsf{X}} \mathbf{d}) \mathcal{U}_{\mathsf{X}} \mathbf{J} \longrightarrow \mathbf{w}_{\mathsf{X}} \mathbf{v}$$

where $\alpha^{(j)}$ is the i^{th} column of A.

$$\nabla f(\mathbf{x}) = 2\mathbf{A}^{\mathsf{T}} \mathbf{A} \mathbf{x} - \mathbf{y}$$

What is the time complexity of a gradient oracle for $\nabla f(\mathbf{x})$?





(dxy) (x1) = (dx1)

DECENT METHODS

Greedy approach: Given a starting point \mathbf{x} , make a small adjustment that decreases $f(\mathbf{x})$. Treparticular, $\mathbf{x} \leftarrow \mathbf{x} + \underline{\eta} \mathbf{v}$ and $f(\mathbf{x} + \eta \mathbf{v})$. $f(\mathbf{x} + \eta \mathbf{v}) < f(\mathbf{x})$

What property do I want in v?

Leading question: When η is small, what's an approximation for $f(\mathbf{x} + \mathbf{y}) - f(\mathbf{x})$?

$$f(\underline{x + \eta v) - f(x)} \approx n D_v f(x)$$

$$= N \cdot (v^{\top} \nabla f(x))$$

DIRECTIONAL DERIVATIVES

$$D_{\mathbf{v}}f(\mathbf{x}) = \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{v}) - f(\mathbf{x})}{t} = \nabla f(\mathbf{x})^{\mathsf{T}}\mathbf{v}.$$

So:

$$f(x + \eta v) - f(x) \approx M(v^{\tau} \nabla f(x))$$

How should we choose v so that $\underline{f(x + \eta v)} < f(x)$?

$$A = -A f(x) \qquad A_{\downarrow} A f(x) = -A f(x) |_{\gamma}$$

GRADIENT DESCENT

Prototype algorithm:

For
$$i = 0, ..., T$$

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$$

• Return $\mathbf{x}^{(7)}$

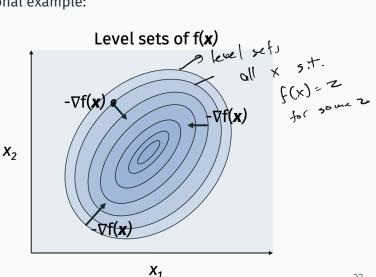
 η is a step-size parameter, which is often adapted on the go. For now, assume it is fixed ahead of time.

GRADIENT DESCENT INTUITION

7 f(x (0)) 1 dimensional example:

GRADIENT DESCENT INTUITION

2 dimensional example:



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KEY RESULTS

For a convex function $f(\mathbf{x})$: For sufficiently small η and a sufficiently large number of iterations T, gradient descent will converge to a near global minimum:

$$f(\mathbf{x}^{(T)}) \leq f(\mathbf{x}^*) + \epsilon.$$

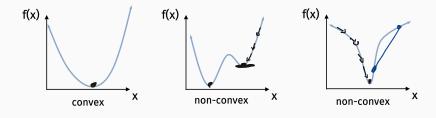
Examples: least squares regression, logistic regression, kernel regression, SVMs.

For a non-convex function f(x): For sufficiently small η and a sufficiently large number of iterations T, gradient descent will converge to a near stationary point:

$$\|\nabla f(\mathbf{x}^{(T)})\|_2 \leq e$$
.

Examples: neural networks, matrix completion problems, mixture models.

CONVEX VS. NON-CONVEX



One issue with non-convex functions is that they can have local minima. Even when they don't, convergence analysis requires different assumptions than convex functions.

APPROACH FOR THIS UNIT

We care about <u>how fast</u> gradient descent and related methods converge, not just that they do converge.

- Bounding iteration complexity requires placing some assumptions on $f(\mathbf{x})$.
- Stronger assumptions lead to better bounds on the convergence.

Understanding these assumptions can help us design faster variants of gradient descent (there are many!).

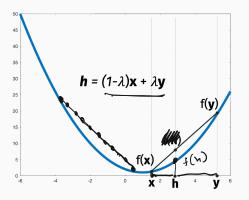
Today, we will start with **convex functions** only.

CONVEXITY

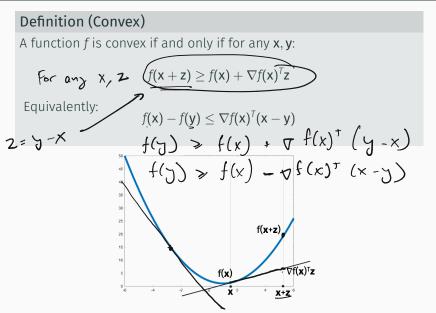
Definition (Convex)

A function f is convex iff for any $\mathbf{x}, \mathbf{y}, \lambda \in [0, 1]$:

$$(1 - \lambda) \cdot f(\mathbf{x}) + \lambda \cdot f(\mathbf{y}) \ge f((\underline{1 - \lambda}) \cdot \underline{\mathbf{x}} + \underline{\lambda} \cdot \underline{\mathbf{y}})$$



GRADIENT DESCENT



Assume:

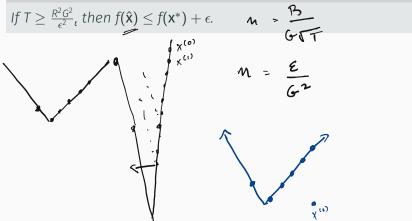
- f is convex.
- Lipschitz function: for all x, $\|\nabla f(x)\|_2 \leq G$.
- Starting radius: $\|\underline{\mathbf{x}^* \mathbf{x}^{(0)}}\|_2$

Gradient descent:

- · Choose number of steps <u>T.</u>
- $\eta = \frac{R}{G\sqrt{T}}$
- For i = 0, ..., T:
 - $\cdot \mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} \eta \nabla f(\mathbf{x}^{(i)})$
- Return $\hat{\mathbf{x}} = \arg\min_{i} f(\mathbf{x}^{(i)})$.



Claim (GD Convergence Bound)



Proof is made tricky by the fact that $f(\mathbf{x}^{(i)})$ does not improve monotonically. We can "overshoot" the minimum.

Claim (GD Convergence Bound)

If
$$T \ge \frac{R^2G^2}{\epsilon^2}$$
 and $\eta = \frac{R}{G\sqrt{T}}$, then $f(\hat{\mathbf{x}}) \le f(\mathbf{x}^*) + \epsilon$.

Claim 1: For all $i = 0, \dots, T$,

 $\mathbf{Z} = \mathbf{x}^{(i)} - \mathbf{M} \ \forall \ \mathcal{Y} (\mathbf{x}^{(i)})$

Claim 1: For all
$$i = 0, \ldots, T$$
,

$$\int_{\Gamma} f(x^{(i)}) - f(x^{*}) \leq \frac{\|x^{(i)} - x^{*}\|_{2}^{2} - \|x^{(i+1)} - x^{*}\|_{2}^{2}}{2\eta} + \frac{\eta G^{2}}{2}$$

$$\|x^{(i+1)} - x^{*}\|_{2}^{2} - \|x^{(i)} - m\nabla f(x^{(i)}) - x^{*}\|_{2}^{2}$$

$$= \|x^{(i)} - x^{*}\|_{2}^{2} + \|m\nabla f(x^{(i)})\|_{2}^{2} - 2m \nabla f(x^{(i)})^{\dagger}(x^{(i)} - x^{*})$$

$$\nabla f(x^{(i)})^{\dagger}(x^{(i)} - x^{*}) \leq \|x^{(i)} - x^{*}\|_{2}^{2} - \|x^{(i+1)} - x^{*}\|_{2}^{2} + mC^{2}$$

$$f(x^{(i)}) - f(x^{*}) \leq \nabla f(x^{(i)})^{\dagger}(x^{(i)} - x^{*})$$

Claim (GD Convergence Bound)

If
$$T = \underbrace{\frac{R^2G^2}{\epsilon^2}}$$
 and $\eta = \frac{R}{G\sqrt{T}} \not \in \frac{\epsilon}{G^2}$, then $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

Claim 1: For all $i = 0, \ldots, T$,

$$f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \le \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(i+1)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2\eta}$$
Telescoping sum:
$$\sum_{i=0}^{T-1} \left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right] \le \frac{\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{T\eta G^2}{2}$$

$$\frac{1}{T} \sum_{i=0}^{T-1} \left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right] \le \frac{R^2}{2T\eta} + \frac{\eta G^2}{2} = \frac{RG}{T}$$

$$\frac{R^2}{2T} = \frac{RG}{T}$$

Claim (GD Convergence Bound)

If
$$T \ge \frac{R^2G^2}{\epsilon^2}$$
 and $\eta = \frac{R}{G\sqrt{T}} = \frac{\epsilon}{G^2}$, then $f(\hat{\mathbf{x}}) \le f(\mathbf{x}^*) + \epsilon$.

Final step:

$$\int_{T} \int_{T=0}^{T-1} \left[f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right] \leq \epsilon$$

$$\left[\frac{1}{T} \sum_{i=0}^{T-1} f(\mathbf{x}^{(i)}) \right] - \underbrace{f(\mathbf{x}^*)}_{T} \leq \epsilon$$

We always have that $\min_{i} f(\mathbf{x}^{(i)}) \leq \frac{1}{i} \sum_{i=0}^{T-1} f(\mathbf{x}^{(i)})$, so this is what we return:

$$f(\hat{\mathbf{x}}) = \min_{i \in 1, \dots, T} f(\mathbf{x}^{(i)}) \leq f(\mathbf{x}^*) + \epsilon.$$

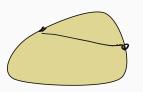
$$\frac{1}{T} \sum_{i=0}^{T-1} f(\mathbf{x}^{(i)}) \Rightarrow \frac{1}{T} \sum_{i=0}^{T-1} f(\mathbf{x}^{(i)}) = f(\hat{\mathbf{x}})$$

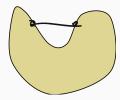
CONSTRAINED CONVEX OPTIMIZATION

Typical goal: Solve a <u>convex minimization problem</u> with additional convex constraints.

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x})$$

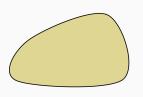
where S is a convex set.





Which of these is convex?

CONSTRAINED CONVEX OPTIMIZATION





Definition (Convex set)

A set S is convex if for any $\mathbf{x}, \mathbf{y} \in S, \lambda \in [0, 1]$:

$$(1-\lambda)x + \lambda y \in S.$$

PROBLEM WITH GRADIENT DESCENT

Gradient descent:

- For i = 0, ..., T: • $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$
- Return $\hat{\mathbf{x}} = \arg\min_{i} f(\mathbf{x}^{(i)})$.



Even if we start with $\mathbf{x}^{(0)} \in \mathcal{S}$, there is no guarantee that $\mathbf{x}^{(0)} - \eta \nabla f(\mathbf{x}^{(0)})$ will remain in our set.

Extremely simple modification: Force $\mathbf{x}^{(i)}$ to be in \mathcal{S} by projecting onto the set.

CONSTRAINED FIRST ORDER OPTIMIZATION

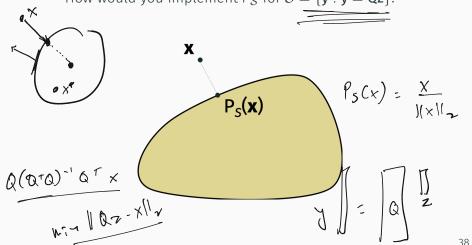
Given a function f to minimize and a convex constraint set S, assume we have:

- Function oracle: Evaluate f(x) for any x.
- Gradient oracle: Evaluate $\nabla f(\mathbf{x})$ for any \mathbf{x} .
- Projection oracle: Evaluate $P_{\mathcal{S}}(\mathbf{x})$ for any \mathbf{x} .

$$P_{\mathcal{S}}(\mathbf{x}) = \underset{\mathbf{y} \in \mathcal{S}}{\operatorname{arg min}} \|\underline{\mathbf{x} - \mathbf{y}}\|_{2}$$

PROJECTION ORACLES

- How would you implement $P_{\mathcal{S}}$ for $\mathcal{S} = \{\mathbf{y} : \|\mathbf{y}\|_2 \le 1\}$.
- How would you implement P_S for $S = \{y : y = Qz\}$.



PROJECTED GRADIENT DESCENT

Given function $f(\mathbf{x})$ and set \mathcal{S} , such that $\|\nabla f(\mathbf{x})\|_2 \leq G$ for all $\mathbf{x} \in \mathcal{S}$ and starting point $\mathbf{x}^{(0)}$ with $\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2 \leq R$.

Projected gradient descent:

• Select starting point $\mathbf{x}^{(0)}$, $\eta = \frac{R}{G\sqrt{T}}$.

• For
$$i = 0$$
, \overline{I} :
• $z = x^{(i)} - \eta \nabla f(x^{(i)})$
• $x^{(i+1)} = P_{\mathcal{S}}(z)$

• Return $\hat{\mathbf{x}} = \operatorname{arg\,min}_i f(\mathbf{x}^{(i)})$.

Claim (PGD Convergence Bound)

If
$$f, S$$
 are convex and $T \ge \frac{R^2 G^2}{\epsilon_-^2}$, then $f(\hat{\mathbf{x}}) \le \underline{f(\mathbf{x}^*) + \epsilon}$.

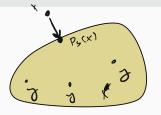
PROJECTED GRADIENT DESCENT ANALYSIS

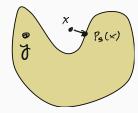
Analysis is almost identical to standard gradient descent! We just need one additional claim:

Claim (Contraction Property of Convex Projection)

If S is convex, then for $\underline{any} \ \mathbf{y} \in S$,

$$\|y - P_{\mathcal{S}}(x)\|_2 \leq \|y - x\|_2.$$





Claim (PGD Convergence Bound)

If
$$f, S$$
 are convex and $T \ge \frac{R^2G^2}{\epsilon^2}$, then $f(\hat{\mathbf{x}}) \le f(\mathbf{x}^*) + \epsilon$.

Claim 1: For all
$$i = 0, ..., T$$
,
$$\underbrace{f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*)}_{\mathbf{x}^{(i)}} \leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - (\mathbf{z}^2 - \mathbf{x}^*\|_2^2)}{2\eta} + \frac{\eta G^2}{2}$$

$$\leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(i+1)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$

Same telescoping sum argument:

$$m \in \{(x^{(i)}) : \{(x^{(i)}) : \{(x^{(i)}) : (x^{(i)}) \} \} = \frac{1}{T} \sum_{i=0}^{T-1} f(x^{(i)}) \} = f(x^*) \le \frac{R^2}{2T\eta} + \frac{\eta G^2}{2}. \le \epsilon$$