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Lecture 3: Huge-scale optimization problems

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Nonlinear Optimization: problems sizes

Class	Operations	Dimension	Iter.Cost	Memory	
Small-size	All	$10^{0} - 10^{2}$	$n^4 ightarrow n^3$	Kilobyte:	10 ³
Medium-size	A^{-1}	$10^{3} - 10^{4}$	$n^3 ightarrow n^2$	Megabyte:	10 ⁶
Large-scale	Ax	$10^{5} - 10^{7}$	$n^2 ightarrow n$	Gigabyte:	10 ⁹
Huge-scale	x + y	$10^8 - 10^{12}$	$n \rightarrow \log n$	Terabyte:	10 ¹²

Sources of Huge-Scale problems

- Internet (New)
- Telecommunications (New)
- Finite-element schemes (Old)
- Partial differential equations (Old)

Very old optimization idea: Coordinate Search

Problem: $\min_{x \in \mathbb{R}^n} f(x)$ (*f* is convex and differentiable).

Coordinate relaxation algorithm

For $k \ge 0$ iterate

• Choose active coordinate i_k .

 Q Update x_{k+1} = x_k − h_k∇_{ik} f(x_k)e_{ik} ensuring f(x_{k+1}) ≤ f(x_k). (e_i is *i*th coordinate vector in Rⁿ.)

Main advantage: Very simple implementation.

Possible strategies

- Ocyclic moves. (Difficult to analyze.)
- Random choice of coordinate (Why?)
- Oboose coordinate with the maximal directional derivative.

Complexity estimate: assume

$$\|
abla f(x) -
abla f(y)\| \le L \|x - y\|, \quad x, y \in R^n.$$

Let us choose $h_k = rac{1}{L}$. Then

$$egin{array}{rll} f(x_k)-f(x_{k+1})&\geq&rac{1}{2L}|
abla_{i_k}f(x_k)|^2&\geq&rac{1}{2nL}\|
abla f(x_k)\|^2\ &\geq&rac{1}{2nLR^2}(f(x_k)-f^*)^2. \end{array}$$

Hence, $f(x_k) - f^* \leq \frac{2nLR^2}{k}$, $k \geq 1$. (For Grad.Method, drop *n*.) This is the only known theoretical result known for CDM!

Criticism

Theoretical justification:

- Complexity bounds are not known for the most of the schemes.
- The only justified scheme needs computation of the <u>whole gradient</u>. (Why don't use GM?)

Computational complexity:

- <u>Fast differentiation</u>: if function is defined by a sequence of operations, then $C(\nabla f) \leq 4C(f)$.
- Can we do anything without computing the function's values?

Result: CDM are almost out of the computational practice.

Google problem

Let $E \in R^{n imes n}$ be an incidence matrix of a graph. Denote $e = (1, \dots, 1)^T$ and

$$\bar{E} = E \cdot \operatorname{diag} (E^T e)^{-1}.$$

Thus, $\bar{E}^T e = e$. Our problem is as follows:

Find
$$x^* \ge 0$$
: $\overline{E}x^* = x^*$.

Optimization formulation:

$$f(x) \stackrel{\text{def}}{=} \frac{1}{2} \|\bar{E}x - x\|^2 + \frac{\gamma}{2} [\langle e, x \rangle - 1]^2 \rightarrow \min_{x \in \mathbb{R}^n}$$

Huge-scale problems

Main features

- The size is very big $(n \ge 10^7)$.
- The data is distributed in space.
- The requested parts of data are not always available.
- The data is changing in <u>time</u>.

Consequences

Simplest operations are expensive or infeasible:

- Update of the full vector of variables.
- Matrix-vector multiplication.
- Computation of the objective function's value, etc.

Structure of the Google Problem

Let ua look at the gradient of the objective:

$$abla_i f(x) = \langle a_i, g(x) \rangle + \gamma[\langle e, x \rangle - 1], \ i = 1, \dots, n,$$

$$g(x) = \overline{E}x - x \in \mathbb{R}^n, \quad (\overline{E} = (a_1, \ldots, a_n)).$$

Main observations:

- The coordinate move x₊ = x − h_i∇_if(x)e_i needs O(p_i) a.o. (p_i is the number of nonzero elements in a_i.)
- $d_i \stackrel{\text{def}}{=} \operatorname{diag} \left(\nabla^2 f \stackrel{\text{def}}{=} \bar{E}^T \bar{E} + \gamma e e^T \right)_i = \gamma + \frac{1}{p_i}$ are available. We can use them for choosing the step sizes $(h_i = \frac{1}{d_i})$.

Reasonable coordinate choice strategy? <u>Random!</u>

Random coordinate descent methods (RCDM)

$$\min_{x \in R^N} f(x), \quad (f \text{ is convex and differentiable})$$

Main Assumption:

$$|f_i'(x+h_ie_i)-f_i'(x)|\leq L_i|h_i|,\quad h_i\in R,\ i=1,\ldots,N,$$
 where e_i is a coordinate vector. Then

$$f(x + h_i e_i) \leq f(x) + f'_i(x)h_i + \frac{L_i}{2}h_i^2$$
. $x \in R^N, h_i \in R$.

Define the coordinate steps: $T_i(x) \stackrel{\text{def}}{=} x - \frac{1}{L_i} f'_i(x) e_i$. Then,

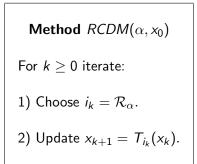
$$f(x) - f(T_i(x)) \geq \frac{1}{2L_i} [f'_i(x)]^2, \quad i = 1, \dots, N.$$

Random coordinate choice

We need a special random counter \mathcal{R}_{α} , $\alpha \in R$:

Prob
$$[i] = p_{\alpha}^{(i)} = L_i^{\alpha} \cdot \left[\sum_{j=1}^N L_j^{\alpha}\right]^{-1}, \quad i = 1, \dots, N.$$

Note: \mathcal{R}_0 generates uniform distribution.



Complexity bounds for RCDM

We need to introduce the following norms for $x, g \in R^N$:

$$\|x\|_{\alpha} = \left[\sum_{i=1}^{N} L_{i}^{\alpha} [x^{(i)}]^{2}\right]^{1/2}, \quad \|g\|_{\alpha}^{*} = \left[\sum_{i=1}^{N} \frac{1}{L_{i}^{\alpha}} [g^{(i)}]^{2}\right]^{1/2}$$

After k iterations, $RCDM(\alpha, x_0)$ generates random output x_k , which depends on $\xi_k = \{i_0, \ldots, i_k\}$. Denote $\phi_k = E_{\xi_{k-1}}f(x_k)$.

Theorem. For any
$$k \ge 1$$
 we have

$$\phi_k - f^* \le \frac{2}{k} \cdot \left[\sum_{j=1}^N L_j^\alpha\right] \cdot R_{1-\alpha}^2(x_0),$$
where $R_\beta(x_0) = \max_x \left\{ \max_{x_* \in X^*} \|x - x_*\|_\beta : f(x) \le f(x_0) \right\}.$

Interpretation

1. $\alpha = 0$. Then $S_0 = N$, and we get

$$\phi_k - f^* \leq \frac{2N}{k} \cdot R_1^2(x_0).$$

Note

• We use the metric
$$||x||_1^2 = \sum_{i=1}^N L_i[x^{(i)}]^2$$
.

- A matrix with diagonal $\{L_i\}_{i=1}^N$ can have its norm equal to n.
- Hence, for GM we can guarantee the same bound. But its cost of iteration is much higher!

Interpretation

2. $\alpha = \frac{1}{2}$. Denote

$$D_{\infty}(x_0) = \max_{x} \left\{ \max_{y \in X^*} \max_{1 \le i \le N} |x^{(i)} - y^{(i)}| : f(x) \le f(x_0) \right\}.$$

Then, $R^2_{1/2}(x_0) \leq S_{1/2}D^2_\infty(x_0),$ and we obtain

$$\phi_k - f^* \leq \frac{2}{k} \cdot \left[\sum_{i=1}^N L_i^{1/2}\right]^2 \cdot D_\infty^2(x_0).$$

Note:

- For the first order methods, the worst-case complexity of minimizing over a box depends on *N*.
- Since $S_{1/2}$ can be bounded, RCDM can be applied in situations when the usual GM fail.

Interpretation

3. $\alpha = 1$. Then $R_0(x_0)$ is the size of the initial level set in the standard Euclidean norm. Hence,

$$\phi_k - f^* \leq \frac{2}{k} \cdot \left[\sum_{i=1}^N L_i\right] \cdot R_0^2(x_0) \equiv \frac{2N}{k} \cdot \left[\frac{1}{N}\sum_{i=1}^N L_i\right] \cdot R_0^2(x_0).$$

Rate of convergence of GM can be estimated as

$$f(x_k)-f^*\leq \frac{\gamma}{k}R_0^2(x_0),$$

where γ satisfies condition $f''(x) \preceq \gamma \cdot I$, $x \in R^N$.

Note: maximal eigenvalue of symmetric matrix can reach its trace.

In the worst case, the rate of convergence of GM is the same as that of RCDM.

Minimizing the strongly convex functions

Theorem. Let f(x) be strongly convex with respect to $\|\cdot\|_{1-\alpha}$ with convexity parameter $\sigma_{1-\alpha} > 0$.

Then, for $\{x_k\}$ generated by $RCDM(\alpha, x_0)$ we have

$$\phi_k - \phi^* \leq \left(1 - \frac{\sigma_{1-\alpha}}{S_{\alpha}}\right)^k (f(x_0) - f^*).$$

Proof: Let x_k be generated by *RCDM* after *k* iterations. Let us estimate the expected result of the next iteration.

$$f(x_k) - E_{i_k}(f(x_{k+1})) = \sum_{i=1}^{N} p_{\alpha}^{(i)} \cdot [f(x_k) - f(T_i(x_k))]$$

$$\geq \sum_{\substack{i=1\\ 2L_i}}^{N} \frac{p_{\alpha}^{(i)}}{2L_i} [f'_i(x_k)]^2 = \frac{1}{2S_{\alpha}} (\|f'(x_k)\|_{1-\alpha}^*)^2$$

$$\geq \frac{\sigma_{1-\alpha}}{S_{\alpha}} (f(x_k) - f^*).$$

It remains to compute expectation in ξ_{k-1} .

Confidence level of the answers

Note: We have proved that the expected values of random $f(x_k)$ are good.

Can we guarantee anything after a single run?

Confidence level: Probability $\beta \in (0, 1)$, that some statement about random output is correct.

Main tool: Chebyschev inequality $(\xi \ge 0)$:

Prob
$$[\xi \geq T] \leq \frac{E(\xi)}{T}$$
.

Our situation:

$$\operatorname{Prob}\left[f(x_k) - f^* \ge \epsilon\right] \le \frac{1}{\epsilon} [\phi_k - f^*] \le 1 - \beta.$$

We need $\phi_k - f^* \le \epsilon \cdot (1 - \beta)$. Too expensive for $\beta \to 1$?

Regularization technique

Consider $f_{\mu}(x) = f(x) + \frac{\mu}{2} ||x - x_0||_{1-\alpha}^2$. It is strongly convex. Therefore, we can obtain $\phi_k - f_{\mu}^* \le \epsilon \cdot (1-\beta)$ in

$$O\left(\frac{1}{\mu}S_{\alpha}\ln\frac{1}{\epsilon\cdot(1-\beta)}
ight)$$
 iterations.

Theorem. Define $\alpha = 1$, $\mu = \frac{\epsilon}{4R_0^2(x_0)}$, and choose

$$k \geq 1 + \frac{8S_1R_0^2(x_0)}{\epsilon} \left[\ln \frac{2S_1R_0^2(x_0)}{\epsilon} + \ln \frac{1}{1-\beta} \right].$$

Let x_k be generated by $RCDM(1, x_0)$ as applied to f_{μ} . Then

$$\operatorname{Prob}(f(x_k) - f^* \leq \epsilon) \geq \beta.$$

Note: $\beta = 1 - 10^{-p} \Rightarrow \ln 10^p = 2.3p.$

Implementation details: Random Counter

Given the values L_i , i = 1, ..., N, generate efficiently random $i \in \{1, ..., N\}$ with probabilities **Prob** $[i = k] = L_k / \sum_{j=1}^N L_j$. **Solution:** a) Trivial $\Rightarrow O(N)$ operations. b). Assume $N = 2^p$. Define p + 1 vectors $S_k \in R^{2^{p-k}}$, k = 0, ..., p: $S_0^{(i)} = L_i$, i = 1, ..., N. $S_k^{(i)} = S_{k-1}^{(2i)} + S_{k-1}^{(2i-1)}$, $i = 1, ..., 2^{p-k}$, k = 1, ..., p.

Algorithm: Make the choice in *p* steps, from top to bottom.

• If the element *i* of S_k is chosen, then choose in S_{k-1} either 2*i* or 2i - 1 in accordance to probabilities $\frac{S_{k-1}^{(2i)}}{S_k^{(i)}}$ or $\frac{S_{k-1}^{(2i-1)}}{S_k^{(i)}}$. **Difference:** for $n = 2^{20} > 10^6$ we have $p = \log_2 N = 20$.

Sparse problems

Problem: $\min_{x \in Q} f(x)$, where Q is closed and convex in \mathbb{R}^N , and • $f(x) = \Psi(Ax)$, where Ψ is a simple convex function: $\Psi(y_1) \ge \Psi(y_2) + \langle \Psi'(y_2), y_1 - y_2 \rangle$, $y_1, y_2 \in \mathbb{R}^M$, • $A : \mathbb{R}^N \to \mathbb{R}^M$ is a sparse matrix. Let $p(x) \stackrel{\text{def}}{=} \#$ of nonzeros in x. Sparsity coefficient: $\gamma(A) \stackrel{\text{def}}{=} \frac{p(A)}{MN}$. Example 1: Matrix-vector multiplication

- Computation of vector Ax needs p(A) operations.
- Initial complexity MN is reduced in $\gamma(A)$ times.

Gradient Method

$$x_0 \in Q, \quad x_{k+1} = \pi_Q(x_k - hf'(x_k)), \quad k \geq 0.$$

Main computational expenses

- Projection of simple set Q needs O(N) operations.
- Displacement $x_k \rightarrow x_k hf'(x_k)$ needs O(N) operations.
- $f'(x) = A^T \Psi'(Ax)$. If Ψ is simple, then the main efforts are spent for two matrix-vector multiplications: 2p(A).

Conclusion: As compared with *full* matrices, we accelerate in $\gamma(A)$ times.

Note: For Large- and Huge-scale problems, we often have $\gamma(A) \approx 10^{-4} \dots 10^{-6}$. **Can we get more?**

Sparse updating strategy

Main idea

- After update $x_+ = x + d$ we have $y_+ \stackrel{\text{def}}{=} Ax_+ = Ax + Ad$.
- What happens if *d* is *sparse*?

Denote
$$\sigma(d) = \{j : d^{(j)} \neq 0\}$$
. Then $y_+ = y + \sum_{j \in \sigma(d)} d^{(j)} \cdot Ae_j$.

Its complexity, $\kappa_A(d) \stackrel{\text{def}}{=} \sum_{j \in \sigma(d)} p(Ae_j)$, can be VERY small! $\kappa_A(d) = M \sum_{j \in \sigma(d)} \gamma(Ae_j) = \gamma(d) \cdot \frac{1}{p(d)} \sum_{j \in \sigma(d)} \gamma(Ae_j) \cdot MN$ $\leq \gamma(d) \max_{1 \leq j \leq m} \gamma(Ae_j) \cdot MN.$

If $\gamma(d) \leq c\gamma(A)$, $\gamma(A_j) \leq c\gamma(A)$, then $\left\lfloor \kappa_A(d) \leq c^2 \cdot \gamma^2(A) \cdot MN \right\rfloor$. Expected acceleration: $(10^{-6})^2 = 10^{-12} \Rightarrow 1 \sec \approx 32\,000$ years

When it can work?

- Simple methods: No full-vector operations! (Is it possible?)
- Simple problems: Functions with *sparse* gradients.

Examples

Quadratic function $f(x) = \frac{1}{2} \langle Ax, x \rangle - \langle b, x \rangle$. The gradient $f'(x) = Ax - b, \quad x \in \mathbb{R}^N$,

is *not* sparse even if A is sparse.

Piece-wise linear function g(x) = max [⟨a_i, x⟩ - b⁽ⁱ⁾]. Its subgradient f'(x) = a_{i(x)}, i(x) : f(x) = ⟨a_{i(x)}, x⟩ - b^{(i(x))}, can be sparse if a_i is sparse!

But: We need a fast procedure for updating max-operations.

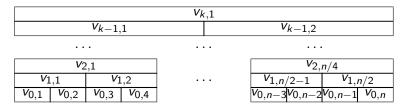
Fast updates in short computational trees

Def: Function f(x), $x \in \mathbb{R}^n$, is *short-tree representable*, if it can be computed by a short binary tree with the height $\approx \ln n$.

Let $n = 2^k$ and the tree has k + 1 levels: $v_{0,i} = x^{(i)}$, i = 1, ..., n. Size of the next level halves the size of the previous one:

$$v_{i+1,j} = \psi_{i+1,j}(v_{i,2j-1}, v_{i,2j}), \quad j = 1, \dots, 2^{k-i-1}, \ i = 0, \dots, k-1,$$

where $\psi_{i,j}$ are some bivariate functions.



Main advantages

• Important examples (symmetric functions)

$$\begin{split} f(x) &= \|x\|_p, \quad p \ge 1, \quad \psi_{i,j}(t_1, t_2) \equiv \left[|t_1|^p + |t_2|^p \right]^{1/p}, \\ f(x) &= \ln\left(\sum_{i=1}^n e^{x^{(i)}}\right), \quad \psi_{i,j}(t_1, t_2) \equiv \ln\left(e^{t_1} + e^{t_2}\right), \\ f(x) &= \max_{1 \le i \le n} x^{(i)}, \qquad \psi_{i,j}(t_1, t_2) \equiv \max\left\{t_1, t_2\right\}. \end{split}$$

- The binary tree requires only n-1 auxiliary cells.
- Its value needs n-1 applications of $\psi_{i,j}(\cdot, \cdot)$ (\equiv operations).
- If x₊ differs from x in one entry only, then for re-computing f(x₊) we need only k ≡ log₂ n operations.

Thus, we can have pure subgradient minimization schemes with Sublinear Iteration Cost

Simple subgradient methods

- I. Problem: $f^* \stackrel{\text{def}}{=} \min_{x \in Q} f(x)$, where
 - Q is a closed and convex and $||f'(x)|| \le L(f)$, $x \in Q$,
 - the optimal value f^* is known.

Consider the following optimization scheme (B.Polyak, 1967):

$$x_0 \in Q, \quad x_{k+1} \; = \; \pi_Q \left(x_k - rac{f(x_k) - f^*}{\|f'(x_k)\|^2} f'(x_k)
ight), \quad k \geq 0.$$

Denote $f_k^* = \min_{0 \le i \le k} f(x_i)$. Then for any $k \ge 0$ we have:

$$f_k^* - f^* \leq \frac{L(f) \|x_0 - \pi_{X_*}(x_0)\|}{(k+1)^{1/2}},$$

$$||x_k - x^*|| \le ||x_0 - x^*||, \quad \forall x^* \in X_*.$$

Proof:

Let us fix $x^* \in X_*$. Denote $r_k(x^*) = ||x_k - x^*||$. Then

$$\begin{aligned} r_{k+1}^2(x^*) &\leq \left\| x_k - \frac{f(x_k) - f^*}{\|f'(x_k)\|^2} f'(x_k) - x^* \right\|^2 \\ &= r_k^2(x^*) - 2 \frac{f(x_k) - f^*}{\|f'(x_k)\|^2} \langle f'(x_k), x_k - x^* \rangle + \frac{(f(x_k) - f^*)^2}{\|f'(x_k)\|^2} \\ &\leq r_k^2(x^*) - \frac{(f(x_k) - f^*)^2}{\|f'(x_k)\|^2} \leq r_k^2(x^*) - \frac{(f_k^* - f^*)^2}{L^2(f)}. \end{aligned}$$

From this reasoning, $||x_{k+1} - x^*||^2 \le ||x_k - x^*||^2$, $\forall x^* \in X^*$. **Corollary:** Assume X_* has recession direction d_* . Then

$$\|x_k - \pi_{X_*}(x_0)\| \leq \|x_0 - \pi_{X_*}(x_0)\|, \quad \langle d_*, x_k \rangle \geq \langle d_*, x_0 \rangle.$$

(Proof: consider $x^* = \pi_{X_*}(x_0) + \alpha d_*$, $\alpha \ge 0$.)

Constrained minimization (N.Shor (1964) & B.Polyak)

II. Problem: $\min_{x \in Q} \{ f(x) : g(x) \le 0 \},$ where

- Q is closed and convex,
- f, g have uniformly bounded subgradients.

Consider the following method. It has step-size parameter h > 0.

If
$$g(x_k) > h \|g'(x_k)\|$$
, then (A): $x_{k+1} = \pi_Q \left(x_k - \frac{g(x_k)}{\|g'(x_k)\|^2} g'(x_k) \right)$,
else (B): $x_{k+1} = \pi_Q \left(x_k - \frac{h}{\|f'(x_k)\|} f'(x_k) \right)$.

Let $\mathcal{F}_k \subseteq \{0, \dots, k\}$ be the set (B)-iterations, and $f_k^* = \min_{i \in \mathcal{F}_k} f(x_i)$. **Theorem:** If $k > ||x_0 - x^*||^2 / h^2$, then $\mathcal{F}_k \neq \emptyset$ and

$$f_k^* - f(x) \leq hL(f), \quad \max_{i\in \mathcal{F}_k} g(x_i) \leq hL(g).$$

Computational strategies

1. Constants L(f), L(g) are known (e.g. Linear Programming) We can take $h = \frac{\epsilon}{\max\{L(f), L(g)\}}$. Then we need to decide on the number of steps N (easy!).

Note: The standard advice is $h = \frac{R}{\sqrt{N+1}}$ (much more difficult!)

2. Constants L(f), L(g) are not known

- Start from a guess.
- Restart from scratch each time we see the guess is wrong.
- The guess is doubled after restart.

3. Tracking the record value f_k^*

Double run.

Other ideas are welcome!

Application examples

Observations:

- Very often, Large- and Huge- scale problems have repetitive sparsity patterns and/or limited connectivity.
 - Social networks.
 - Mobile phone networks.
 - Truss topology design (local bars).
 - Finite elements models (2D: four neighbors, 3D: six neighbors).
- 2 For *p*-diagonal matrices $\kappa(A) \leq p^2$.

Nonsmooth formulation of Google Problem

Main property of spectral radius $(A \ge 0)$

If $A \in \mathbb{R}^{n \times n}_+$, then $\rho(A) = \min_{x \ge 0} \max_{1 \le i \le n} \frac{1}{x^{(i)}} \langle e_i, Ax \rangle$. The minimum is attained at the corresponding eigenvector.

Since $\rho(\bar{E}) = 1$, our problem is as follows:

$$f(x) \stackrel{\text{def}}{=} \max_{1 \leq i \leq N} [\langle e_i, \overline{E}x \rangle - x^{(i)}] \rightarrow \min_{x \geq 0}.$$

Interpretation: Maximizing the self-esteem! Since $f^* = 0$, we can apply Polyak's method with sparse updates. **Additional features;** the optimal set X^* is a *convex cone*. If $x_0 = e$, then the whole sequence is separated from zero:

$$\langle x^*, e \rangle \leq \langle x^*, x_k \rangle \leq \|x^*\|_1 \cdot \|x_k\|_{\infty} = \langle x^*, e \rangle \cdot \|x_k\|_{\infty}.$$

Goal: Find $\bar{x} \ge 0$ such that $\|\bar{x}\|_{\infty} \ge 1$ and $f(\bar{x}) \le \epsilon$. (First condition is satisfied automatically.)

Computational experiments: Iteration Cost

We compare Polyak's GM with sparse update (GM_s) with the standard one (GM).

Setup: Each agent has exactly *p* random friends. Thus, $\kappa(A) \approx p^2$.

Iteration Cost: $GM_s \approx p^2 \log_2 N$, $GM \approx pN$.

Time for 10^4 iterations ($p = 32$)									
	N	$\kappa(A)$	GM _s	GM					
	1024	1632	3.00	2.98					
	2048	1792	3.36	6.41					
	4096	1888	3.75	15.11					
	8192	1920	4.20	139.92					
	16384	1824	4.69	408.38					

Time for 10^3 iterations ($p = 16$)							
N	$\kappa(A)$	GM _s	GM				
131072	576	0.19	213.9				
262144	592	0.25	477.8				
524288	592	0.32	1095.5				
1048576	608	0.40	2590.8				
1							

1 sec \approx 100 min!