Complexity analysis framework of adaptive stochastic optimization methods via martingales.

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Stochastic Complexity Analysis

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Unconstrained Optimization

Minimize $f(x) : \mathbb{R}^n \to \mathbb{R}$

- We will assume throughout that f is sufficiently smooth and nonconvex, unless specified.
- When f(x) is deterministic, standard methods are 1. line search,
 2. trust region and 3. cubicly regularized Newton.
- When f(x) is stochastic, standard method is stochastic gradient descent and variants.
- When f(x) has biased noise and/or no derivative information, we use other methods (e.g. black box optimization).
- How can adaptive deterministic methods be used and analyzed in nondeterministic (possibly black box) settings?

Generic Adaptive Deterministic Method

0. Initialization

Choose constants $\eta \in (0, 1)$, $\gamma \in (1, \infty)$, and $\overline{\alpha} \in (0, \infty)$. Choose an initial iterate $x_0 \in \mathbb{R}^n$ and stepsize parameter $\alpha_0 \in (0, \overline{\alpha}]$.

1. Determine model and compute step

Choose a local model m_k of f around x_k . Compute a step $s_k(\alpha_k)$ such that the model reduction $m_k(x_k) - m_k(x_k + s_k(\alpha_k)) \ge 0$ is sufficiently large.

2. Check for sufficient reduction in f

Check if $f(x_k) - f(x_k + s_k(\alpha_k))$ is sufficiently large relative to $m_k(x_k) - m_k(x_k + s_k(\alpha_k))$ using a condition parameterized by η .

3. Successful iteration

If true (along with other potential requirements), then set $x_{k+1} \leftarrow x_k + s_k(\alpha_k)$ and $\alpha_{k+1} \leftarrow \min\{\gamma \alpha_k, \overline{\alpha}\}.$

4. Unsuccessful iteration

Otherwise, $x_{k+1} \leftarrow x_k$ and $\alpha_{k+1} \leftarrow \gamma^{-1} \alpha_k$.

5. Next iteration

Set $k \leftarrow k+1$.

Particular Methods

For line search method

•
$$m_k(x_k+s) = f(x_k) + \nabla f(x_k)^T s + \frac{1}{2\alpha_k} s^T H s, H \succ 0$$

•
$$s_k(\boldsymbol{\alpha}_k) = -\boldsymbol{\alpha}_k H^{-1} \nabla f(x_k)$$

• Sufficient reduction: $f(x_k) - f(x_k + s_k(\boldsymbol{\alpha_k})) \ge -\eta \nabla f(x_k)^T s_k(\boldsymbol{\alpha_k})$

For trust region method

•
$$m_k(x_k + s) = f(x_k) + \nabla f(x_k)^T s + \frac{1}{2}s^T H s, \ H \sim \nabla^2 f(x_k)$$

•
$$s_k(\alpha_k) = \arg\min_{s: ||s|| \le \alpha_k} m_k(x_k + s)$$

• Sufficient reduction:
$$\frac{f(x_k) - f(x_k + s_k(\boldsymbol{\alpha}_k))}{m_k(x_k) - m_k(x_k + s_k(\boldsymbol{\alpha}_k))} \ge \eta$$

For cubicly regularized Newton method

- $m_k(x_k+s) = f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s + \frac{1}{3\alpha_k} ||s||^3$,
- $s_k(\alpha_k) = \arg\min_s m_k(x_k + s)$
- Sufficient reduction: $\frac{f(x_k) f(x_k + s_k(\alpha_k))}{m_k(x_k) m_k(x_k + s_k(\alpha_k))} \geq \eta$

What can happen?



Figure: Illustration of successful (left) and unsuccessful (right) steps in a trust region method.

Why analyze adaptive methods in stochastic setting?

- For gradient descent $x_{k+1} = x_k \alpha_k \nabla f(x_k)$ small enough step $\alpha_k \leq \frac{1}{L}$ always works.
- For inexact gradient descent $x_{k+1} = x_k \alpha_k g_k$, $g_k \approx \nabla f(x_k)$ bound on α_k is harder to determine.
- Suppose a descent direction condition, e.g. $\|\nabla f(x_k) g_k\| \le \theta \|\nabla f(x_k)\|$, holds only w.p. 1δ . What kind of convergence result we can guaranate then?
- It takes $\mathcal{O}(\frac{1}{\epsilon^2})$ iterations until $\|\nabla f(x_k)\| \leq \epsilon$. So if for each of the first $\mathcal{O}(\frac{1}{\epsilon^2})$ iterations g_k is a descent direction, then the algorithm works!!
- Thus convergence result holds with probability $(1-\delta)^{\mathcal{O}(\frac{1}{\epsilon^2})}$.
- But what happens if the descent condition is failed even once?

First and Second order model requirements

Use a model $m_k(x_k + s) = f_k + g_k^T s + \frac{1}{2}s^T H s.$

First order model conditions

• $|f(x_k) - f_k| \leq \mathcal{O} ||s||^2$

•
$$\|\nabla f(x_k) - g_k\| \leq \mathcal{O}\|s\|^1$$

• $\|\nabla^2 f(x_k) - H_k\| \leq \mathcal{O}\|s\|^0$

Second order model conditions

•
$$|f(x_k) - f_k| \le \mathcal{O} ||s||^3$$

• $||\nabla f(x_k) - g_k|| \le \mathcal{O} ||s||^2$

•
$$\|\nabla^2 f(x_k) - H_k\| \leq \mathcal{O}\|s\|^1$$

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We consider three different cases:

- Model conditions hold deterministically this is already known and analyzed.
- Conditions on f hold deterministically, and on g and H hold w.p. 1δ .
- Conditions on f, g and H hold w.p. 1δ .

Analysis should consider what can happens when model conditions fail to hold.

Framework for Convergence Rate Analysis, Case 1

- $\{\Phi_k\} \ge 0$ a sequence whose role is to measure progress of the algorithm.
- $\{W_k\}$ is a sequence of indicators; specifically, for all $k \in \mathbb{N}$, if iteration k is successful, then $W_k = 1$, and $W_k = -1$ otherwise.
- $\{\alpha_k\} \ge 0$ a sequence of step size values obeying $\alpha_{k+1} = \gamma^{W_k} \alpha_k$
- T_{ε} , the *stopping time*, is the index of the first iterate that satisfies a desired ε -convergence criterion.

Condition 1

The following statements hold with respect to $\{(\Phi_k, \alpha_k, W_k)\}$ and T_{ε} .

• There exists a scalar $\underline{\alpha}_{\varepsilon} \in (0, \infty)$ such that for each $k \in \mathbb{N}$, $\alpha_k \leq \underline{\alpha}_{\varepsilon}$ implies $W_k = 1$. Therefore, $\alpha_k \geq \underline{\alpha}_{\varepsilon}$ for all $k \in \mathbb{N}$.

2 There exists a nondecreasing function $h_{\varepsilon} : [0, \infty) \to (0, \infty)$ such that, for all $k < T_{\varepsilon}$, if k is successful, then $\Phi_k - \Phi_{k+1} \ge h_{\varepsilon}(\alpha_k)$.

Under Condition 1

$$T_{\varepsilon} \leq \mathcal{O}\left(\frac{\Phi_0}{h_{\varepsilon}(\underline{\alpha}_{\varepsilon})}\right)$$

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Generic Adaptive Stochastic Method

Initialization

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1. Determine model and compute step

Choose a random local model m_k of f around x_k . Compute a step $s_k(\alpha_k)$ such that the model reduction $m_k(x_k) - m_k(x_k + s_k(\alpha_k)) \ge 0$ is sufficiently large.

2. Check for sufficient reduction in f

Compute estimates $f_k^0 \sim f(x_k)$ and $f_k^s \sim f(x_k + s_k(\alpha_k))$ and check if $f_k^0 - f_k^s$ is sufficiently large relative to $m_k(x_k) - m_k(x_k + s_k(\alpha_k))$ using a condition parameterized by η .

3. Successful iteration

If true (along with other potential requirements), then set $x_{k+1} \leftarrow x_k + s_k(\alpha_k)$ and $\alpha_{k+1} \leftarrow \min\{\gamma \alpha_k, \overline{\alpha}\}.$

4. Unsuccessful iteration

Otherwise, $x_{k+1} \leftarrow x_k$ and $\alpha_{k+1} \leftarrow \gamma^{-1} \alpha_k$.

5. Next iteration

Set $k \leftarrow k+1$.

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Framework for adaptive stochastic methods

What can happen under random models (Case 2)?



(a) Good model; good estimates. True successful steps. (b) Bad model; good estimates. Unsuccessful steps.

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Casting the Algorithm as a Stochastic Process, Case 2

- $\{\Phi_k\} \ge 0$ a random sequence whose role is to measure progress of the algorithm.
- $\{W_k\}$ is a sequence of random indicators; specifically, for all $k \in \mathbb{N}$, if iteration k is successful, then $W_k = 1$, and $W_k = -1$ otherwise.
- $\{\alpha_k\} \ge 0$ a random sequence of step size values that obeying $\alpha_{k+1} = \gamma^{W_k} \alpha_k$
- T_{ε} , the random stopping time, is the index of the first iterate that satisfies a desired ε -convergence criterion.

 $\{\Phi_k, \alpha_k, W_k\}$ is a stochastic process and T_{ϵ} is its stopping time.

Recall Condition 1

The statement in red no longer hold with respect to $\{(\Phi_k, \alpha_k, W_k)\}$ and T_{ε} .

1 There exists a scalar $\underline{\alpha}_{\varepsilon} \in (0, \infty)$ such that for each $k \in \mathbb{N}$ such that $\alpha_k \leq \gamma \underline{\alpha}_{\varepsilon}$, the iteration is guaranteed to be successful, i.e., $W_k = 1$. Therefore, $\alpha_k \geq \underline{\alpha}_{\varepsilon}$ for all $k \in \mathbb{N}$.

2 There exists a nondecreasing function $h_{\varepsilon} : [0, \infty) \to (0, \infty)$ such that, for all $k < T_{\varepsilon}$, if k is successful then $\Phi_k - \Phi_{k+1} \ge h_{\varepsilon}(\alpha_k)$.

The α_k Process

Modifying Condition 1

There exists a constant $\underline{\alpha}_{\varepsilon} \in (0, \infty)$ such that, for $k < T_{\varepsilon}$

$$\alpha_{k+1} \ge \gamma^{W_k} \alpha_k,$$

where $\mathbb{P}(W_k = 1 | \alpha_k \leq \underline{\alpha}_{\varepsilon}) \geq 1 - \delta$.



Bounding the total number of iterations



Main Ideas:

- α_k may become arbitrarily small, but it tends to increase up to $\underline{\alpha}_{\varepsilon}$.
- Large steps imply large function decrease, i.e. each successful iteration with accurate model and $\alpha_k \geq \underline{\alpha}_{\varepsilon}$ brings $h_{\varepsilon}(\underline{\alpha}_{\varepsilon})$ improvement, so their total number is bounded.
- The number of small upward steps is bounded by the small downward steps, but downwards steps are bounded by upward steps (because of the new Condition 1).
- The number of successful iterations with accurate models and $\alpha_k \geq \underline{\alpha}_{\varepsilon}$ is constant fraction of the total number of iterations.

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Bounding the total number of iterations



Main Ideas:

- α_k may become arbitrarily small, but it tends to increase up to $\underline{\alpha}_{\varepsilon}$.
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Bounding the total number of iterations



Main Ideas:

- α_k may become arbitrarily small, but it tends to increase up to $\underline{\alpha}_{\varepsilon}$.
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- The number of successful iterations with accurate models and $\alpha_k \geq \underline{\alpha}_{\varepsilon}$ is constant fraction of the total number of iterations.

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Complexity bounds

 $\{\Phi_k, \alpha_k, W_k\}$ is a stochastic process and T_{ϵ} is its stopping time.

Condition 1

- For all $k < T_{\varepsilon}$ such that $\alpha_k \leq \underline{\alpha}_{\varepsilon}, W_k = 1 \text{ w.p.} 1 \delta$.
- (2) There exists a nondecreasing function $h_{\varepsilon} : [0, \infty) \to (0, \infty)$ such that, for all $k < T_{\varepsilon}$, if k is successful then $\Phi_k \Phi_{k+1} \ge h_{\varepsilon}(\alpha_k)$.

Theorem

Under Condition 1,

$$\mathbb{E}[T_{\varepsilon}] \leq \mathcal{O}\left(\frac{1}{1-2\delta} \frac{\Phi_0}{h_{\varepsilon}(\underline{\alpha}_{\varepsilon})}\right)$$

Moreover,

$$\mathbb{P}(T_{\varepsilon} \geq \boldsymbol{N}) \leq e^{\left(-\frac{(\delta-\hat{\delta})^2}{2}\boldsymbol{N}\right)}, \forall \boldsymbol{N} \geq \mathcal{O}\left(\frac{1}{1-2\hat{\delta}}\frac{\Phi_0}{h_{\varepsilon}(\underline{\alpha}_{\varepsilon})}\right)$$

Complexity bounds for particular cases

Line Search

For the line search algorithm with random first order models, accurate w.p $1-\delta$

• applied to nonconvex f(x)

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta}\frac{f(x_0)-f_*)}{\varepsilon^2}\right), \quad T_{\varepsilon} = \min\{k: \|\nabla f(x_k)\| \le \varepsilon\}$$

• applied to convex f(x)

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta}\frac{f(x_0)-f_*)}{\varepsilon}\right), \quad T_{\varepsilon} = \min\{k: f(x_k)-f_* \le \varepsilon\}$$

• and strongly convex f(x)

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta} \frac{f(x_0) - f_*)}{\log(\varepsilon)}\right), \quad T_{\varepsilon} = \min\{k : f(x_k) - f_* \le \varepsilon\}$$

Complexity bounds for particular cases

Trust region and Regularized Newton

• For the trust region method with random first order models, accurate w.p. $1-\delta$

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta}\frac{f(x_0)-f_*)}{\varepsilon^2}\right), \quad T_{\varepsilon} = \min\{k: \|\nabla f(x_k)\| \le \varepsilon\}$$

• with random second order models, accurate w.p. $1 - \delta$

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta} \frac{f(x_0) - f_*)}{\varepsilon^3}\right), \ T_{\varepsilon} = \min\{k : \|\nabla f(x_k)\|, -\lambda_{\min}(\nabla^2 f(x_k)) \le \varepsilon\}$$

• For cubicly regularized Newton method with random first order models accurate w.p. $1-\delta$

$$T_{\varepsilon} \approx \mathcal{O}\left(\frac{1}{1-2\delta} \frac{f(x_0) - f_*)}{\varepsilon^{\frac{3}{2}}}\right), \quad T_{\varepsilon} = \min\{k : \|\nabla f(x_k)\| \le \varepsilon\}$$

What can happen under random function estimates, Case 3



(c) Good model; bad estimates. Unsuccessful steps. (d) Bad model; bad estimates. False successful steps: *f* can increase!

Assumptions on Stochastic Process, Case 3

- $\{\Phi_k\} \ge 0$ a random sequence whose role is to measure progress of the algorithm.
- $\{W_k\}$ is a sequence of random indicators; specifically, for all $k \in \mathbb{N}$, if iteration k is successful, then $W_k = 1$, and $W_k = -1$ otherwise.
- $\{\alpha_k\} \ge 0$ a random sequence of step size values that obeying $\alpha_{k+1} = \gamma^{W_k} \alpha_k$
- T_{ε} , the random stopping time, is the index of the first iterate that satisfies a desired ε -convergence criterion.

 $\{\Phi_k, \alpha_k, W_k\}$ is a stochastic process and T_{ϵ} is its stopping time.

Recall Condition 1

The statements in red no longer hold with respect to $\{(\Phi_k, \alpha_k, W_k)\}$ and T_{ε} .

 $\square \underline{\alpha}_{\varepsilon} \in (0,\infty) \text{ such that, for } k < T_{\varepsilon} \text{ for which } \alpha_k \leq \underline{\alpha}_{\varepsilon},$

$$\alpha_{k+1} \ge \gamma^{W_k} \alpha_k$$
, where $W_k = 1$ w.p. $1 - \delta$.

2 There exists a nondecreasing function h_ε : [0,∞) → (0,∞) such that, for all k < T_ε, if k is successful, Φ_k − Φ_{k+1} ≥ h_ε(α_k).

Assumptions on Stochastic Process, Case 3

- $\{\Phi_k\} \ge 0$ a random sequence whose role is to measure progress of the algorithm.
- $\{W_k\}$ is a sequence of random indicators; specifically, for all $k \in \mathbb{N}$, if iteration k is successful, then $W_k = 1$, and $W_k = -1$ otherwise.
- $\{\alpha_k\} \ge 0$ a random sequence of step size values that obeying $\alpha_{k+1} = \gamma^{W_k} \alpha_k$
- T_{ε} , the random *stopping time*, is the index of the first iterate that satisfies a desired ε -convergence criterion.
- $\{\Phi_k, \alpha_k, W_k\}$ is a stochastic process and T_{ϵ} is its stopping time.

New Condition 1

The statements in red no longer hold with respect to $\{(\Phi_k, \alpha_k, W_k)\}$ and T_{ε} .

 $\underbrace{ \mathbf{0} }_{\varepsilon} \in (0,\infty) \text{ such that, for } k < T_{\varepsilon} \text{ for which } \alpha_k \leq \underline{\alpha}_{\varepsilon},$

$$\alpha_{k+1} \ge \gamma^{W_k} \alpha_k$$
, where $W_k = 1$ w.p. $1 - \delta$.

2 There exists a nondecreasing function h(·): [0,∞) → (0,∞) such that, until the stopping time:

$$\mathbb{E}(\Phi_{k+1}|\operatorname{past}) \le \Phi_k - h(\alpha_k).$$

Bounding expected stopping time

Main Idea: This is a renewal-reward process and Φ_k is a supermartingale - $\mathbb{E}[\Phi_{k+1}| \text{ past}] \leq \Phi_k - h_{\varepsilon}(\alpha_k)$ and, thus,

- $\Phi_0 \ge \mathbb{E}[\sum_{i=0}^{T_{\epsilon}} h(\alpha_i)].$
- T_{ϵ} is a stopping time!
- Applying Wald's Identity we can bound the number of renewals that will occur before T_{ϵ} .
- Multiply by the expected renewal time.
- We have the following results

Theorem (Blanchet, Cartis, Menickelly, S. '17)

Let Condition 1 hold. Then

$$\mathbb{E}[T_{\varepsilon}] \leq \frac{1-\delta}{1-2\delta} \cdot \frac{\Phi_0}{h(\underline{\alpha}_{\varepsilon})} + 1.$$

Stochastic TR: First-order convergence rate.

• α_k is the trust region radius.

•
$$\Phi_k = \nu (f(x_k) - f_{\min}) + (1 - \nu) \alpha_k^2$$

• $T_{\epsilon} = \inf\{k \ge 0 : \|\nabla f(x_k)\| \le \epsilon\}.$

Theorem

(Blanchet-Cartis-Menickelly-S. '17)

$$\mathbb{E}[T_{\epsilon}] \leq \mathcal{O}\left(\frac{1-\delta}{1-2\delta}\left(\frac{L}{\epsilon^2}\right)\right),\,$$

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Stochastic TR: Second-order convergence rate

• α_k is the trust region radius.

•
$$\Phi_k = \nu (f(x_k) - f_{\min}) + (1 - \nu) \alpha_k^3.$$

• $T_{\epsilon} = \inf\{k \ge 0 : \max\{\|\nabla f(x_k)\|, -\lambda_{\min}(\nabla^2 f(x_k))\} \le \epsilon\}.$

Theorem

(Blanchet-Cartis-Menickelly-S. '17)

$$\mathbb{E}[T_{\epsilon}] \leq \mathcal{O}\left(\frac{1-\delta}{1-2\delta}\left(\frac{L}{\epsilon^3}\right)\right),\,$$

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Stochastic line search: nonconvex case

• α_k - the step size parameter, δ_k additional parameter meant to approximate $\alpha_k \|\nabla f(x_k)\|^2$.

•
$$\Phi_k = \nu (f(x_k) - f_{\min}) + (1 - \nu) \alpha_k \|\nabla f(x_k)\|^2 + (1 - \nu) \theta \delta_k^2$$

•
$$T_{\epsilon} = \inf\{k \ge 0 : \|\nabla f(x_k)\| \le \epsilon\}.$$

Theorem

(Paquette-S. '18)

$$\mathbb{E}[T_{\epsilon}] \leq \mathcal{O}\left(\frac{1-\delta}{1-2\delta}\left(\frac{L^3}{\epsilon^2}\right)\right),\,$$

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Stochastic line search: convex case

• α_k - the step size parameter, δ_k additional parameter meant to approximate $\alpha_k \|\nabla f(x_k)\|^2$.

•
$$\Phi_k = \nu (f(x_k) - f_{\min}) + (1 - \nu) \alpha_k \|\nabla f(x_k)\|^2 + (1 - \nu) \theta \delta_k^2$$

•
$$T_{\epsilon} = \inf\{k : f(x_k) - f^* < \varepsilon\}.$$

•
$$\Psi_k = \frac{1}{\nu \varepsilon} - \frac{1}{\Phi_k}.$$

Theorem

(Paquette-S. '18)

$$\mathbb{E}[T_{\epsilon}] \leq \mathcal{O}\left(\frac{1-\delta}{1-2\delta}\left(\frac{L^3}{\varepsilon}\right)\right),\,$$

Stochastic line search: strongly convex case

• α_k - the step size parameter, δ_k additional parameter meant to approximate $\alpha_k \|\nabla f(x_k)\|^2$.

•
$$\Phi_k = \nu (f(x_k) - f_{\min}) + (1 - \nu) \alpha_k \|\nabla f(x_k)\|^2 + (1 - \nu) \theta \delta_k^2$$

•
$$T_{\epsilon} = \inf\{k : f(x_k) - f^* < \varepsilon\}.$$

•
$$\Psi_k = \log(\Phi_k) - \log(\nu \varepsilon).$$

Theorem

(Paquette-S. '18)

$$\mathbb{E}[T_{\epsilon}] \leq \mathcal{O}\left(\frac{1-\delta}{1-2\delta}\log\left(\frac{L^3}{\varepsilon}\right)\right),\,$$

Cubicly regularized Newton

• $\Phi_k = \nu(f(x_k) - f_{\min}) + (1 - \nu)\alpha_k \|\nabla f(x_k)\|^{3/2} + ???.$ • $T_{\epsilon} = \inf\{k : \|\nabla f(x_{k+1})\| < \epsilon\}.$

 T_ϵ is NOT a stopping time. Need to modify Condition 1 again.

Conclusions and Remarks

- We have a versatile framework based on bounding stoping time of a martingale which can be used to derive expected complexity bounds for adaptive stochastic methods.
- Algorithms can converge even with constant (and quite large) probability of "iteration failure."
- To do: High probability results for stochastic case.
- To do: Weaker conditions for stochastic case.
- To do: Stochastic Cubicly regularized Newton and optimal Trust Region method.

Thanks for listening!

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