Mathematics of Data: From Theory to Computation

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Lecture 3: Large-scale optimization algorithms

Laboratory for Information and Inference Systems (LIONS)
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EE-556 (Fall 2020)

Recall: Gradient descent

Problem (Unconstrained convex problem)

Consider the following convex minimization problem:

$$f^\star = \min_{\mathbf{x}\in\mathbb{R}^p} f(\mathbf{x})$$

- f *is a convex function that is*
  - *proper :* $\forall \mathbf{x} \in \mathbb{R}^p$, $-\infty < f(\mathbf{x})$ *and there exists* $\mathbf{x} \in \mathbb{R}^p$ *such that* $f(x) < +\infty$.
  - *closed :* *The epigraph* $\text{epi} f = \{(\mathbf{x}, t) \in \mathbb{R}^{p+1}, f(\mathbf{x}) \leq t\}$ *is closed.*
  - *smooth :* f *is differentiable and its gradient* ∇f *is* L*-Lipschitz.*
- *The solution set* $\mathcal{S}^\star := \{\mathbf{x}^\star \in \text{dom}\,(f) : f(\mathbf{x}^\star) = f^\star\}$ *is nonempty.*

Gradient descent (GD)

Choose a starting point $\mathbf{x}^0$ and iterate

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k)$$

where α_k is a step-size to be chosen so that $\mathbf{x}^k$ converges to $\mathbf{x}^\star$.

Convergence rate of gradient descent

Theorem

Let f be a twice-differentiable convex function, if

f is L-smooth,	$\alpha = \frac{1}{L}$:	$f(\mathbf{x}^k) - f(\mathbf{x}^\star)$	$\leq \frac{2L}{k+4}$	$\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2$
f is L-smooth and μ-strongly convex,	$\alpha = \frac{2}{L+\mu}$:	$\|\mathbf{x}^k - \mathbf{x}^\star\|_2$	$\leq \left(\frac{L-\mu}{L+\mu}\right)^k$	$\|\mathbf{x}^0 - \mathbf{x}^\star\|_2$
f is L-smooth and μ-strongly convex,	$\alpha = \frac{1}{L}$:	$\|\mathbf{x}^k - \mathbf{x}^\star\|_2$	$\leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}}$	$\|\mathbf{x}^0 - \mathbf{x}^\star\|_2$

Note that $\frac{L-\mu}{L+\mu} = \frac{\kappa-1}{\kappa+1}$, where $\kappa := \frac{L}{\mu}$ is the condition number of $\nabla^2 f$.

Information theoretic lower bounds [17]

What is the **best** achievable rate for a **first-order** method?

$f \in \mathcal{F}_L^\infty$: ∞-differentiable and L-smooth

It is possible to construct a function in $\mathcal{F}_L^\infty$, for which **any** first order method must satisfy

$$f(\mathbf{x}^k) - f(\mathbf{x}^\star) \geq \frac{3L}{32(k+1)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2 \quad \text{for all } k \leq (p-1)/2$$

$f \in \mathcal{F}_{L,\mu}^\infty$: ∞-differentiable, L-smooth and μ-strongly convex

It is possible to construct a function in $\mathcal{F}_{L,\mu}^\infty$, for which **any** first order method must satisfy

$$\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \geq \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2$$

Gradient descent is $O(1/k)$ for $\mathcal{F}_L^\infty$ and it is slower for $\mathcal{F}_{L,\mu}^\infty$, hence it does not achieve the lower bounds!

Accelerated gradient descent algorithm

Problem

Is it possible to design first-order methods with convergence rates matching the theoretical lower bounds?

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Solution [Nesterov's accelerated scheme]

Accelerated Gradient Descent (AGD) methods achieve optimal convergence rates.

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Accelerated Gradient algorithm for L-smooth (AGD-L)

1. Set $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}\,(f)$ and $t_0 := 1$.
2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \frac{(t_k - 1)}{t_{k+1}}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

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Accelerated Gradient algorithm for L-smooth and μ-strongly convex (AGD-μL)

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$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L}\nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \alpha(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

where $\alpha = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$.

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where $\alpha = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$.

Remark: ○ AGD is not monotone, but the cost-per-iteration is essentially the same as GD.

Global convergence of AGD [17]

Theorem (f is convex with Lipschitz gradient)

If f is L-smooth or L-smooth and μ-strongly convex, the sequence $\{\mathbf{x}^k\}_{k\geq 0}$ generated by **AGD-L** *satisfies*

$$f(\mathbf{x}^k) - f^\star \leq \frac{4L}{(k+2)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2, \ \forall k \geq 0. \tag{1}$$

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AGD-L is **optimal** *for L-smooth but NOT for L-smooth and μ-strongly convex!*

Theorem (f is strongly convex with Lipschitz gradient)

If f is L-smooth and μ-strongly convex, the sequence $\{\mathbf{x}^k\}_{k\geq 0}$ generated by **AGD-μL** *satisfies*

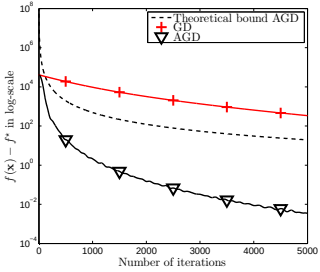
$$f(\mathbf{x}^k) - f^\star \leq L\left(1 - \sqrt{\frac{\mu}{L}}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2,\ \forall k \geq 0 \tag{2}$$

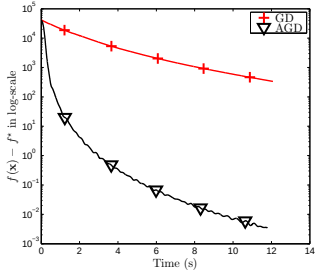
$$\|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \sqrt{\frac{2L}{\mu}}\left(1 - \sqrt{\frac{\mu}{L}}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2,\ \forall k \geq 0. \tag{3}$$

Observations:
- AGD-L's iterates are not guaranteed to converge.
- AGD-L does not have a **linear** convergence rate for L-smooth and μ-strongly convex.
- AGD-μL does, but needs to know μ.
- AGD achieves the iteration lowerbound within a constant!

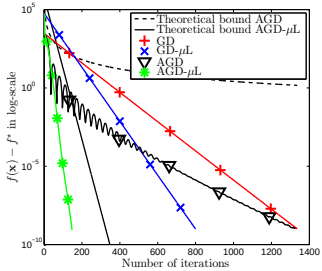
Example: Ridge regression

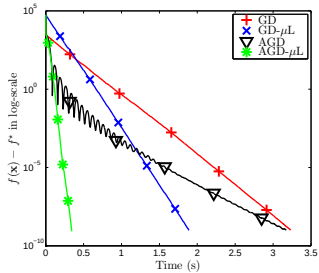
Case 1: $n = 500, p = 2000, \rho = 0$





Case 2: $n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T\mathbf{A})$





Gradient descent vs. Accelerated gradient descent

Assumptions, step sizes and convergence rates

Gradient descent:

$$f \text{ is } L\text{-smooth}, \quad \alpha = \frac{1}{L}: \qquad f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2L}{k+4}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2.$$

Accelerated Gradient Descent:

$$f \text{ is } L\text{-smooth}, \quad \alpha = \frac{1}{L}: \qquad f(\mathbf{x}^k) - f(x^\star) \leq \frac{4L}{(k+2)^2}\|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2, \ \forall k \geq 0.$$

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Observations:

- We require α_t to be a function of L.
- It may not be possible to know exactly the Lipschitz constant.
- Adaptation to local geometry $\rightarrow$ may lead to larger steps.

Adaptive first-order methods and *Newton method

Adaptive methods

Adaptive methods converge with fast rates without knowing the smoothness constant.

They do so by making use of the information from gradients and their norms.

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Adaptive methods converge with fast rates without knowing the smoothness constant.

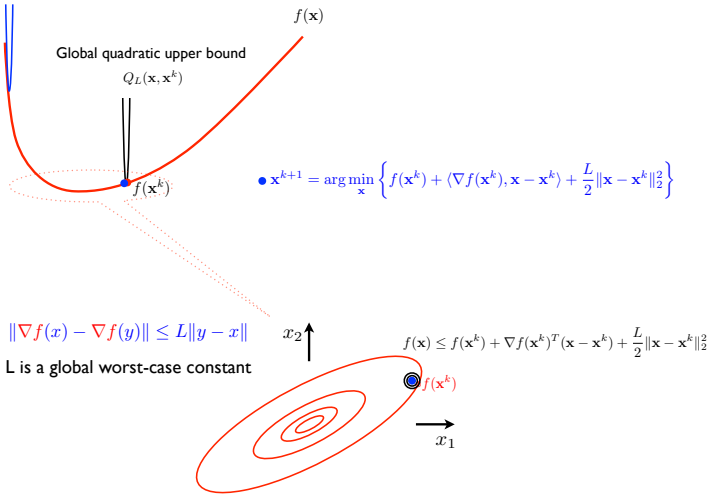
They do so by making use of the information from gradients and their norms.

*Newton method

Higher-order information, e.g., Hessian, gives a finer characterization of local behavior.

Newton method achieves asymptotically better local rates, but for additional cost.

How can we better adapt to the local geometry?



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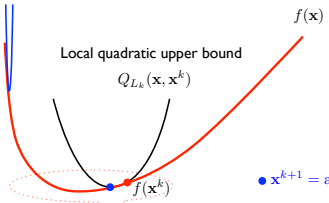


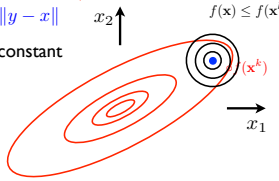
- $\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L_k}{2} \|\mathbf{x} - \mathbf{x}^k\|_2^2 \right\}$

$\|\nabla f(x) - \nabla f(y)\| \leq L\|y - x\|$

L is a global worst-case constant

$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{L_k}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

applies only locally



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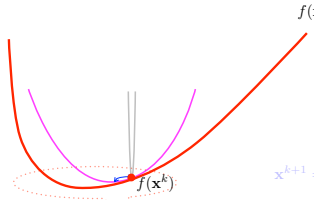

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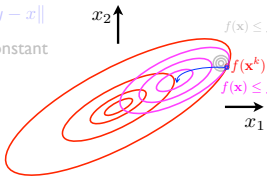

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$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{1}{2}\|\mathbf{x} - \mathbf{x}^k\|_{H_k^{-1}}^2$$

Variable metric gradient descent algorithm

Variable metric gradient descent algorithm

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point and $\mathbf{H}_0 \succ 0$.
2. For $k = 0, 1, \cdots$, perform:

$$\begin{cases} \mathbf{d}^k & := -\mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k), \\ \mathbf{x}^{k+1} & := \mathbf{x}^k + \alpha_k \mathbf{d}^k, \end{cases}$$

where $\alpha_k \in (0, 1]$ is a given step size.

3. Update $\mathbf{H}_{k+1} \succ 0$ if necessary.

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Common choices of the variable metric $\mathbf{H}_k$

- $\mathbf{H}_k := \lambda_k \mathbf{I} \implies$ gradient descent method.
- $\mathbf{H}_k := \mathbf{D}_k$ (a positive diagonal matrix) $\implies$ adaptive gradient methods.
- $\mathbf{H}_k := \nabla^2 f(\mathbf{x}^k) \implies$ Newton method.
- $\mathbf{H}_k \approx \nabla^2 f(\mathbf{x}^k) \implies$ quasi-Newton method.

Adaptive gradient methods

Intuition

Adaptive gradient methods adapt locally by setting $\mathbf{H}_k$ as a function of past gradient information.

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Adaptive gradient methods adapt locally by setting $\mathbf{H}_k$ as a function of past gradient information.

- Roughly speaking, $\mathbf{H}_k = \text{function}(\nabla f(\mathbf{x}^1), \nabla f(\mathbf{x}^2), \cdots, \nabla f(\mathbf{x}^k))$
- Some well-known examples:

AdaGrad [7]

$$\mathbf{H}_k = \sqrt{\sum_{t=1}^{k} (\nabla f(\mathbf{x}^t)^\top \nabla f(\mathbf{x}^t))}$$

*RmsProp [24]

$$\mathbf{H}_k = \sqrt{\beta \mathbf{H}_{k-1} + (1-\beta)\text{diag}(\nabla f(\mathbf{x}^k))^2}$$

*ADAM [12]

$$\hat{\mathbf{H}}_k = \beta \hat{\mathbf{H}}_{k-1} + (1-\beta)\text{diag}(\nabla f(\mathbf{x}^k))^2$$
$$\mathbf{H}_k = \sqrt{\hat{\mathbf{H}}_k / (1-\beta^k)}$$

AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \lambda_k \mathbf{I}$

- If $\mathbf{H}_k = \lambda_k \mathbf{I}$, it becomes gradient descent method with adaptive step-size $\frac{\alpha_k}{\lambda_k}$.

How step-size adapts?

If gradient $\|\nabla f(\mathbf{x}^k)\|$ is large/small $\rightarrow$ AdaGrad adjusts step-size α_k/λ_k smaller/larger

Adaptive gradient descent (AdaGrad with $\mathbf{H}_k = \lambda_k \mathbf{I}$) [13]

1. Set $Q^0 = 0$.
2. For $k = 0, 1, \ldots$, iterate

$$\begin{cases} Q^k & = Q^{k-1} + \|\nabla f(\mathbf{x}^k)\|^2 \\ \mathbf{H}_k & = \sqrt{Q^k} I \\ \mathbf{x}^{k+1} & = \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

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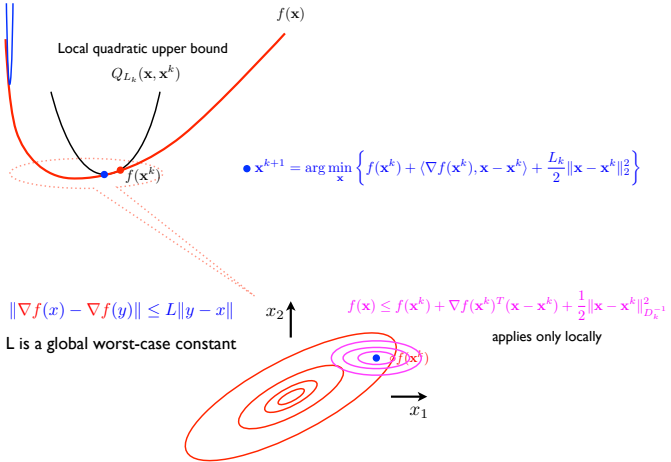
Adaptation through first-order information

- When $H_k = \lambda_k I$, AdaGrad estimates local geometry through gradient norms.
- Akin to estimating a local quadratic upper bound (majorization / minimization) using gradient history.

AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

Adaptation strategy with a positive diagonal matrix $\mathbf{D}_k$

Adaptive step-size + coordinate-wise extension = adaptive step-size for each coordinate



AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

- Suppose $\mathbf{H}_k$ is diagonal,

$$\mathbf{H}_k := \begin{bmatrix} \lambda_{k,1} & & 0 \\ & \ddots & \\ 0 & & \lambda_{k,d} \end{bmatrix},$$

- For each coordinate i, we have different step-size $\frac{\alpha_k}{\lambda_{k,i}}$ is the step-size.

Adaptive gradient descent(AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$)

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Adaptation across each coordinate

- When $\mathbf{H}_k = \mathbf{D}_k$, we adapt across each coordinate individually.
- Essentially, we have a finer treatment of the function we want to optimize.

Convergence rate for AdaGrad

Original convergence for a different function class

Consider a proper, convex function f such that it is G-Lipschitz continuous (NOT L-smooth). Let $D = \max_k \|\mathbf{x}^k - \mathbf{x}^\star\|_2$ and $\alpha_k = \frac{D}{\sqrt{2}}$. Define $\bar{\mathbf{x}}^k = (\sum_{i=1}^k \mathbf{x}^i)/k$. Then,

$$f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star) \leq \frac{1}{k}\sqrt{2D^2 \sum_{i=1}^k \|\nabla f(\mathbf{x}^i)\|_2^2} \leq \frac{\sqrt{2}DG}{\sqrt{k}}$$

A more familiar convergence result [13]

Assume f is L-smooth, $D = \max_t \|\mathbf{x}^k - \mathbf{x}^\star\|_2$ and $\alpha_k = \frac{D}{\sqrt{2}}$. Define $\bar{\mathbf{x}}^k = (\sum_{i=1}^k \mathbf{x}^i)/k$. Then,

$$f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star) \leq \frac{1}{k}\sqrt{2D^2 \sum_{i=1}^k \|\nabla f(\mathbf{x}^i)\|_2^2} \leq \frac{4D^2 L}{k}$$

AcceleGrad - Adaptive gradient + Accelerated gradient [14]

Motivation behind AcceleGrad

Is it possible to achieve acceleration for when f is L-smooth, without knowing the Lipschitz constant?

- The answer is yes! See advanced material (AcceleGrad) at the end.
- A rough comparison of the accelerated methods:

Accelerated Gradient algorithm

1. Choose $\mathbf{x}^0 = \mathbf{y}^0 \in \mathrm{dom}\,(f)$
2. For $k = 0, 1, \ldots$, iterate

$$\begin{cases} \mathbf{x}^{k+1} & = \mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} + \gamma_{k+1}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

for some proper choice of α and γ_{k+1}.

AcceleGrad (Accelerated Adaptive Gradient Method)

1. Set $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$
2. For $k = 0, 1, \ldots$, iterate

$$\begin{cases} \tau_k & := 1/\alpha_k \\ \mathbf{x}^{k+1} & = \tau_k \mathbf{z}^k + (1-\tau_k)\mathbf{y}^k \\ \mathbf{z}^{k+1} & = \mathbf{z}^k - \alpha_k \eta_k \nabla f(\mathbf{x}^k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} - \eta_k \nabla f(\mathbf{x}^k) \end{cases}$$

for $\alpha_k = (k+1)/4$ and

$$\eta_k = \frac{2D}{\sqrt{G^2 + \sum_{i=0}^{k} (\alpha_k)^2 \|\nabla f(\mathbf{x}^k)\|^2}}.$$

Performance of optimization algorithms

Time-to-reach ϵ

`time-to-reach` ϵ `= number of iterations to reach` ϵ $\times$ `per iteration time`

The **speed** of numerical solutions depends on two factors:

- **Convergence rate** determines the number of iterations needed to obtain an ϵ-optimal solution.
- **Per-iteration time** depends on the information oracles, implementation, and the computational platform.

In general, convergence rate and per-iteration time are inversely proportional.
Finding the **fastest** algorithm is tricky!

Performance of optimization algorithms (convex)

A non-exhaustive comparison:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
L-smooth	Gradient descent	Sublinear $(1/k)$	One gradient
	AdaGrad	Sublinear $(1/k)$	One gradient
	Accelerated GD	Sublinear $(1/k^2)$	One gradient
	AcceleGrad	Sublinear $(1/k^2)$	One gradient
	Newton method	Sublinear $(1/k)$, Quadratic	One gradient, one linear system
L-smooth and μ-strongly convex	Gradient descent	Linear (e^{-k})	One gradient
	Accelerated GD	Linear (e^{-k})	One gradient
	Newton method	Linear (e^{-k}), Quadratic	One gradient, one linear system

Gradient descent:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k),$$

where the stepsize is chosen appropriately, $\alpha \in (0, \frac{2}{L})$

AdaGrad:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha^k \nabla f(\mathbf{x}^k),$$

where scalar version of the step size is $\alpha^k = \frac{D}{\sqrt{\sum_{i=1}^{k} \|\nabla f(x^i)\|^2}}$

Performance of optimization algorithms (convex)

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Accelerated gradient descent:

$$\mathbf{x}^{k+1} = \mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k)$$
$$\mathbf{y}^{k+1} = \mathbf{x}^{k+1} + \gamma_{k+1}(\mathbf{x}^{k+1} - \mathbf{x}^k).$$

for some proper choice of α and γ_{k+1}.

AcceleGrad:

$$\mathbf{x}^{k+1} = \tau_k \mathbf{z}^k + (1-\tau_k)\mathbf{y}^k$$
$$\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha_k \eta_k \nabla f(\mathbf{x}^k)$$
$$\mathbf{y}^{k+1} = \mathbf{x}^{k+1} - \eta_k \nabla f(\mathbf{x}^k).$$

for $\alpha_k = (k+1)/4$, $\tau_k = 1/\alpha_k$ and $\eta_k = \dfrac{2D}{\sqrt{G^2 + \sum_{i=0}^{k} (\alpha_k)^2 \|\nabla f(\mathbf{x}^k)\|^2}}$.

Performance of optimization algorithms (convex)

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The main computation of the Newton method requires the solution of the linear system

$$\nabla^2 f(\mathbf{x}^k)\mathbf{p}^k = -\nabla f(\mathbf{x}^k)\ .$$

The gradient method for non-convex optimization

Remarks:
- Gradient descent does not match lower bounds in convex setting.
- How about non-convex problems?

Lower bounds for non-convex problems [4]

Assume f is L-gradient Lipschitz and non-convex. Then any first-order method must satisfy,

$$\|\nabla f(\mathbf{x}^k)\|^2 = \Omega\left(\frac{1}{k}\right)$$

Observations:
- Gradient descent is optimal for non-convex problems, up to some constant factor!
- Acceleration for non-convex, L-Lipschitz gradient functions is not as meaningful.

Recall: Gradient descent

Problem (Unconstrained optimization problem)

Consider the following minimization problem:

$$f^\star = \min_{\mathbf{x}\in\mathbb{R}^p} f(\mathbf{x})$$

$f(\mathbf{x})$ *is proper and closed.*

Gradient descent

Choose a starting point $\mathbf{x}^0$ and iterate

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k)$$

where α_k is a step-size to be chosen so that $\mathbf{x}^k$ converges to $\mathbf{x}^\star$.

	f **is** L**-smooth & convex**	f **is** L**-gradient Lipschitz & non-convex**
GD	$O(1/k)$ (fast)	$O(1/k)$ (optimal)
AGD	$O(1/k^2)$ (optimal)	$O(1/k)$ (optimal) [10]

Recall: Gradient descent

Problem (Unconstrained optimization problem)

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AGD	$O(1/k^2)$ (optimal)	$O(1/k)$ (optimal) [10]

Why should we study anything else?

Statistical learning with streaming data

- Recall that statistical learning seeks to find a $h^\star \in \mathcal{H}$ that minimizes the *expected* risk,

$$h^\star \in \arg\min_{h \in \mathcal{H}} \left\{ R(h) := \mathbb{E}_{(\mathbf{a},b)} \left[L(h(\mathbf{a}), b) \right] \right\}.$$

Abstract gradient method

$$h^{k+1} = h^k - \alpha_k \nabla R(h^k) = h^k - \alpha_k \mathbb{E}_{(\mathbf{a},b)} [\nabla L(h^k(\mathbf{a}), b)].$$

This can not be implemented in practice as the distribution of $(\mathbf{a}, b)$ is unknown.

Statistical learning with streaming data

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This can not be implemented in practice as the distribution of $(\mathbf{a}, b)$ is unknown.

- In practice, data can arrive in a *streaming* way.

A parametric example: Markowitz portfolio optimization

$$\mathbf{x}^\star := \min_{\mathbf{x} \in \mathcal{X}} \left\{ \mathbb{E}\left[|b - \langle \mathbf{x}, \mathbf{a} \rangle|^2 \right] \right\}$$

- $h_{\mathbf{x}}(\cdot) = \langle \mathbf{x}, \cdot \rangle$
- $b \in \mathbb{R}$ is the desired return & $\mathbf{a} \in \mathbb{R}^p$ are the stock returns
- $\mathcal{X}$ is intersection of the standard simplex and the constraint: $\langle \mathbf{x}, \mathbb{E}[\mathbf{a}] \rangle \geq \rho$.

Stochastic programming

Problem (**Mathematical formulation**)

Consider the following convex minimization problem:

$$f^\star = \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \mathbb{E}[f(\mathbf{x},\theta)] \right\}$$

- θ *is a random vector whose probability distribution is supported on set* Θ.
- $f(\mathbf{x}) := \mathbb{E}[f(\mathbf{x},\theta)]$ *is proper, closed, and convex.*
- *The solution set* $\mathcal{S}^\star := \{\mathbf{x}^\star \in \operatorname{dom}(f) : f(\mathbf{x}^\star) = f^\star\}$ *is nonempty.*

Stochastic gradient descent (SGD)

Stochastic gradient descent (SGD)

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k\in\mathbb{N}} \in]0, +\infty[^{\mathbb{N}}$.
2. For $k = 0, 1, \ldots$ perform:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$$

- $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient:

$$\mathbb{E}[G(\mathbf{x}^k, \theta_k)] = \nabla f(\mathbf{x}^k).$$

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- $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient:

$$\mathbb{E}[G(\mathbf{x}^k, \theta_k)] = \nabla f(\mathbf{x}^k).$$

Remarks:

- The cost of computing $G(\mathbf{x}^k, \theta_k)$ is n times cheaper than that of $\nabla f(\mathbf{x}^k)$.
- As $G(\mathbf{x}^k, \theta_k)$ is an unbiased estimate of the full gradient, SGD would perform well.
- We assume $\{\theta_k\}$ are jointly independent.
- SGD is not a monotonic descent method.

Example: Convex optimization with finite sums

Convex optimization with finite sums

The problem

$$\arg\min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{j=1}^{n} f_j(\mathbf{x}) \right\},$$

can be rewritten as

$$\arg\min_{\mathbf{x}\in\mathbb{R}^p} \{ f(\mathbf{x}) := \mathbb{E}_i[f_i(\mathbf{x})] \}, \qquad i \text{ is uniformly distributed over } \{1, 2, \cdots, n\}.$$

A stochastic gradient descent (SGD) variant for finite sums

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f_i(\mathbf{x}^k) \qquad i \text{ is uniformly distributed over} \{1, ..., n\}$$

Remarks:

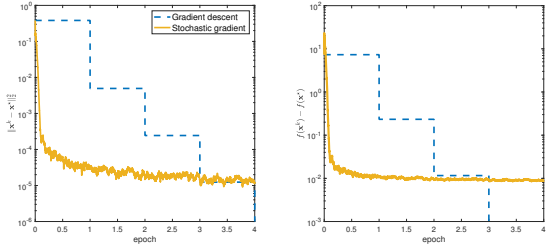
- Note: $\mathbb{E}_i[\nabla f_i(\mathbf{x}^k)] = \sum_{j=1}^{n} \nabla f_j(\mathbf{x}^k)/n = \nabla f(\mathbf{x}^k)$.
- The computational cost of SGD per iteration is p.

Synthetic least-squares problem

$$\min_{\mathbf{x}} \left\{ f(\mathbf{x}) := \frac{1}{2n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 : \mathbf{x} \in \mathbb{R}^p \right\}$$

Setup

- $\mathbf{A} := \mathrm{randn}(n, p)$ - standard Gaussian $\mathcal{N}(0, \mathbb{I})$, with $n = 10^4$, $p = 10^2$.
- $\mathbf{x}^\natural$ is 50 sparse with zero mean Gaussian i.i.d. entries, normalized to $\|\mathbf{x}^\natural\|_2 = 1$.
- $\mathbf{b} := \mathbf{A}\mathbf{x}^\natural + \mathbf{w}$, where $\mathbf{w}$ is Gaussian white noise with variance 1.



- 1 epoch $= 1$ pass over the full gradient

Convergence of SGD when the objective is not strongly convex

Theorem (decaying step-size [22])

Assume

- $\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \leq D^2$ *for all* k,
- $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] \leq M^2$ *(bounded gradient),*
- $\alpha_k = \alpha_0/\sqrt{k}$.

Then

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \leq \left(\frac{D^2}{\alpha_0} + \alpha_0 M^2\right) \frac{2 + \log k}{\sqrt{k}}.$$

Observation: ∘ $\mathcal{O}(1/\sqrt{k})$ rate is optimal for SGD if we do not consider the strong convexity.

Convergence of SGD for strongly convex problems I

Theorem (strongly convex objective, fixed step-size [3])

Assume

- f *is* μ*-strongly convex and* L*-smooth,*
- $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2]_2 \leq \sigma^2 + M\|\nabla f(\mathbf{x}^k)\|_2^2$ *(bounded variance),*
- $\alpha_k = \alpha \leq \frac{1}{LM}$.

Then

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \leq \frac{\alpha L \sigma^2}{2\mu} + (1 - \mu\alpha)^{k-1} \left(f(\mathbf{x}^1) - f^\star\right).$$

Observations:

- Converge fast (linearly) to a neighborhood around $\mathbf{x}^\star$
- Zero variance ($\sigma = 0$) $\Longrightarrow$ linear convergence
- Smaller step-sizes α $\Longrightarrow$ converge to a better point, but with a slower rate

Convergence of SGD for strongly convex problems II

Theorem (strongly convex objective, decaying step-size [3])

Assume

- f *is* μ*-strongly convex and* L*-smooth,*
- $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2]_2 \leq \sigma^2 + M\|\nabla f(\mathbf{x}^k)\|_2^2$ *(bounded variance),*
- $\alpha_k = \frac{c}{k_0+k}$ *with some appropriate constants* c *and* k_0*.*

Then

$$\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \leq \frac{C}{k+1},$$

where C *is a constant independent of* k*.*

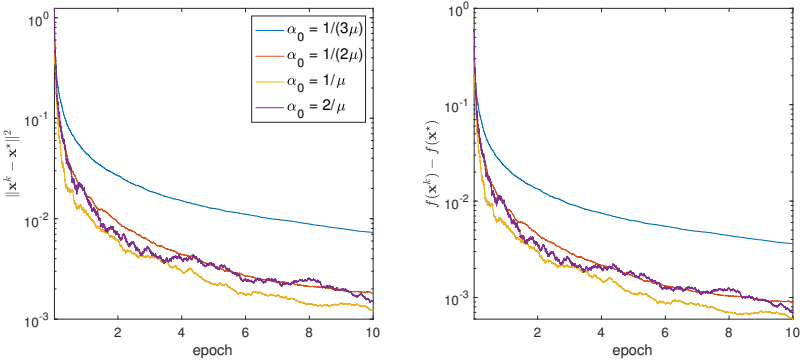
Observations:

- Using the smooth property,

$$\mathbb{E}[f(\mathbf{x}^k) - f(\mathbf{x}^\star)] \leq L\mathbb{E}[\|\mathbf{x}^k - \mathbf{x}^\star\|^2] \leq \frac{C}{k+1}.$$

- The rate is optimal if $\sigma^2 > 0$ with the assumption of strongly-convexity.

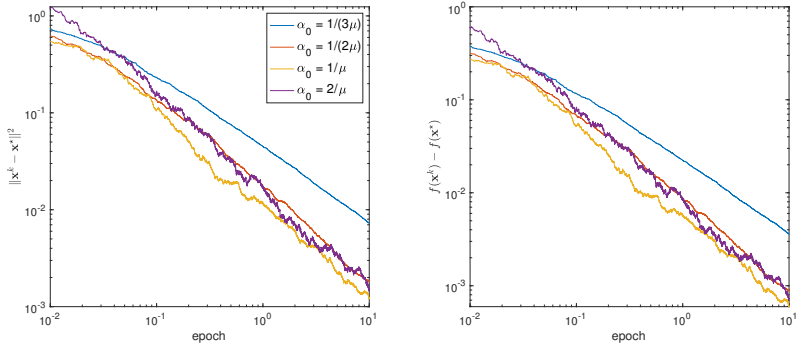
Example: SGD with different step sizes



Setup

- Synthetic least-squares problem as before
- $\alpha_k = \alpha_0/(k + k_0)$.

Example: SGD with different step sizes



Setup

- Synthetic least-squares problem as before
- $\alpha_k = \alpha_0/(k + k_0)$.

Observation: - $\alpha_0 = 1/\mu$ is the best choice.

Comparison with GD

$$f^\star := \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{j=1}^{n} f_j(\mathbf{x}) \right\}.$$

- f: μ-strongly convex with L-Lipschitz smooth.

	rate	iteration complexity	cost per iteration	total cost
GD	ρ^k	$\log(1/\epsilon)$	n	$n\log(1/\epsilon)$
SGD	$1/k$	$1/\epsilon$	1	$1/\epsilon$

Remark:
- SGD is more favorable when n is large — large-scale optimization problems

Motivation for SGD with Averaging

- SGD iterates tend to oscillate around global minimizers
- Averaging iterates can reduce the oscillation effect
- Two types of averaging:

$$\bar{\mathbf{x}}^k = \frac{1}{k}\sum_{j=1}^{k} \alpha_j \mathbf{x}^j \quad \text{(vanilla averaging)}$$

$$\bar{\mathbf{x}}^k = \frac{\sum_{j=1}^{k} \alpha_j \mathbf{x}^j}{\sum_{j=1}^{k} \alpha_j} \quad \text{(weighted averaging)}$$

Convergence for SGD-A I: non-strongly convex case

Stochastic gradient method with averaging (SGD-A)

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k\in\mathbb{N}} \in]0, +\infty[^{\mathbb{N}}$.
2a. For $k = 0, 1, \ldots$ perform:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$$

2b. $\bar{\mathbf{x}}^k = (\sum_{j=0}^k \alpha_j)^{-1} \sum_{j=0}^k \alpha_j \mathbf{x}^j$.

Theorem (Convergence of SGD-A [16])

Let $D = \|\mathbf{x}^0 - \mathbf{x}^\star\|$ *and* $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] \leq M^2$.
Then,

$$\mathbb{E}[f(\bar{\mathbf{x}}^{k+1}) - f(\mathbf{x}^\star)] \leq \frac{D^2 + M^2 \sum_{j=0}^k \alpha_j^2}{2 \sum_{j=0}^k \alpha_j}.$$

In addition, choosing $\alpha_k = D/(M\sqrt{k+1})$, *we get,*

$$\mathbb{E}[f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star)] \leq \frac{MD(2 + \log k)}{\sqrt{k}}.$$

Observation: ○ Same convergence rate with vanilla SGD.

Convergence for SGD-A II: strongly convex case

Stochastic gradient method with averaging (SGD-A)

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $(\alpha_k)_{k\in\mathbb{N}} \in]0, +\infty[^{\mathbb{N}}$.
2a. For $k = 0, 1, \ldots$ perform:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k).$$

2b. $\bar{\mathbf{x}}^k = \frac{1}{k}\sum_{j=1}^{k} \mathbf{x}^j$.

Theorem (Convergence of SGD-A [21])

Assume

- f *is* μ*-strongly convex,*
- $\mathbb{E}[\|G(\mathbf{x}^k, \theta_k)\|^2] \leq M^2$,
- $\alpha_k = \alpha_0/k$ *for some* $\alpha_0 \geq 1/\mu$.

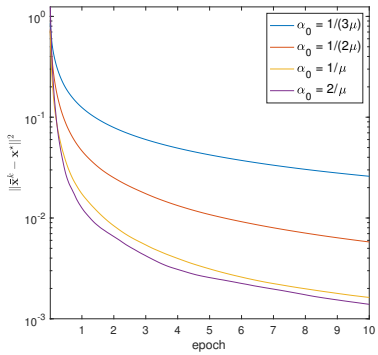
Then

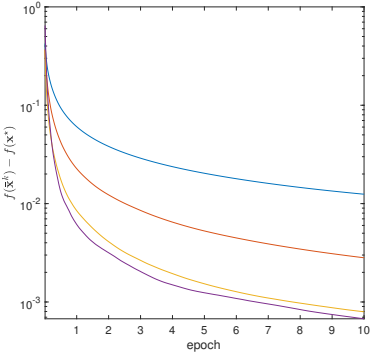
$$\mathbb{E}[f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star)] \leq \frac{\alpha_0 M^2(1 + \log k)}{2k}.$$

Observation: ○ Same convergence rate with vanilla SGD.

Example: SGD-A method with different step sizes

$$\min_{\mathbf{x}} \left\{ f(\mathbf{x}) := \frac{1}{2n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 : \mathbf{x} \in \mathbb{R}^p \right\}$$





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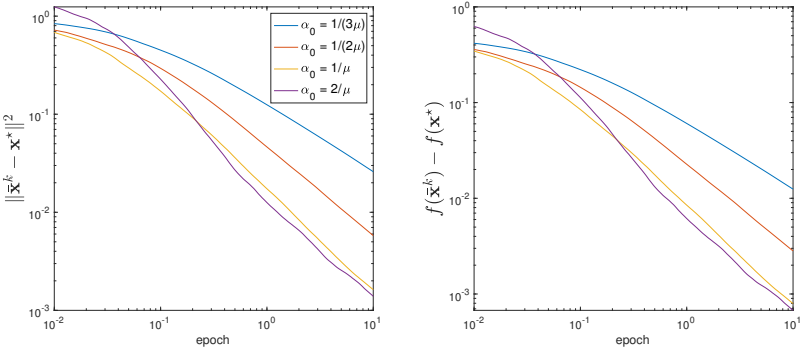

Setup

- Synthetic least-squares problem as before
- $\alpha_k = \alpha_0/(k + k_0)$.

Observations:

- SGD-A is more stable than SGD.
- $\alpha_0 = 2/\mu$ is the best choice.

Least mean squares algorithm

Least-square regression problem

Solve

$$\mathbf{x}^\star \in \arg\min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{2}\mathbb{E}_{(\mathbf{a},b)}(\langle \mathbf{a}, \mathbf{x}\rangle - b)^2 \right\},$$

given i.i.d. samples $\{(\mathbf{a}_j, b_j)\}_{j=1}^n$ (particularly in a streaming way).

Stochastic gradient method with averaging

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $\alpha > 0$.

2a. For $k = 1, \ldots, n$ perform:

$$\mathbf{x}^k = \mathbf{x}^{k-1} - \alpha \left(\langle \mathbf{a}_k, \mathbf{x}^{k-1}\rangle - b_k \right) \mathbf{a}_k.$$

2b. $\bar{\mathbf{x}}^k = \frac{1}{k+1} \sum_{j=0}^k \mathbf{x}^j$.

$O(1/n)$ convergence rate, without strongly convexity [2]

Let $\|\mathbf{a}_j\|_2 \leq R$ and $|\langle \mathbf{a}_j, \mathbf{x}^\star\rangle - b_j| \leq \sigma$ a.s.. Pick $\alpha = 1/(4R^2)$. Then

$$\mathbb{E} f(\bar{\mathbf{x}}^{n-1}) - f^* \leq \frac{2}{n} \left(\sigma\sqrt{p} + R\|\mathbf{x}^0 - \mathbf{x}^\star\|_2 \right)^2.$$

Popular SGD Variants

- Mini-batch SGD: For each iteration,

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \frac{1}{b} \sum_{\theta \in \Gamma} G(\mathbf{x}^k, \theta).$$

  - α_k: step-size
  - b : mini-batch size
  - Γ : a set of random variables θ of size b

- Accelerated SGD (Nesterov accelerated technique)

- SGD with Momentum

- Adaptive stochastic methods: AdaGrad...

SGD - Non-convex stochastic optimization

- SGD is not as well-studied for non-convex problems as for convex problems.
- There is a gap between SGD's practical performance and theoretical understanding.
- Recall SGD update rule:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta)$$

Theorem (A well-known result for SGD & Non-convex problems [9])

Let f be a non-convex and L-smooth function. Set $\alpha_k = \min\left\{\frac{1}{L}, \frac{C}{\sigma\sqrt{T}}\right\}$, $\forall k = 1, ..., T$, where σ^2 is the variance of the gradients and $C > 0$ is constant. Then,

$$\mathbb{E}[\|\nabla f(\mathbf{x}^R)\|^2] = O\left(\frac{\sigma}{\sqrt{T}}\right),$$

where $\mathbb{P}(R = k) = \frac{2\alpha_k - L\alpha_k^2}{\sum_{k=1}^{T}(2\alpha_k - L\alpha_k^2)}$.

Wrap up!

- The remaining slides in this lecture are advanced material.

*Enhancements

Two enhancements

1. Line-search for estimating L for both GD and AGD.
2. Restart strategies for AGD.

*Enhancements

Two enhancements

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2. Restart strategies for AGD.

When do we need a line-search procedure?

We can use a line-search procedure for both GD and AGD when

- L is **known** but it is expensive to evaluate;
- The global constant L usually does not capture the local behavior of f or it is **unknown**.

*Enhancements

Two enhancements

1. Line-search for estimating L for both GD and AGD.
2. Restart strategies for AGD.

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We can use a line-search procedure for both GD and AGD when

- L is **known** but it is expensive to evaluate;
- The global constant L usually does not capture the local behavior of f or it is **unknown**.

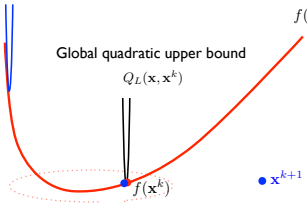
Line-search

At each iteration, we try to find a constant L_k that satisfies:

$$f(\mathbf{x}^{k+1}) \leq Q_{L_k}(\mathbf{x}^{k+1}, \mathbf{y}^k) := f(\mathbf{y}^k) + \langle \nabla f(\mathbf{y}^k), \mathbf{x}^{k+1} - \mathbf{y}^k \rangle + \frac{L_k}{2} \|\mathbf{x}^{k+1} - \mathbf{y}^k\|_2^2.$$

Here: $L_0 > 0$ is given (e.g., $L_0 := c \frac{\|\nabla f(\mathbf{x}^1) - \nabla f(\mathbf{x}^0)\|_2}{\|\mathbf{x}^1 - \mathbf{x}^0\|_2}$) for $c \in (0, 1]$.

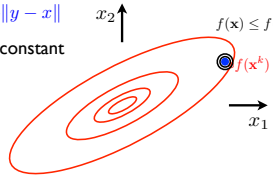
*How can we better adapt to the local geometry?



- $\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2} \|\mathbf{x} - \mathbf{x}^k\|_2^2 \right\}$

$\|\nabla f(x) - \nabla f(y)\| \leq L\|y - x\|$

L is a global worst-case constant



$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

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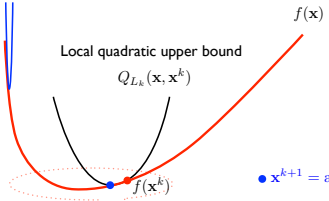

- $\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L_k}{2} \|\mathbf{x} - \mathbf{x}^k\|_2^2 \right\}$

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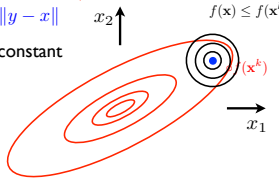
$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \nabla f(\mathbf{x}^k)^T(\mathbf{x} - \mathbf{x}^k) + \frac{L_k}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

applies only locally



*Enhancements

Why do we need a restart strategy?

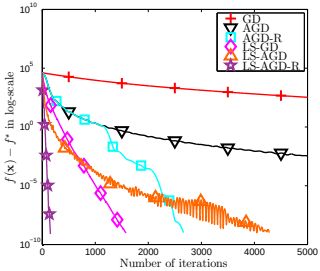
- AGD-μL requires knowledge of μ and AGD-L does not have optimal convergence for strongly convex f.
- AGD is non-monotonic (i.e., $f(\mathbf{x}^{k+1}) \leq f(\mathbf{x}^k)$ is not always satisfied).
- AGD has a periodic behavior, where the momentum depends on the local condition number $\kappa = L/\mu$.
- A **restart strategy** tries to reset this momentum whenever we observe high periodic behavior. We often use function values but other strategies are possible.

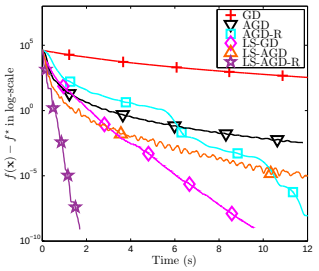
Restart strategies

1. **O'Donoghue - Candes's strategy [19]:** There are at least three options: Restart with fixed number of iterations, restart based on objective values, and restart based on a gradient condition.
2. **Giselsson-Boyd's strategy [11]:** Do not require $t_k = 1$ and do not necessary require function evaluations.
3. **Fercoq-Qu's strategy [8]:** Unconditional periodic restart for strongly convex functions. Do not require the strong convexity parameter.

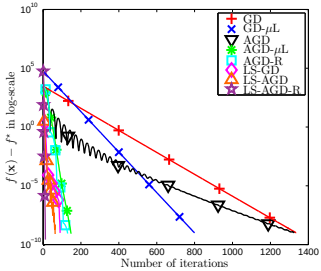
⋆Example: Ridge regression

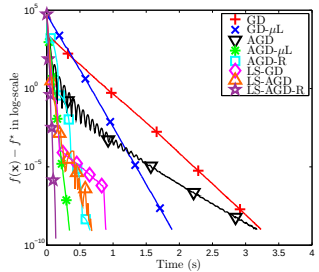
Case 1: $n = 500, p = 2000, \rho = 0$





Case 2: $n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T\mathbf{A})$





*AcceleGrad - Adaptive gradient + Accelerated gradient [14]

Motivation behind AcceleGrad

Is it possible to achieve acceleration when f is L-smooth, without knowing the Lipschitz constant?

AcceleGrad (Accelerated Adaptive Gradient Method)

Input : $\mathbf{x}^0 \in \mathcal{K}$, diameter D, weights $\{\alpha_k\}_{k\in\mathbb{N}}$, learning rate $\{\eta_k\}_{k\in\mathbb{N}}$

1. Set $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$

2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \tau_k & := 1/\alpha_k \\ \mathbf{x}^{k+1} & = \tau_k \mathbf{z}^k + (1-\tau_k)\mathbf{y}^k, \text{define } \mathbf{g}_k := \nabla f(\mathbf{x}^{k+1}) \\ \mathbf{z}^{k+1} & = \Pi_{\mathcal{K}}(\mathbf{z}^k - \alpha_k \eta_k \mathbf{g}_k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} - \eta_k \mathbf{g}_k \end{cases}$$

Output : $\overline{\mathbf{y}}^k \propto \sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1}$

where $\Pi_{\mathcal{K}}(\mathbf{y}) = \arg\min_{\mathbf{x}\in\mathcal{K}} \langle \mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}\rangle$ (projection onto $\mathcal{K}$).

Remark: ◦ This is essentially the **MD + GD** scheme [1], with an adaptive step size!

*AcceleGrad - Properties and convergence

Learning rate and weight computation

Assume that function f has uniformly bounded gradient norms $\|\nabla f(\mathbf{x}^k)\|^2 \leq G^2$, i.e., f is G-Lipschitz continuous. AcceleGrad uses the following weights and learning rate:

$$\alpha_k = \frac{k+1}{4}, \quad \eta_k = \frac{2D}{\sqrt{G^2 + \sum_{\tau=0}^{k} \alpha_\tau^2 \|\nabla f(\mathbf{x}_{\tau+1})\|^2}}$$

- Similar to RmsProp, AcceleGrad assignes greater weights to recent gradients.

Convergence rate of AcceleGrad

Assume that f is convex and L-smooth. Let K be a convex set with bounded diameter D, and assume $\mathbf{x}^\star \in K$. Define $\bar{\mathbf{y}}^k = (\sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1})/(\sum_{i=0}^{k-1} \alpha_i)$. Then,

$$f(\bar{\mathbf{y}}^k) - \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) \leq O\left(\frac{DG + LD^2 \log(LD/G)}{k^2}\right)$$

If f is only convex and G-Lipschitz, then

$$f(\bar{\mathbf{y}}^k) - \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) \leq O\left(GD\sqrt{\log k}/\sqrt{k}\right)$$

⋆Example: Logistic regression

Problem (Logistic regression)

Given $\mathbf{A} \in \{0,1\}^{n \times p}$ *and* $\mathbf{b} \in \{-1,+1\}^n$*, solve:*

$$f^\star := \min_{\mathbf{x},\beta} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^{n} \log\left(1 + \exp\left(-\mathbf{b}_j(\mathbf{a}_j^T \mathbf{x} + \beta)\right)\right) \right\}.$$

Real data

- Real data: a4a with $\mathbf{A} \in \mathbb{R}^{n \times d}$, where $n = 4781$ data points, $d = 122$ features
- All methods are run for $T = 10000$ iterations

*RMSProp - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

What could be improved over AdaGrad?

1. Gradients have equal weights in step size.
2. Consider a *steep* function, flat around minimum $\rightarrow$ slow convergence at flat region.

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AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$

1. Set $\mathbf{Q}_0 = 0$.
2. For $k = 0, 1, \ldots$, iterate

$$\begin{cases} \mathbf{Q}^k &= \mathbf{Q}^{k-1} + \operatorname{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

RMSProp

1. Set $\mathbf{Q}_0 = 0$.
2. For $k = 0, 1, \ldots$, iterate

$$\begin{cases} \mathbf{Q}^k &= \beta \mathbf{Q}^{k-1} + (1-\beta) \operatorname{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

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- RMSProp uses weighted averaging with constant β
- Recent gradients have greater importance

*ADAM - Adaptive moment estimation

Over-simplified idea of ADAM

RMSProp + 2nd order moment estimation = ADAM

*ADAM - Adaptive moment estimation

Over-simplified idea of ADAM

RMSProp + 2nd order moment estimation = ADAM

ADAM

Input. Step size α, exponential decay rates $\beta_1, \beta_2 \in [0, 1)$

1. Set $\mathbf{m}_0, \mathbf{v}_0 = 0$

2. For $k = 0, 1, \ldots$, iterate

$$
\begin{cases}
\mathbf{g}_k & = \nabla f(\mathbf{x}^{k-1}) \\
\mathbf{m}_k & = \beta_1 \mathbf{m}_{k-1} + (1-\beta_1)\mathbf{g}_k \leftarrow \text{1st order estimate} \\
\mathbf{v}_k & = \beta_2 \mathbf{v}_{k-1} + (1-\beta_2)\mathbf{g}_k^2 \leftarrow \text{2nd order estimate} \\
\hat{\mathbf{m}}_k & = \mathbf{m}_k/(1-\beta_1^k) \leftarrow \text{Bias correction} \\
\hat{\mathbf{v}}_k & = \mathbf{v}_k/(1-\beta_2^k) \leftarrow \text{Bias correction} \\
\mathbf{H}_k & = \sqrt{\hat{\mathbf{v}}_k} + \epsilon \\
\mathbf{x}^{k+1} & = \mathbf{x}^k - \alpha \hat{\mathbf{m}}_k / \mathbf{H}_k
\end{cases}
$$

Output : $\mathbf{x}^k$

(Every vector operation is an element-wise operation)

*Non-convergence of ADAM and a new method: AmsGrad

- It has been shown that ADAM may not converge for *some* objective functions [20].
- An ADAM alternative is proposed that is proved to be convergent [20].

AmsGrad

Input. Step size $\{\alpha_k\}_{k\in\mathbb{N}}$, exponential decay rates $\{\beta_{1,k}\}_{k\in\mathbb{N}}$, $\beta_2 \in [0,1)$

1. Set $\mathbf{m}_0 = 0, \mathbf{v}_0 = 0$ and $\hat{\mathbf{v}}_0 = 0$

2. For $k = 1, 2, \ldots$, iterate

$$\begin{cases} \mathbf{g}_k & = G(\mathbf{x}^k, \theta) \\ \mathbf{m}_k & = \beta_{1,k}\mathbf{m}_{k-1} + (1-\beta_{1,k})\mathbf{g}_k \leftarrow \text{1st order estimate} \\ \mathbf{v}_k & = \beta_2\mathbf{v}_{k-1} + (1-\beta_2)\mathbf{g}_k^2 \leftarrow \text{2nd order estimate} \\ \hat{\mathbf{v}}_k & = \max\{\hat{\mathbf{v}}_{k-1}, \mathbf{v}_k\} \text{ and } \hat{\mathbf{V}}_k = \mathsf{diag}(\hat{\mathbf{v}}_k) \\ \mathbf{H}_k & = \sqrt{\hat{\mathbf{v}}_k} \\ \mathbf{x}^{k+1} & = \Pi_{\mathcal{X}}^{\sqrt{\hat{\mathbf{V}}_k}}(\mathbf{x}^k - \alpha_k \hat{\mathbf{m}}_k / \mathbf{H}_k) \end{cases}$$

Output : $\mathbf{x}^k$

where $\Pi_{\mathcal{K}}^{\mathbf{A}}(\mathbf{y}) = \arg\min_{\mathbf{x}\in\mathcal{K}} \langle (\mathbf{x}-\mathbf{y}), \mathbf{A}(\mathbf{x}-\mathbf{y})\rangle$ (weighted projection onto $\mathcal{K}$).
(Every vector operation is an element-wise operation)

*AdaGrad & AmsGrad for non-convex optimization

Theorem (AdaGrad convergence rate: stochastic, non-convex [25])

Assume f is non-convex and L-smooth, such that $\|\nabla f(\mathbf{x})\|^2 \leq G^2$ and $f^\star = \inf_{\mathbf{x}} f(\mathbf{x}) > \infty$. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x},\theta) - \nabla f(\mathbf{x})\|^2 | \mathbf{x}\right] \leq \sigma^2$. Then with probability $1-\delta$,

$$\min_{i \in \{1,..,k-1\}} \|\nabla f(\mathbf{x}^i)\|^2 = \tilde{O}\left(\frac{\sigma}{\delta^{3/2}\sqrt{k}}\right)$$

- **Note:** As $1-\delta \to 1$, the rate deteriorates by a factor of $\delta^{-3/2}$.

Theorem (AmsGrad convergence rate 1: stochastic, non-convex [5])

Let $\mathbf{g}_k = G(x^k, \theta)$. Assume $|\mathbf{g}_{1,i}| > c > 0$, $\forall i \in [d]$ and $\|\mathbf{g}_k\| \leq G$. Consider a non-increasing sequence $\beta_{1,k}$ and $\beta_{1,k} \leq \beta_1 \in [0,1)$. Set $\alpha_k = 1/\sqrt{k}$. Then,

$$\min_{i \in \{1,..,k-1\}} \mathbb{E}\left[\|\nabla f(\mathbf{x}^i)\|^2\right] = O\left(\frac{\log k}{\sqrt{k}}\right).$$

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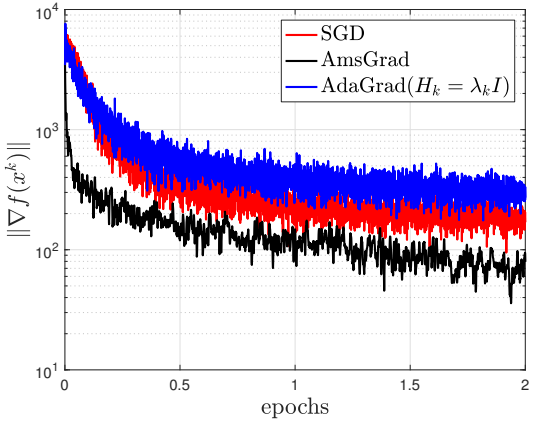
Theorem (AmsGrad convergence rate 2: stochastic, non-convex [26])

Consider $f : \mathbb{R}^d \to \mathbb{R}$ to be non-convex ans L-smooth. Assume $\|G(\mathbf{x},\theta)\|_\infty \leq G_\infty$ and set $\alpha_k = 1/\sqrt{dT}$. Also define $\mathbf{x}_{out} = \mathbf{x}^k$, for $k = 1,\dots,T$ with probability $\alpha^k / \sum_{i=1}^T \alpha_i$. Then,

$$\mathbb{E}\left[\|\nabla f(\mathbf{x}_{out})\|^2\right] = O\left(\sqrt{\frac{d}{T}}\right).$$

*Example: Logistic regression with non-convex regularizer

- Synthetic data: $\mathbf{A} \in \mathbb{R}^{n \times d}$, $n = 2000$, $d = 200$.
- Batch size: 20 samples.
- Algorithms: SGD, AdaGrad, AmsGrad.



*Adaptive methods for stochastic optimization

Remark

- Adaptive methods have extensive applications in stochastic optimization.
- We will see **another nature** of adaptive methods in this lecture.
- Mild additional assumption: **bounded variance** of gradient estimates.

*AdaGrad for stochastic optimization

- Only modification: $\nabla f(\mathbf{x}) \Rightarrow G(\mathbf{x}, \theta)$

AdaGrad with $\mathbf{H}_k = \lambda_k \mathbf{I}$ [13]

1. Set $Q^0 = 0$.

2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} Q^k & = Q^{k-1} + \|G(\mathbf{x}^k, \theta)\|^2 \\ \mathbf{H}_k & = \sqrt{Q^k}\mathbf{I} \\ \mathbf{x}^{k+1} & = \mathbf{x}_t - \alpha_k \mathbf{H}_k^{-1} G(\mathbf{x}^k, \theta) \end{cases}$$

Theorem (Convergence rate: stochastic, convex optimization [13])

Assume f is convex and L-smooth, such that minimizer of f lies in a convex, compact set $\mathcal{K}$ with diameter D. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x}, \theta) - \nabla f(\mathbf{x})\|^2 | \mathbf{x}\right] \leq \sigma^2$. Then,

$$\mathbb{E}[f(\mathbf{x}^k)] - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) = O\left(\frac{\sigma D}{\sqrt{k}}\right)$$

- AdaGrad is **adaptive** also in the sense that it adapts to nature of the oracle.

*AcceleGrad for stochastic optimization

- Similar to AdaGrad, replace $\nabla f(\mathbf{x}) \Rightarrow G(\mathbf{x}, \theta)$

AcceleGrad (Accelerated Adaptive Gradient Method)

Input : $\mathbf{x}^0 \in \mathcal{K}$, diameter D, weights $\{\alpha_k\}_{k\in\mathbb{N}}$, learning rate $\{\eta_k\}_{k\in\mathbb{N}}$

1. Set $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$

2. For $k = 0, 1, \ldots,$ iterate

$$\begin{cases} \tau_k & := 1/\alpha_k \\ \mathbf{x}^{k+1} & = \tau_t \mathbf{z}^k + (1-\tau_k)\mathbf{y}^k, \text{define } \mathbf{g}_k := \nabla f(\mathbf{x}^{k+1}) \\ \mathbf{z}^{k+1} & = \Pi_{\mathcal{K}}(\mathbf{z}^k - \alpha_k \eta_k \mathbf{g}_k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} - \eta_k \mathbf{g}_k \end{cases}$$

Output : $\overline{\mathbf{y}}^k \propto \sum_{i=0}^{k-1} \alpha_i \mathbf{y}^{i+1}$

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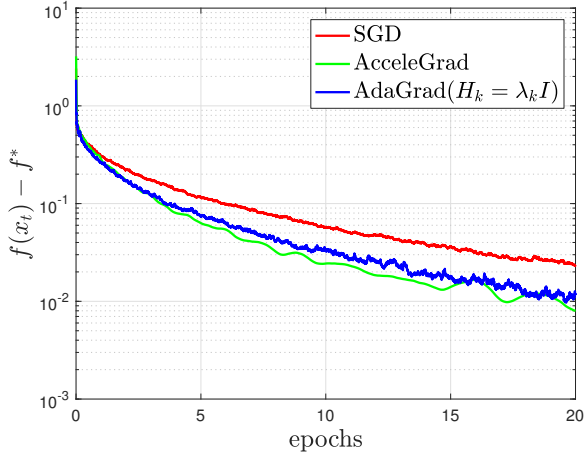
Assume f is convex and G-Lipschitz and that minimizer of f lies in a convex, compact set $\mathcal{K}$ with diameter D. Also consider bounded variance for unbiased gradient estimates, i.e., $\mathbb{E}\left[\|G(\mathbf{x},\theta) - \nabla f(\mathbf{x})\|^2 | \mathbf{x}\right] \leq \sigma^2$. Then,

$$\mathbb{E}[f(\overline{\mathbf{y}}^k)] - \min_{\mathbf{x}} f(\mathbf{x}) = O\left(\frac{GD\sqrt{\log k}}{\sqrt{k}}\right).$$

*Example: Synthetic least squares

- $\mathbf{A} \in \mathbb{R}^{n \times d}$, where $n = 200$ and $d = 50$.
- Number of epochs: 20.
- Algorithms: SGD, AdaGrad & AcceleGrad.



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- Fast (local) convergence but expensive per iteration cost
- **Useful** when warm-started near a solution

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Local quadratic approximation using the Hessian

- Obtain a local quadratic approximation using the second-order Taylor series approximation to $f(\mathbf{x}^k + \mathbf{p})$:

$$f(\mathbf{x}^k + \mathbf{p}) \approx f(\mathbf{x}^k) + \langle \mathbf{p}, \nabla f(\mathbf{x}^k) \rangle + \frac{1}{2} \langle \mathbf{p}, \nabla^2 f(\mathbf{x}^k) \mathbf{p} \rangle$$

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- The Newton direction is the vector $\mathbf{p}^k$ that minimizes $f(\mathbf{x}^k + \mathbf{p})$; assuming the Hessian $\nabla^2 f_k$ to be **positive definite**:

$$\nabla^2 f(\mathbf{x}^k) \mathbf{p}^k = -\nabla f(\mathbf{x}^k) \quad \Leftrightarrow \quad \mathbf{p}^k = -\left(\nabla^2 f(\mathbf{x}^k)\right)^{-1} \nabla f(\mathbf{x}^k)$$

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- A unit step-size $\alpha_k = 1$ can be chosen near convergence:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \left(\nabla^2 f(\mathbf{x}^k)\right)^{-1} \nabla f(\mathbf{x}^k) \, .$$

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Remark

- For $f \in \mathcal{F}_L^{2,1}$ but $f \notin \mathcal{F}_{L,\mu}^{2,1}$, the Hessian may not always be positive definite.

*(Local) Convergence of Newton method

Lemma

Assume f is a twice differentiable convex function with minimum at $\mathbf{x}^\star$ such that:

- $\nabla^2 f(\mathbf{x}^\star) \succeq \mu \mathbf{I}$ *for some* $\mu > 0$,
- $\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\|_{2\to 2} \leq M\|\mathbf{x} - \mathbf{y}\|_2$ *for some constant* $M > 0$ *and all* $\mathbf{x}, \mathbf{y} \in \mathrm{dom}(f)$.

Moreover, assume the starting point $\mathbf{x}^0 \in \mathrm{dom}(f)$ *is such that* $\|\mathbf{x}^0 - \mathbf{x}^\star\|_2 < \frac{2\mu}{3M}$.
Then, the Newton method iterates converge **quadratically**:

$$\|\mathbf{x}^{k+1} - \mathbf{x}^\star\| \leq \frac{M\|\mathbf{x}^k - \mathbf{x}^\star\|_2^2}{2\left(\mu - M\|\mathbf{x}^k - \mathbf{x}^\star\|_2\right)}.$$

Remark

This is the fastest convergence rate we have seen so far, but it requires to solve a $p \times p$ linear system at each iteration, $\nabla^2 f(\mathbf{x}^k)\mathbf{p}^k = -\nabla f(\mathbf{x}^k)$!

*Locally quadratic convergence of the Newton method–I

Newton's method local quadratic convergence - Proof [18]

Since $\nabla f(\mathbf{x}^\star) = 0$ we have

$$\begin{aligned}\mathbf{x}^{k+1} - \mathbf{x}^\star &= \mathbf{x}^k - \mathbf{x}^\star - (\nabla^2 f(\mathbf{x}^k))^{-1}\nabla f(\mathbf{x}^k) \\ &= (\nabla^2 f(\mathbf{x}^k))^{-1}\left(\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^\star) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star))\right)\end{aligned}$$

By Taylor's theorem, we also have

$$\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star) = \int_0^1 \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^\star - \mathbf{x}^k))(\mathbf{x}^k - \mathbf{x}^\star)dt$$

Combining the two above, we obtain

$$\begin{aligned}&\|\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^\star) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star))\| \\ &= \left\| \int_0^1 \left(\nabla^2 f(\mathbf{x}^k) - \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^\star - \mathbf{x}^k))\right)(\mathbf{x}^k - \mathbf{x}^\star)dt \right\| \\ &\leq \int_0^1 \left\| \nabla^2 f(\mathbf{x}^k) - \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^\star - \mathbf{x}^k)) \right\| \|\mathbf{x}^k - \mathbf{x}^\star\| dt \\ &\leq M\|\mathbf{x}^k - \mathbf{x}^\star\|^2 \int_0^1 t dt = \frac{1}{2}M\|\mathbf{x}^k - \mathbf{x}^\star\|^2\end{aligned}$$

*Locally quadratic convergence of the Newton method–II

Newton's method local quadratic convergence - Proof [18].

- Recall

$$\mathbf{x}^{k+1} - \mathbf{x}^\star = (\nabla^2 f(\mathbf{x}^k))^{-1} \left(\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^\star) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star)) \right)$$

$$\|\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^\star) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^\star))\| \leq \frac{1}{2} M \|\mathbf{x}^k - \mathbf{x}^\star\|^2$$

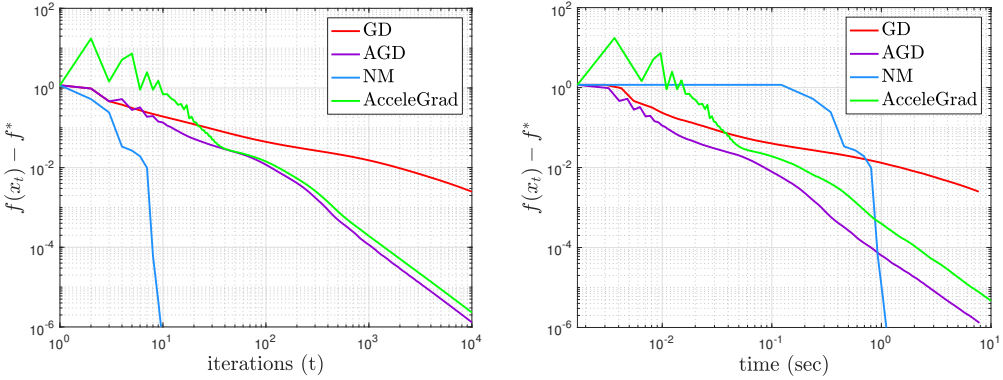
- Since $\nabla^2 f(\mathbf{x}^\star)$ is nonsingular, there must exist a radius r such that $\|(\nabla^2 f(\mathbf{x}^k))^{-1}\| \leq 2\|(\nabla^2 f(\mathbf{x}^\star))^{-1}\|$ for all $\mathbf{x}^k$ with $\|\mathbf{x}^k - \mathbf{x}^\star\| \leq r$.
- Substituting, we obtain

$$\|\mathbf{x}^{k+1} - \mathbf{x}^\star\| \leq M\|(\nabla^2 f(\mathbf{x}^\star))^{-1}\|\|\mathbf{x}^k - \mathbf{x}^\star\|^2 = \widetilde{M}\|\mathbf{x}^k - \mathbf{x}^\star\|^2,$$

  where $\widetilde{M} = M\|(\nabla^2 f(\mathbf{x}^\star))^{-1}\|$.
- If we choose $\|\mathbf{x}^0 - \mathbf{x}^\star\| \leq \min(r, 1/(2\widetilde{M}))$, we obtain by induction that the iterates $\mathbf{x}^k$ converge quadratically to $\mathbf{x}^\star$.

□

*Example: Logistic regression - GD, AGD, AcceleGrad + NM



Parameters

- Newton's method: maximum number of iterations 30, tolerance 10^{-6}.
- For GD, AGD & AcceleGrad: maximum number of iterations 10000, tolerance 10^{-6}.
- Ground truth: Get a high accuracy approximation of $\mathbf{x}^\star$ and $f^\star$ by applying Newton's method for 200 iterations.

Approximating Hessian: Quasi-Newton methods

Quasi-Newton methods use an approximate Hessian oracle and can be more scalable.

- Useful for $f(\mathbf{x}) := \sum_{i=1}^{n} f_i(\mathbf{x})$ with $n \gg p$.

Main ingredients

Quasi-Newton direction:

$$\mathbf{p}^k = -\mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) = -\mathbf{B}_k \nabla f(\mathbf{x}^k).$$

- Matrix $\mathbf{H}_k$, or its inverse $\mathbf{B}_k$, undergoes low-rank updates:
  - Rank 1 or 2 updates: famous Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm.
  - Limited memory BFGS (L-BFGS).
- Line-search: The step-size α_k is chosen to satisfy the **Wolfe conditions**:

$$f(\mathbf{x}^k + \alpha_k \mathbf{p}^k) \leq f(\mathbf{x}^k) + c_1 \alpha_k \langle \nabla f(\mathbf{x}^k), \mathbf{p}^k \rangle \qquad \text{(sufficient decrease)}$$

$$\langle \nabla f(\mathbf{x}^k + \alpha_k \mathbf{p}^k), \mathbf{p}^k \rangle \geq c_2 \langle \nabla f(\mathbf{x}^k), \mathbf{p}^k \rangle \qquad \text{(curvature condition)}$$

  with $0 < c_1 < c_2 < 1$. For quasi-Newton methods, we usually use $c_1 = 0.1$.
- Convergence is guaranteed under the Dennis & Moré condition [6].
- For more details on quasi-Newton methods, see Nocedal&Wright's book [18].

*Quasi-Newton methods

How do we update $\mathbf{B}_{k+1}$?

Suppose we have (note the coordinate change from $\mathbf{p}$ to $\bar{\mathbf{p}}$)

$$m_{k+1}(\bar{\mathbf{p}}) := f(\mathbf{x}^{k+1}) + \langle \nabla f(\mathbf{x}^{k+1}), \bar{\mathbf{p}} - \mathbf{x}^{k+1} \rangle + \frac{1}{2} \left\langle \mathbf{B}_{k+1}(\bar{\mathbf{p}} - \mathbf{x}^{k+1}), (\bar{\mathbf{p}} - \mathbf{x}^{k+1}) \right\rangle .$$

We require the gradient of m_{k+1} to match the gradient of f at $\mathbf{x}^k$ and $\mathbf{x}^{k+1}$.

- $\nabla m_{k+1}(\mathbf{x}^{k+1}) = \nabla f(\mathbf{x}^{k+1})$ as desired;
- For $\mathbf{x}^k$, we have
$$\nabla m_{k+1}(\mathbf{x}^k) = \nabla f(\mathbf{x}^{k+1}) + \mathbf{B}_{k+1}(\mathbf{x}^k - \mathbf{x}^{k+1})$$
which must be equal to $\nabla f(\mathbf{x}^k)$.
- Rearranging, we have that $\mathbf{B}_{k+1}$ must satisfy the **secant equation**
$$\mathbf{B}_{k+1}\mathbf{s}^k = \mathbf{y}^k$$
where $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$ and $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$.
- The secant equation can be satisfied with a positive definite matrix $\mathbf{B}_{k+1}$ only if $\langle \mathbf{s}^k, \mathbf{y}^k \rangle > 0$, which is guaranteed to hold if the step-size α_k satisfies the Wolfe conditions.

*Quasi-Newton methods

BFGS method [18] (from Broyden, Fletcher, Goldfarb & Shanno)

The BFGS method arises from directly updating $\mathbf{H}_k = \mathbf{B}_k^{-1}$. The update on the inverse $\mathbf{B}$ is found by solving

$$\min_{\mathbf{H}} \|\mathbf{H} - \mathbf{H}_k\|_{\mathbf{W}} \quad \text{subject to } \mathbf{H} = \mathbf{H}^T \text{ and } \mathbf{H}\mathbf{y}^k = \mathbf{s}^k \tag{4}$$

The solution is a rank-2 update of the matrix $\mathbf{H}_k$:

$$\mathbf{H}_{k+1} = \mathbf{V}_k^T \mathbf{H}_k \mathbf{V}_k + \eta_k \mathbf{s}^k (\mathbf{s}^k)^T \ ,$$

where $\mathbf{V}_k = \mathbf{I} - \eta_k \mathbf{y}^k (\mathbf{s}^k)^T$.

- Initialization of $\mathbf{H}_0$ is an art. We can choose to set it to be an approximation of $\nabla^2 f(\mathbf{x}^0)$ obtained by finite differences or just a multiple of the identity matrix.

*Quasi-Newton methods

BFGS method [18] (from Broyden, Fletcher, Goldfarb & Shanno)

The BFGS method arises from directly updating $\mathbf{H}_k = \mathbf{B}_k^{-1}$. The update on the inverse $\mathbf{B}$ is found by solving

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The solution is a rank-2 update of the matrix $\mathbf{H}_k$:

$$\mathbf{H}_{k+1} = \mathbf{V}_k^T \mathbf{H}_k \mathbf{V}_k + \eta_k \mathbf{s}^k (\mathbf{s}^k)^T \ ,$$

where $\mathbf{V}_k = \mathbf{I} - \eta_k \mathbf{y}^k (\mathbf{s}^k)^T$.

Theorem (Convergence of BFGS)

Let $f \in \mathcal{C}^2$. Assume that the BFGS sequence $\{\mathbf{x}^k\}$ converges to a point $\mathbf{x}^\star$ and $\sum_{k=1}^{\infty} \|\mathbf{x}^k - \mathbf{x}^\star\| \leq \infty$. Assume also that $\nabla^2 f(\mathbf{x})$ is Lipschitz continuous at $\mathbf{x}^\star$. Then $\mathbf{x}^k$ converges to $\mathbf{x}^\star$ at a **superlinear** *rate.*

Remarks

The proof shows that given the assumptions, the BFGS updates for $\mathbf{B}_k$ satisfy the Dennis & Moré condition, which in turn implies superlinear convergence.

*L-BFGS

Challenges for BFGS

- BFGS approach stores and applies a dense $p \times p$ matrix $\mathbf{H}_k$.
- When p is very large, $\mathbf{H}_k$ can prohibitively expensive to store and apply.

L(imited memory)-BFGS

- Do not store $\mathbf{H}_k$, but keep only the m most recent pairs $\{(\mathbf{s}^i, \mathbf{y}^i)\}$.
- Compute $\mathbf{H}_k \nabla f(\mathbf{x}_k)$ by performing a sequence of operations with $\mathbf{s}^i$ and $\mathbf{y}^i$:
  - Choose a temporary initial approximation $\mathbf{H}_k^0$.
  - Recursively apply $\mathbf{H}_{k+1} = \mathbf{V}_k^T \mathbf{H}_k \mathbf{V}_k + \eta_k \mathbf{s}^k (\mathbf{s}^k)^T$, m times starting from $\mathbf{H}_k^0$:

$$\begin{aligned}\mathbf{H}_k = &\left(\mathbf{V}_{k-1}^T \cdots \mathbf{V}_{k-m}^T\right) \mathbf{H}_k^0 \left(\mathbf{V}_{k-m} \cdots \mathbf{V}_{k-1}\right) \\ &+ \eta_{k-m} \left(\mathbf{V}_{k-1}^T \cdots \mathbf{V}_{k-m+1}^T\right) \mathbf{s}^{k-m} (\mathbf{s}^{k-m})^T \left(\mathbf{V}_{k-m+1} \cdots \mathbf{V}_{k-1}\right) \\ &+ \cdots \\ &+ \eta_{k-1} \mathbf{s}^{k-1} (\mathbf{s}^{k-1})^T\end{aligned}$$

  - From the previous expression, we can compute $\mathbf{H}_k \nabla f(\mathbf{x}^k)$ recursively.
- Replace the oldest element in $\{\mathbf{s}^i, \mathbf{y}^i\}$ with $(\mathbf{s}^k, \mathbf{y}^k)$.
- From practical experience, $m \in (3, 50)$ does the trick.

*L-BFGS: A quasi-Newton method

Procedure for computing $\mathbf{H}_k \nabla f(\mathbf{x}^k)$

0. Recall $\eta_k = 1/\langle \mathbf{y}^k, \mathbf{s}^k \rangle$.
1. $\mathbf{q} = \nabla f(\mathbf{x}^k)$.
2. For $i = k-1, \ldots, k-m$

$$\begin{aligned} \alpha_i &= \eta_i \langle \mathbf{s}^i, \mathbf{q} \rangle \\ \mathbf{q} &= \mathbf{q} - \alpha_i \mathbf{y}^i. \end{aligned}$$

3. $\mathbf{r} = \mathbf{H}_k^0 \mathbf{q}$.
4. For $i = k-m, \ldots, k-1$

$$\begin{aligned} \beta &= \eta_i \langle \mathbf{y}^i, \mathbf{r} \rangle \\ \mathbf{r} &= \mathbf{r} + (\alpha_i - \beta)\mathbf{s}^i. \end{aligned}$$

5. $\mathbf{H}_k \nabla f(\mathbf{x}^k) = \mathbf{r}$.

Remarks

- Apart from the step $\mathbf{r} = \mathbf{H}_k^0 \mathbf{q}$, the algorithm requires only $4mp$ multiplications.
- If $\mathbf{H}_k^0$ is chosen to be diagonal, another p multiplications are needed.
- An effective initial choice is $\mathbf{H}_k^0 = \gamma_k \mathbf{I}$, where

$$\gamma_k = \frac{\langle \mathbf{s}^{k-1}, \mathbf{y}^{k-1} \rangle}{\langle \mathbf{y}^{k-1}, \mathbf{y}^{k-1} \rangle}$$

*L-BFGS: A quasi-Newton method

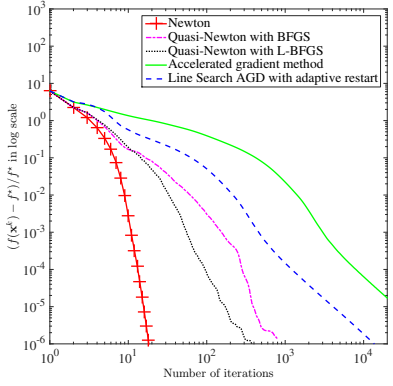
L-BFGS

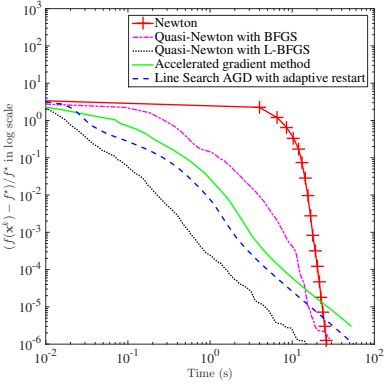
1. Choose starting point $\mathbf{x}^0$ and $m > 0$.
2. For $k = 0, 1, \ldots$
   - **2.a** Choose $\mathbf{H}_k^0$.
   - **2.b** Compute $\mathbf{p}^k = -\mathbf{H}_k \nabla f(\mathbf{x}^k)$ using the previous algorithm.
   - **2.c** Set $\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k \mathbf{p}^k$, where α_k satisfies the Wolfe conditions.
     if $k > m$, discard the pair $\{\mathbf{s}^{k-m}, \mathbf{p}^{k-m}\}$ from storage.
   - **2.d** Compute and store $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$, $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$.

Warning

L-BFGS updates does not guarantee positive semidefiniteness of the variable metric $\mathbf{H}_k$ in contrast to BFGS.

⋆Example: Logistic regression - numerical results





Parameters

- For BFGS, L-BFGS and Newton's method: maximum number of iterations 200, tolerance 10^{-6}. L-BFGS memory $m = 50$.
- For accelerated gradient method: maximum number of iterations 20000, tolerance 10^{-6}.
- Ground truth: Get a high accuracy approximation of $\mathbf{x}^\star$ and $f^\star$ by applying Newton's method for 200 iterations.

*Performance of optimization algorithms

Time-to-reach ϵ

`time-to-reach` ϵ `= number of iterations to reach` ϵ $\times$ `per iteration time`

The **speed** of numerical solutions depends on two factors:

- **Convergence rate** determines the number of iterations needed to obtain an ϵ-optimal solution.
- **Per-iteration time** depends on the information oracles, implementation, and the computational platform.

In general, convergence rate and per-iteration time are inversely proportional.
Finding the **fastest** algorithm is tricky! A non-exhaustive illustration:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
L-smooth	Gradient descent	Sublinear $(1/k)$	One gradient
	Accelerated GD	Sublinear $(1/k^2)$	One gradient
	Quasi-Newton	Superlinear	One gradient, rank-2 update
	Newton method	Sublinear $(1/k)$, Quadratic	One gradient, one linear system
L-smooth and μ-strongly convex	Gradient descent	Linear (e^{-k})	One gradient
	Accelerated GD	Linear (e^{-k})	One gradient
	Quasi-Newton	Superlinear	One gradient, rank-2 update
	Newton method	Linear (e^{-k}), Quadratic	One gradient, one linear system

*Performance of optimization algorithms

A non-exhaustive comparison:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
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	Accelerated GD	Linear (e^{-k})	One gradient
	Quasi-Newton	Superlinear	One gradient, rank-2 update
	Newton method	Linear (e^{-k}), Quadratic	One gradient, one linear system

Accelerated gradient descent:

$$\mathbf{x}^{k+1} = \mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k)$$
$$\mathbf{y}^{k+1} = \mathbf{x}^{k+1} + \alpha_{k+1}(\mathbf{x}^{k+1} - \mathbf{x}^k).$$

for some proper choice of α and α_{k+1}.

*Performance of optimization algorithms

A non-exhaustive comparison:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
L-smooth	Gradient descent	Sublinear $(1/k)$	One gradient
	Accelerated GD	Sublinear $(1/k^2)$	One gradient
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	Quasi-Newton	Superlinear	One gradient, rank-2 update
	Newton method	Linear (e^{-k}), Quadratic	One gradient, one linear system

Main computations of the Quasi-Newton method is given by

$$\mathbf{p}^k = -\mathbf{B}_k^{-1} \nabla f(\mathbf{x}^k) \ ,$$

where $\mathbf{B}_k^{-1}$ is updated at each iteration by adding a rank-2 matrix.

*Performance of optimization algorithms

A non-exhaustive comparison:

Assumptions on f	Algorithm	Convergence rate	Iteration complexity
L-smooth	Gradient descent	Sublinear $(1/k)$	One gradient
	Accelerated GD	Sublinear $(1/k^2)$	One gradient
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L-smooth and μ-strongly convex	Gradient descent	Linear (e^{-k})	One gradient
	Accelerated GD	Linear (e^{-k})	One gradient
	Quasi-Newton	Superlinear	One gradient, rank-2 update
	Newton method	Linear (e^{-k}), Quadratic	One gradient, one linear system

The main computation of the Newton method requires the solution of the linear system

$$\nabla^2 f(\mathbf{x}^k)\mathbf{p}^k = -\nabla f(\mathbf{x}^k) \; .$$

*Randomized Kaczmarz algorithm

Problem

Given a full-column-rank matrix $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $b \in \mathbb{R}^n$, solve the linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}.$$

Notations: $\mathbf{b} := (b_1, \ldots, b_n)^T$ and $\mathbf{a}_j^T$ is the j-th row of $\mathbf{A}$.

Randomized Kaczmarz algorithm (RKA)

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$.
2. For $k = 0, 1, \ldots$ perform:
2a. Pick $j_k \in \{1, \cdots, n\}$ randomly with $\Pr(j_k = i) = \|\mathbf{a}_i\|_2^2 / \|\mathbf{A}\|_F^2$
2b. $\mathbf{x}^{k+1} = \mathbf{x}^k - \left(\langle \mathbf{a}_{j_k}, \mathbf{x}^k \rangle - b_{j_k}\right) \mathbf{a}_{j_k} / \|\mathbf{a}_{j_k}\|_2^2$.

Linear convergence [23]

Let $\mathbf{x}^\star$ be the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ and $\kappa = \|\mathbf{A}\|_F \|\mathbf{A}^{-1}\|$. Then

$$\mathbb{E}\|\mathbf{x}^k - \mathbf{x}^\star\|_2^2 \leq (1 - \kappa^{-2})^k \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2$$

- RKA can be seen as a particular case of SGD [15].

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