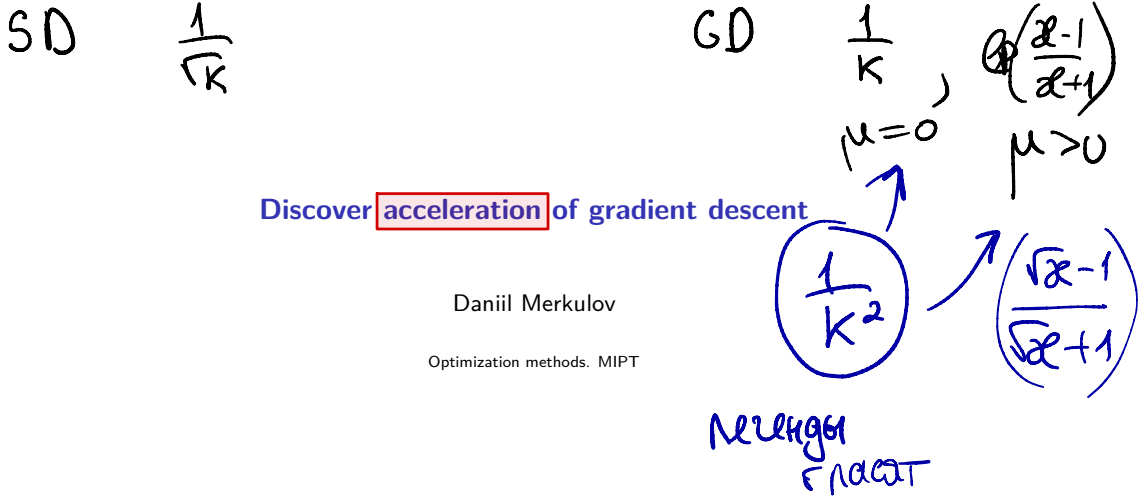
Discover acceleration of gradient descent

Daniil Merkulov

Optimization methods. MIPT



Coordinate shift

Consider the following quadratic optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}^d_{++}.$$

$x^* = A^{-1} b$

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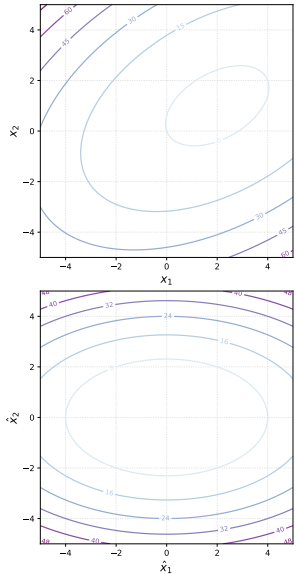
- Firstly, without loss of generality we can set $c = 0$, which will or affect optimization process.



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$$A = Q \Lambda Q^T$$

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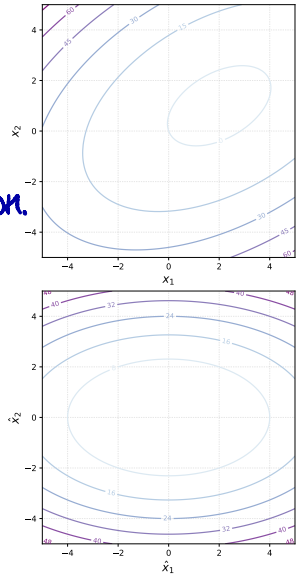

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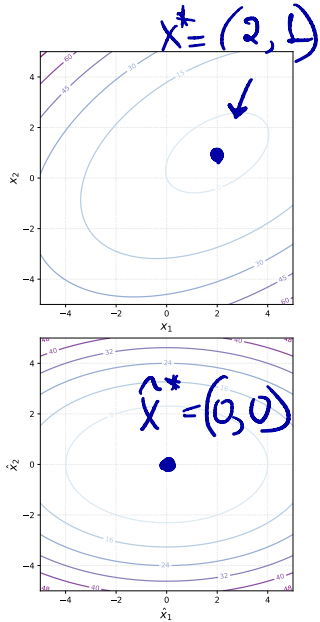
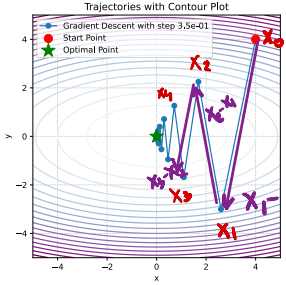
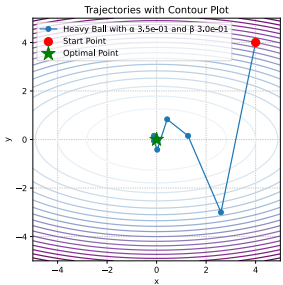
- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^T(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.

$$\begin{aligned} f(\hat{x}) &= \frac{1}{2}(Q\hat{x} + x^*)^\top A(Q\hat{x} + x^*) - b^\top(Q\hat{x} + x^*) \\ &= \frac{1}{2}\hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2}(x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^* \\ &= \frac{1}{2}\hat{x}^T \Lambda \hat{x} \end{aligned}$$



Polyak Heavy ball method





Let's introduce the idea of momentum, proposed by Polyak in 1964. Recall that the momentum update is

$$x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta(x_k - x_{k-1}).$$

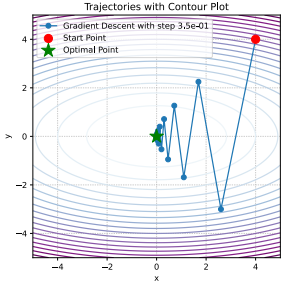
$$x_k = x_{k-1} - \alpha \nabla f(x_{k-1}) + \beta(x_{k-1} - x_{k-2})$$

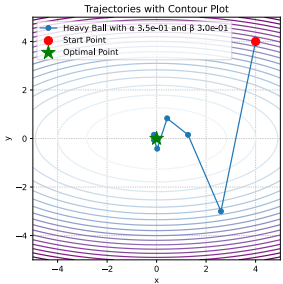
$$= x_k - \alpha \nabla f(x_k) + \beta \cdot (-\alpha \nabla f(x_{k-1}) + \beta(x_{k-1} - x_{k-2}))$$

$$= x_k - \alpha \nabla f(x_k) - \alpha \cdot \beta \nabla f(x_{k-1}) + \beta^2 (x_{k-1} - x_{k-2}) =$$

$$= x_k - \alpha \left[\nabla f(x_k) + \beta \cdot \nabla f(x_{k-1}) + \beta^2 \nabla f(x_{k-2}) + \beta^3 \dots \right]$$

Polyak Heavy ball method





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$$\nabla f(x_k) = \nabla f(\hat{x}_k) = \Lambda \hat{x}_k$$

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Which is in our case is

$$\hat{x}_{k+1} = \hat{x}_k - \alpha \Lambda \hat{x}_k + \beta(\hat{x}_k - \hat{x}_{k-1}) = (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta \hat{x}_{k-1}$$

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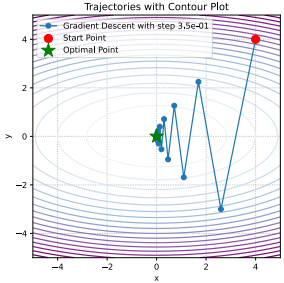

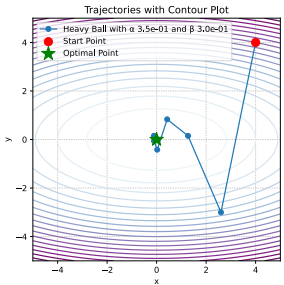

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$$\hat{x}_{k+1} = \hat{x}_k - \alpha\Lambda\hat{x}_k + \beta(\hat{x}_k - \hat{x}_{k-1}) = (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta\hat{x}_{k-1}$$

This can be rewritten as a follows

$$\begin{cases} \hat{x}_{k+1} = (I - \alpha\Lambda + \beta I)\hat{x}_k - \beta\hat{x}_{k-1}, \\ \hat{x}_k = \hat{x}_k. \end{cases}$$

Let's use the following notation $\hat{z}_k = \begin{bmatrix} \hat{x}_{k+1} \\ \hat{x}_k \end{bmatrix}$. Therefore $\hat{z}_{k+1} = M\hat{z}_k$, where the iteration matrix M is:

$$M = \begin{bmatrix} I - \alpha\Lambda + \beta I & -\beta I \\ I & 0_d \end{bmatrix}.$$

Reduction to a scalar case

Note, that M is $2d \times 2d$ matrix with 4 block-diagonal matrices of size $d \times d$ inside. It means, that we can rearrange the order of coordinates to make M block-diagonal in the following form. Note that in the equation below, the matrix M denotes the same as in the notation above, except for the described permutation of rows and columns. We use this slight abuse of notation for the sake of clarity.

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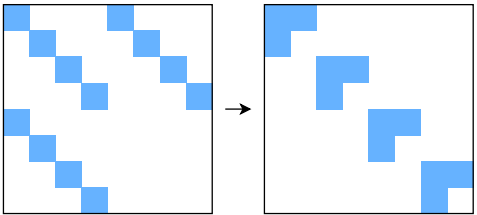


Figure 1: Illustration of matrix M rearrangement

$$\begin{bmatrix} \hat{x}_k^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \to \begin{bmatrix} \hat{x}_k^{(1)} \\ \hat{x}_{k-1}^{(1)} \\ \vdots \\ \hat{x}_k^{(d)} \\ \hat{x}_{k-1}^{(d)} \end{bmatrix} \qquad M = \begin{bmatrix} M_1 & & & \\ & M_2 & & \\ & & \dots & \\ & & & M_d \end{bmatrix}$$

where $\hat{x}_k^{(i)}$ is i-th coordinate of vector $\hat{x}_k \in \mathbb{R}^d$ and M_i stands for 2×2 matrix. This rearrangement allows us to study the dynamics of the method independently for each dimension. One may observe, that the asymptotic convergence rate of the $2d$-dimensional vector sequence of $\hat{z}_k$ is defined by the worst convergence rate among its block of coordinates. Thus, it is enough to study the optimization in a one-dimensional case.

Reduction to a scalar case

For i-th coordinate with λ_i as an i-th eigenvalue of matrix W we have:

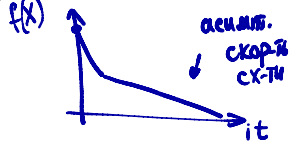
$$M_i = \begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix}.$$

The method will be convergent if $\rho(M) < 1$, and the optimal parameters can be computed by optimizing the spectral radius

$$\alpha^*, \beta^* = \arg\min_{\alpha,\beta} \max_{\lambda \in [\mu, L]} |\lambda(M)|$$

$$\alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^2.$$

It can be shown, that for such parameters the matrix M has complex eigenvalues, which forms a conjugate pair, so the distance to the optimum (in this case, $\|z_k\|$), generally, will not go to zero monotonically.



Heavy ball quadratic convergence

We can explicitly calculate the eigenvalues of M_i:

$$\lambda_1^M, \lambda_2^M = \lambda\left(\begin{bmatrix} 1-\alpha\lambda_i+\beta & -\beta \\ 1 & 0 \end{bmatrix}\right) = \frac{1+\beta-\alpha\lambda_i \pm \sqrt{(1+\beta-\alpha\lambda_i)^2 - 4\beta}}{2}.$$

When α and β are optimal (α^*, β^*), the eigenvalues are complex-conjugated pair $(1+\beta-\alpha\lambda_i)^2 - 4\beta \leq 0$, i.e. $\beta \geq (1-\sqrt{\alpha\lambda_i})^2$.

$$\mathrm{Re}(\lambda_1^M) = \frac{L+\mu-2\lambda_i}{(\sqrt{L}+\sqrt{\mu})^2}; \quad \mathrm{Im}(\lambda_1^M) = \frac{\pm 2\sqrt{(L-\lambda_i)(\lambda_i-\mu)}}{(\sqrt{L}+\sqrt{\mu})^2}; \quad |\lambda_1^M| = \frac{L-\mu}{(\sqrt{L}+\sqrt{\mu})^2}.$$

And the convergence rate does not depend on the stepsize and equals to $\sqrt{\beta^*}$.

Heavy ball method summary

- Ensures accelerated convergence for strongly convex quadratic problems

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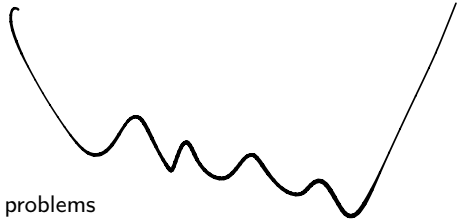

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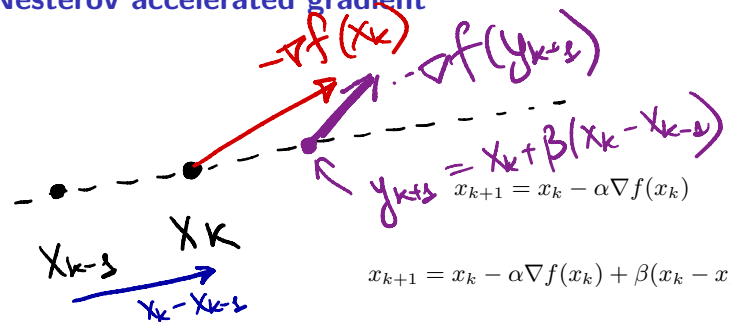
2 схеми HB, NAG

- Ensures accelerated convergence for strongly convex quadratic problems
- Local accelerated convergence was proved in the original paper.
- Recently was proved, that there is no global accelerated convergence for the method.
- Method was not extremely popular until the ML boom
- Nowadays, it is de-facto standard for practical acceleration of gradient methods, even for the non-convex problems (neural network training)

Nesterov accelerated gradient



$$x_{k+1} = x_k - \alpha\nabla f(x_k) \tag{GD}$$

$$x_{k+1} = x_k - \alpha\nabla f(x_k) + \beta(x_k - x_{k-1}) \tag{HB}$$

$$\begin{cases} y_{k+1} = x_k + \beta(x_k - x_{k-1}) \\ x_{k+1} = y_{k+1} - \alpha\nabla f(y_{k+1}) \end{cases} \tag{NAG}$$

$x_{k+1} = x_k + \beta(x_k - x_{k-1}) - \alpha\cdot\nabla f\left(x_k + \beta(x_k - x_{k-1})\right)$ $\frac{1}{k^2}$

(1981)

$\exp\left(\frac{\sqrt{2}-1}{\sqrt{2}+1}\right)$

Nesterov accelerated gradient

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Nesterov's Accelerated Gradient Descent on L-smooth convex function
Proof approach 1

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Content

Problem setup: smooth unconstrained convex optimisation

$$(\mathcal{P}) \ : \ \operatorname*{argmin}_{\boldsymbol{x}} f(\boldsymbol{x}).$$

- We consider Euclidean space
- $f : \mathbb{R}^n \to \mathbb{R}$
- f is $L-$smooth
  - f is continuously differentiable $f \in \mathcal{C}^1$, i.e., $\nabla f(\boldsymbol{x})$ exists for all $\boldsymbol{x} \in \operatorname{dom} f$
  - ∇f is L-Lipschitz $L > 0$ is the least upper bound in $\frac{\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\|}{\|\boldsymbol{x} - \boldsymbol{y}\|} \leq L$

$$\forall \boldsymbol{a}, \boldsymbol{b} \in \operatorname{dom} f \ : \ f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b} \rangle + \frac{L}{2}\|\boldsymbol{a} - \boldsymbol{b}\|_2^2 .$$

- f is convex — all local minima of $\mathcal{P}$ are global minima

$$(\forall \boldsymbol{x} \in \operatorname{dom} f)(\forall \boldsymbol{y} \in \operatorname{dom} f)\Big\{ f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle \Big\}$$

- Details of convexity, L-smoothness, see here

Gradient Descent (GD)

- Notation

$$f_k \coloneqq f(\boldsymbol{x}_k)$$
$$f^* \coloneqq f(\boldsymbol{x}^*)$$

- GD: start with initial point $\boldsymbol{x}_0 \in \mathbb{R}^n$, iterates

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha_k \nabla f(\boldsymbol{x}_k).$$

For sufficiently small stepsize ($\alpha_k < \frac{2}{L}$), the sequence $\{\boldsymbol{x}_k\}_{k \in \mathbb{N}}$ converges to a stationary point of f.

As f is convex, the sequence converges to the global minimizer $\boldsymbol{x}^*$ (if exists).

- GD convergence as $f_k - f^* \leq \mathcal{O}\Big(\frac{1}{k}\Big)$

Nesterov's Accelerated Gradient Descent (NAGD)

$$(\mathcal{P}) \ : \ \min_{\boldsymbol{x}} f(\boldsymbol{x})$$

- Start with initial point $\boldsymbol{y}_0 = \boldsymbol{x}_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$, iterates

convex

$$\text{Gradient update} \quad \boldsymbol{y}_{k+1} = \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) \tag{1}$$

$$\text{Extrapolation} \quad \boldsymbol{x}_{k+1} = (1-\gamma_k)\boldsymbol{y}_{k+1} + \gamma_k \boldsymbol{y}_k \tag{2}$$

$$\text{Extrapolation weight} \quad \gamma_k = \frac{1-\lambda_k}{\lambda_{k+1}} \tag{3}$$

$$\text{Extrapolation weight} \quad \lambda_k = \frac{1+\sqrt{1+4\lambda_{k-1}^2}}{2} \tag{4}$$

Note that here fix stepsize is used: $\alpha_k = \frac{1}{L} \forall k$.

- **Theorem**. If $f : \mathbb{R}^n \to \mathbb{R}$ is L-smooth and convex, the sequences $\{f(\boldsymbol{y}_k)\}_k$ produced by NAGD converges to the optimal value f^* at the rate $\mathcal{O}\left(\frac{1}{k^2}\right)$ as

R

$$f(\boldsymbol{y}_k) - f^* \ \leq \ \frac{2L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{k^2}.$$

  - The convergence rate $\mathcal{O}\left(\frac{1}{k^2}\right)$ is optimal. I.e., no 1st-order algo. can perform better than NAGD in terms of convergence rate. All 1st-order algorithm can only be at most as good as NAGD. Proof here.
  - If f is nonconvex, the sequence $\{f(\boldsymbol{y}_k)\}_k$ produced by NAGD converges to the closest stationary point with the same convergence rate.

NAGD converges rate $\mathcal{O}\left(\frac{1}{k^2}\right)$ proof 1/6 **Stage 1: make use of convexity & smoothness**

- f cvx: $(\forall \boldsymbol{x}\forall \boldsymbol{y})\Big\{f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y}-\boldsymbol{x}\rangle\Big\}$ gives

$$-f(\boldsymbol{y}) \leq -f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{x}-\boldsymbol{y}\rangle \tag{5}$$

- f L-smooth $(\forall \boldsymbol{a}\forall \boldsymbol{b})\Big\{f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \langle \nabla f(\boldsymbol{b}), \boldsymbol{a}-\boldsymbol{b}\rangle + \frac{L}{2}\|\boldsymbol{a}-\boldsymbol{b}\|_2^2\Big\}$, with $\boldsymbol{a} = \boldsymbol{x} - \frac{1}{L}\nabla f(\boldsymbol{x}), \boldsymbol{b} = \boldsymbol{x}$,

$$f\Big(\boldsymbol{x} - \frac{1}{L}\nabla f(\boldsymbol{x})\Big) - f(\boldsymbol{x}) \;\leq\; -\frac{1}{L}\|\nabla f(\boldsymbol{x})\|_2^2 + \frac{1}{2L}\|\nabla f(\boldsymbol{x})\|_2^2 = \frac{-1}{2L}\|\nabla f(\boldsymbol{x})\|_2^2. \tag{6}$$

- (5) + (6) will cancel $-f(\boldsymbol{x})$ and give

$$f\Big(\boldsymbol{x} - \frac{1}{L}\nabla f(\boldsymbol{x})\Big) - f(\boldsymbol{y}) \;\leq\; \frac{-1}{2L}\|\nabla f(\boldsymbol{x})\|_2^2 + \langle \nabla f(\boldsymbol{x}), \boldsymbol{x}-\boldsymbol{y}\rangle. \tag{7}$$

- Put $\boldsymbol{x} = \boldsymbol{x}_k$, $\boldsymbol{y} = \boldsymbol{x}^*$ in (7)

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* \;\leq\; \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k-\boldsymbol{x}^*\rangle. \tag{8}$$

- put $\boldsymbol{x} = \boldsymbol{x}_k$, $\boldsymbol{y} = \boldsymbol{y}_k$ in (7)

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f(\boldsymbol{y}_k) \;\leq\; \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k-\boldsymbol{y}_k\rangle. \tag{9}$$

- Proof overview: (8), (9) link $f(\boldsymbol{y}_{k+1}), f(\boldsymbol{y}_k)$ and f^*. We see $\nabla f(\boldsymbol{x}_k)$ appear in (8), (9) but not in the convergence result, so we eliminate $\nabla f(\boldsymbol{x}_k)$ in (8), (9).

Proof 2/6 **Stage 2: eliminate gradient**

$$\boldsymbol{y}_{k+1} = \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) \tag{1}$$

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* \le \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{x}^*\rangle. \tag{8}$$

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f(\boldsymbol{y}_k) \le \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k\rangle. \tag{9}$$

- Simplify notation, let $\delta_k := f(\boldsymbol{y}_k) - f^*$, then

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) \overset{(1)}{=} f(\boldsymbol{y}_{k+1}) \tag{10}$$

$$f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* \overset{(10),\delta_k}{=} \delta_{k+1} \tag{11}$$

$$\begin{aligned} f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f(\boldsymbol{y}_k) &= f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* - \Big(f(\boldsymbol{y}_k) - f^*\Big) \\ &= \delta_{k+1} - \delta_k \end{aligned} \tag{12}$$

$$\nabla f(\boldsymbol{x}_k) \overset{(1)}{=} -L(\boldsymbol{y}_{k+1} - \boldsymbol{x}_k) \tag{13}$$

$$\|\nabla f(\boldsymbol{x}_k)\|_2^2 \overset{(13)}{=} L^2\|\boldsymbol{y}_{k+1} - \boldsymbol{x}_k\|_2^2 \tag{14}$$

- Put (11,13,14) into (8)

$$\delta_{k+1} \le -\frac{L}{2}\|\boldsymbol{y}_{k+1} - \boldsymbol{x}_k\|_2^2 - L\langle \boldsymbol{y}_{k+1} - \boldsymbol{x}_k, \boldsymbol{x}_k - \boldsymbol{x}^*\rangle. \tag{15}$$

- Put (12,13,14) into (9)

$$\delta_{k+1} - \delta_k \le -\frac{L}{2}\|\boldsymbol{y}_{k+1} - \boldsymbol{x}_k\|_2^2 - L\langle \boldsymbol{y}_{k+1} - \boldsymbol{x}_k, \boldsymbol{x}_k - \boldsymbol{y}_k\rangle. \tag{16}$$

Proof 3/6 **Stage 3: form telescoping sum**

$$\begin{aligned} \lambda_k &= \tfrac{1}{2}\left(1+\sqrt{1+4\lambda_{k-1}^2}\right) && (4)\\ \delta_{k+1} &\le -\tfrac{L}{2}\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 - L\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \boldsymbol{x}_k-\boldsymbol{x}^*\rangle && (15)\\ \delta_{k+1}-\delta_k &\le -\tfrac{L}{2}\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 - L\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \boldsymbol{x}_k-\boldsymbol{y}_k\rangle && (16)\end{aligned}$$

- **Tricky step**: consider (15) + (λ_k-1)(16).

$$\text{Left-hand size of (15)} + (\lambda_k-1)(16) \;=\; \delta_{k+1} + (\lambda_k-1)(\delta_{k+1}-\delta_k) \;=\; \lambda_k\delta_{k+1} - (\lambda_k-1)\delta_k.$$

- Right-hand side of (15) + (λ_k-1)(16)

$$\begin{aligned} & -\frac{L}{2}\,\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 \; - L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k\,,\ \boldsymbol{x}_k-\boldsymbol{x}^*\Big\rangle \;+\; (\lambda_k-1)\left(\frac{-L}{2}\,\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 \; - L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k\,,\ \boldsymbol{x}_k-\boldsymbol{y}_k\Big\rangle\right)\\ =\;& -\frac{\lambda_k L}{2}\,\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 \; - L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k\,,\ \boldsymbol{x}_k-\boldsymbol{x}^*+(\lambda_k-1)(\boldsymbol{x}_k-\boldsymbol{y}_k)\Big\rangle\\ =\;& -\frac{\lambda_k L}{2}\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 - L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\Big\rangle\end{aligned}$$

- By LHS = RHS $\lambda_k\delta_{k+1} - (\lambda_k-1)\delta_k \;\le\; -\frac{\lambda_k L}{2}\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 - L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\Big\rangle$.
  Multiply the inequality with λ_k:

$$\begin{aligned} \lambda_k^2\delta_{k+1} - \lambda_k(\lambda_k-1)\delta_k \;&\le\; -\frac{\lambda_k^2 L}{2}\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 - \lambda_k L\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\Big\rangle\\ &=\; -\frac{L}{2}\left(\lambda_k^2\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 + 2\lambda_k\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\Big\rangle\right). \qquad (\#)\end{aligned}$$

- (4) gives $(2\lambda_k-1)^2 = 1+4\lambda_{k-1}^2 \iff 4\lambda_k^2-4\lambda_k+1 = 1+4\lambda_{k-1}^2 \iff \lambda_{k-1}^2 = \lambda_k(\lambda_k-1)$, put this into (#) gives

$$\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k \le -\frac{L}{2}\left(\lambda_k^2\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 + 2\lambda_k\Big\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\Big\rangle\right) \qquad (17)$$

Proof 4/6

$$\lambda_k = \tfrac{1}{2}\left(1+\sqrt{1+4\lambda_{k-1}^2}\right) \tag{4}$$

$$\lambda_k^2\delta_{k+1} - \lambda_k(\lambda_k-1)\delta_k \leq -\frac{L}{2}\left(\lambda_k^2\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 + 2\lambda_k\left\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\rangle\right) \tag{17}$$

- Inspecting the inner product in (17) we see that it is completing squares (Thanks to Tony Silveti-Falls for figuring it out, 2023 Nov 3).

$$\|\lambda\boldsymbol{a}+\boldsymbol{b}\|_2^2 = \lambda^2\|\boldsymbol{a}\|_2^2 + 2\lambda\langle\boldsymbol{a},\boldsymbol{b}\rangle + \|\boldsymbol{b}\|_2^2 \quad\Longleftrightarrow\quad \lambda^2\|\boldsymbol{a}\|_2^2 + 2\lambda\langle\boldsymbol{a},\boldsymbol{b}\rangle = \|\lambda\boldsymbol{a}+\boldsymbol{b}\|_2^2 - \|\boldsymbol{b}\|_2^2.$$

$$\begin{aligned}
&\lambda_k^2\|\boldsymbol{y}_{k+1}-\boldsymbol{x}_k\|_2^2 + 2\lambda_k\left\langle \boldsymbol{y}_{k+1}-\boldsymbol{x}_k,\ \lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\rangle \\
= &\left\|\lambda(\boldsymbol{y}_{k+1}-\boldsymbol{x}_k)+\lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2 - \left\|\lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2 \\
= &\left\|\lambda_k\boldsymbol{y}_{k+1}-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2 - \left\|\lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2.
\end{aligned}$$

- Using this (17) becomes

$$\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k \leq -\frac{L}{2}\left(\left\|\lambda_k\boldsymbol{y}_{k+1}-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2 - \left\|\lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2\right). \tag{18}$$

- We have $\lambda_k\boldsymbol{x}_k-(\lambda_k-1)\boldsymbol{y}_k = (1-\lambda_{k-1})\boldsymbol{y}_{k-1}+\lambda_{k-1}\boldsymbol{y}_k$.

Proof: $\gamma_k \overset{(3)}{=} \frac{1-\lambda_k}{\lambda_{k+1}} \quad\Longleftrightarrow\quad \gamma_k\lambda_{k+1} = 1-\lambda_k$.

By (2) $\boldsymbol{x}_{k+1} = (1-\gamma_k)\boldsymbol{y}_{k+1}+\gamma_k\boldsymbol{y}_k$ gives $x_{k+1} = \boldsymbol{y}_{k+1}+\gamma_k(\boldsymbol{y}_k-\boldsymbol{y}_{k+1})$, multiply with λ_{k+1} gives
$\lambda_{k+1}x_{k+1} = \lambda_{k+1}\boldsymbol{y}_{k+1}+\lambda_{k+1}\gamma_k(\boldsymbol{y}_k-\boldsymbol{y}_{k+1}) = \lambda_{k+1}\boldsymbol{y}_{k+1}+(1-\lambda_k)(\boldsymbol{y}_k-\boldsymbol{y}_{k+1})$, rearrange gives
$\lambda_{k+1}x_{k+1}-\lambda_{k+1}\boldsymbol{y}_{k+1} = (1-\lambda_k)(\boldsymbol{y}_k-\boldsymbol{y}_{k+1})$, add $\boldsymbol{y}_{k+1}$ on both side gives
$\lambda_{k+1}x_{k+1}-(\lambda_{k+1}-1)\boldsymbol{y}_{k+1} = (1-\lambda_k)\boldsymbol{y}_k+\lambda_k\boldsymbol{y}_{k+1}$. Move counter k by -1 gives the result.

So (18) becomes

$$\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k \leq -\frac{L}{2}\left(\left\|\lambda_k\boldsymbol{y}_{k+1}-(\lambda_k-1)\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2 - \left\|(1-\lambda_{k-1})\boldsymbol{y}_{k-1}+\lambda_{k-1}\boldsymbol{y}_k-\boldsymbol{x}^*\right\|_2^2\right).$$

Proof ... 5/6

We have $\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k \;\leq\; -\frac{L}{2}\left(\left\|\lambda_k \boldsymbol{y}_{k+1} - (\lambda_k - 1)\boldsymbol{y}_k - \boldsymbol{x}^*\right\|_2^2 - \left\|(1-\lambda_{k-1})\boldsymbol{y}_{k-1} + \lambda_{k-1}\boldsymbol{y}_k - \boldsymbol{x}^*\right\|_2^2\right)$.

Rearrange the second term to make the terms in right-hand side have similar form

$$\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k \;\leq\; -\frac{L}{2}\left(\left\|\lambda_k \boldsymbol{y}_{k+1} - (\lambda_k - 1)\boldsymbol{y}_k - \boldsymbol{x}^*\right\|_2^2 - \left\|\lambda_{k-1}\boldsymbol{y}_k - (\lambda_{k-1} - 1)\boldsymbol{y}_{k-1} - \boldsymbol{x}^*\right\|_2^2\right). \tag{19}$$

Let $\boldsymbol{u}_k = \lambda_k \boldsymbol{y}_{k+1} - (\lambda_k - 1)\boldsymbol{y}_k - \boldsymbol{x}^*$ so $\lambda_{k-1}\boldsymbol{y}_k - (\lambda_{k-1} - 1)\boldsymbol{y}_{k-1} - \boldsymbol{x}^* = \boldsymbol{u}_{k-1}$ and (19) becomes

$$\begin{array}{lcll}
\lambda_k^2\delta_{k+1} - \lambda_{k-1}^2\delta_k & \leq & -\frac{L}{2}\left(\|\boldsymbol{u}_k\|_2^2 - \|\boldsymbol{u}_{k-1}\|_2^2\right) & \\
\lambda_1^2\delta_2 - \lambda_0^2\delta_1 & \leq & -\frac{L}{2}\left(\|\boldsymbol{u}_1\|_2^2 - \|\boldsymbol{u}_0\|_2^2\right) & \text{case } k = 1 \\
\lambda_2^2\delta_3 - \lambda_1^2\delta_2 & \leq & -\frac{L}{2}\left(\|\boldsymbol{u}_2\|_2^2 - \|\boldsymbol{u}_1\|_2^2\right) & \text{case } k = 2 \\
 & \vdots & & \\
\lambda_{K-1}^2\delta_K - \lambda_{K-2}^2\delta_{K-1} & \leq & -\frac{L}{2}\left(\|\boldsymbol{u}_{K-1}\|_2^2 - \|\boldsymbol{u}_{K-2}\|_2^2\right) & \text{case } k = K-1 \\
\lambda_{K-1}^2\delta_K - \lambda_0^2\delta_1 & \leq & -\frac{L}{2}\left(\|\boldsymbol{u}_{K-1}\|_2^2 - \|\boldsymbol{u}_0\|_2^2\right) & \text{sum } k = 1 \text{ to } k = K-1 \\
 & = & \frac{L}{2}\left(\|\boldsymbol{u}_0\|_2^2 - \|\boldsymbol{u}_{K-1}\|_2^2\right) & \\
 & \leq & \frac{L}{2}\|\boldsymbol{u}_0\|_2^2 & \|\boldsymbol{u}_{K-1}\|_2^2 \geq 0
\end{array}$$

By definition, $\lambda_0 = 0$, $\boldsymbol{y}_0 = \boldsymbol{x}_0$, $\boldsymbol{u}_0 = \lambda_0\boldsymbol{y}_1 - (\lambda_0 - 1)\boldsymbol{y}_0 - \boldsymbol{x}^* \overset{\lambda_0=0}{=} \boldsymbol{y}_0 - \boldsymbol{x}^* \overset{\boldsymbol{y}_0=\boldsymbol{x}_0}{=} \boldsymbol{x}_0 - \boldsymbol{x}^*$, thus

$$\lambda_{K-1}^2\delta_K \leq \frac{L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \quad\Longrightarrow\quad \delta_K \leq \frac{L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{2\lambda_{K-1}^2}.$$

Proof ... 6/6

Lemma. $\lambda_{k-1} \geq \frac{k}{2}$.
Proof (by induction)

- Case $k = 0$ and $\lambda_0 = 0$. It is trivial $0 \geq 0/2$.
- Case $k = 1$. By definition,
  $\lambda_k = \frac{1+\sqrt{1+4\lambda_{k-1}^2}}{2} = \frac{1+\sqrt{1+4\cdot 0^2}}{2} = 1 > \frac{1}{2} = \frac{k}{2}\Big|_{k=1}$
- Induction hypothesis: assume $\lambda_{n-1} \geq \frac{n}{2}$.
- Case $k = n$

$$\begin{aligned}
\lambda_n &= \frac{1+\sqrt{1+4\lambda_{n-1}^2}}{2} \\
&\geq \frac{1+\sqrt{1+4\left(\frac{n}{2}\right)^2}}{2} \quad \text{[Induction hypothesis]} \\
&= \frac{1+\sqrt{1+n^2}}{2} \\
&> \frac{1+\sqrt{n^2}}{2} \\
&= \frac{1+n}{2}. \quad \square
\end{aligned}$$

With $\lambda_{k-1} \geq \frac{k}{2}$, so

$$\frac{1}{\lambda_{k-1}^2} \leq \frac{4}{k^2}.$$

Therefore $\delta_K \leq \frac{L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{2\lambda_{K-1}^2}$ becomes

$$f(\boldsymbol{y}_K) - f^* \leq \frac{2L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{K^2}.$$

where $f(\boldsymbol{y}_K) - f^* =: \delta_K$. $\square$

Rename K as k gives

$$f(\boldsymbol{y}_k) - f^* \leq \frac{2L\|x_0 - \boldsymbol{x}^*\|_2^2}{k^2}.$$

This { complicated / highly-involved / non-intuitive } proof is now completed.

Last page - summary

For unconstrained convex smooth problem

$$(\mathcal{P}) \ : \ \underset{\boldsymbol{x}}{\operatorname{argmin}} \ f(\boldsymbol{x})$$

with $f : \mathbb{R}^n \to \mathbb{R}$ being convex, L-smooth, the NAGD algorithm starts with initial point $\boldsymbol{x}_0 = \boldsymbol{y}_0 \in \mathbb{R}^n$ and $\lambda_0 = 0$ and iterates the following:

$$\begin{aligned}
\text{Gradient update} \quad \boldsymbol{y}_{k+1} &= \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) \\
\text{Extrapolation} \quad \boldsymbol{x}_{k+1} &= (1-\gamma_k)\boldsymbol{y}_{k+1} + \gamma_k \boldsymbol{y}_k \\
\text{Extrapolation weight} \quad \gamma_k &= \frac{1-\lambda_k}{\lambda_{k+1}} \\
\text{Extrapolation weight} \quad \lambda_k &= \frac{1+\sqrt{1+4\lambda_{k-1}^2}}{2}
\end{aligned}$$

the sequences $\left\{f(\boldsymbol{y}_k)\right\}_{k\in\mathbb{N}}$ produced will converges to the optimal f^* at order of $\mathcal{O}\left(\frac{1}{k^2}\right)$ as

$$f(\boldsymbol{y}_k) - f^* \ \leq \ \frac{2L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{k^2}.$$

The proof can be used for proximal gradient descent.

End of document

Nesterov's accelerated gradient method

on m-strongly convex L-smooth functionconverges at $\mathcal{O}(\exp \frac{-k}{\sqrt{Q}})$

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Content

Nesterov's estimate sequence

$$\Phi_0(\boldsymbol{x}) \coloneqq f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$$

$$\Phi_{k+1}(\boldsymbol{x}) \coloneqq \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)$$

Lemma 1 $\Phi_k(\boldsymbol{x}) \leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)^k \left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right)$

Lemma 2 $\nabla^2 \Phi_k(\boldsymbol{x}) = m\boldsymbol{I}_n$

Lemma 3 $f(\boldsymbol{y}_k) \leq \Phi_k^* \coloneqq \min_{x \in \mathbb{R}^n} \Phi_k(\boldsymbol{x})$

Lemma 4 $\boldsymbol{\nu}_k - \boldsymbol{x}_k = \sqrt{Q}(\boldsymbol{x}_k - \boldsymbol{y}_K)$

NAG convergence rate $f(\boldsymbol{y}_k) - f^* \leq \left(\frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2\right) \exp \frac{-k}{\sqrt{Q}}$

Problem setup: unconstrained strongly convex smooth optimisation

$$(\mathcal{P}) \ : \ \operatorname*{argmin}_{\boldsymbol{x}} \ f(\boldsymbol{x}).$$

- We consider Euclidean space
- $f : \mathbb{R}^n \to \mathbb{R}$ is $L-$smooth
  - f is continuously differentiable — $f \in \mathcal{C}^1$, i.e., $\nabla f(\boldsymbol{x})$ exists for all $\boldsymbol{x} \in \operatorname{dom} f$
  - ∇f is globally L-Lipschitz — $L > 0$ is the least upper bound in $\dfrac{\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\|}{\|\boldsymbol{x} - \boldsymbol{y}\|} \leq L$
  - $(\forall \boldsymbol{a} \in \operatorname{dom} f)(\forall \boldsymbol{b} \in \operatorname{dom} f)\Big\{ f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b} \rangle + \dfrac{L}{2}\|\boldsymbol{a} - \boldsymbol{b}\|_2^2 \Big\}$
- $f : \mathbb{R}^n \to \mathbb{R}$ is m-strongly convex — the global minima of $\mathcal{P}$ is unique
  - f is convex — all local minima of $\mathcal{P}$ are global minima
    - $(\forall \boldsymbol{x} \in \operatorname{dom} f)(\forall \boldsymbol{y} \in \operatorname{dom} f)\Big\{ f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle \Big\}$
  - f is m-strongly convex
    - $f(\boldsymbol{x}) - \dfrac{m}{2}\|\boldsymbol{x}\|_2^2$ is convex
- Details of L-smoothness, convexity, strong convexity, see here

Gradient Descent (GD)

$$(\mathcal{P}) \ : \ \min_{\boldsymbol{x}} f(\boldsymbol{x})$$

- GD starts with initial point $\boldsymbol{x}_0 \in \mathbb{R}^n$, iterates

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - m_k \nabla f(\boldsymbol{x}_k).$$

If stepsize is sufficiently small ($m_k < \frac{2}{L}$), then $\{\boldsymbol{x}_k\}_{k\in\mathbb{N}}$ converges to a stationary point of f.

- f convex $\implies$ {all local minimizers are global} — $\{\boldsymbol{x}_k\}_{k\in\mathbb{N}} \to$ a global minimizer $\boldsymbol{x}^*$ (if it exists)
- f strongly convex $\implies$ {unique minimizer} — global minimizer $\boldsymbol{x}^*$ is unique (if it exists)

- Notation $f^* \coloneqq f(\boldsymbol{x}^*)$ and $Q = \dfrac{L}{m}$.

- **If f is L-smooth and convex**, $f_k - f^* \leq \mathcal{O}\left(\frac{1}{k}\right)$ — convergence rate on $\{f_k\}_{k\in\mathbb{N}}$ is $\mathcal{O}\left(\frac{1}{k}\right)$
  Details

- **If f is L-smooth and m-strongly convex**, $f_k - f^* \leq \mathcal{O}\left(\exp \frac{-k}{Q}\right)$ — convergence rate on $\{f_k\}_{k\in\mathbb{N}}$ is $\mathcal{O}\left(\exp \frac{-k}{Q}\right)$
  Details

Nesterov's accelerated gradient (NAG) method

$$(\mathcal{P}) \ : \ \min_{\boldsymbol{x}} f(\boldsymbol{x})$$

If f is L-smooth and convex

Algorithm 1: NAG (for convex smooth f)

1 Initialize $\boldsymbol{x}_0 \in \mathbb{R}^n$, $\lambda_1 = 1$
2 **while** not converge **do**
3

$$\begin{aligned} \boldsymbol{y}_{k+1} &= \boldsymbol{x}_k - \frac{\nabla f(\boldsymbol{x}_k)}{L} \\ \boldsymbol{x}_{k+1} &= (1-\gamma_k)\boldsymbol{y}_{k+1} + \gamma_k \boldsymbol{y}_k \\ \gamma_k &= \frac{1-\lambda_k}{\lambda_{k+1}} \\ \lambda_k &= \frac{1+\sqrt{1+4\lambda_{k-1}^2}}{2} \end{aligned}$$

Theorem The sequence $\{f(\boldsymbol{x}_k)\}_{k\in\mathbb{N}}$ produced by NAG on convex L-smooth function satisfies

$$f(\boldsymbol{y}_k) - f^* \ \leq \ \left(\frac{1}{k^2}\right).$$

Details

If f is L-smooth and m-strongly convex
Fix $\gamma_k = \dfrac{\sqrt{Q}-1}{\sqrt{Q}+1}$ where $Q = \dfrac{L}{m}$

Algorithm 2: NAG (for strongly convex smooth f)

1 Initialize $\boldsymbol{x}_0 \in \mathbb{R}^n$
2 **while** not converge **do**
3

$$\begin{aligned} \boldsymbol{y}_{k+1} &= \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) \\ \boldsymbol{x}_{k+1} &= \left(1 - \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\right)\boldsymbol{y}_{k+1} + \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\boldsymbol{y}_k \end{aligned}$$

Theorem The sequence $\{f(\boldsymbol{x}_k)\}_{k\in\mathbb{N}}$ produced by NAG on m-strongly convex L-smooth function satisfies

$$f(\boldsymbol{y}_k) - f^* \ \leq \ \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \exp\left(\frac{-k}{\sqrt{Q}}\right).$$

This pdf: prove this.

Convergence rate of NAG - proof idea: Nesterov's estimate sequence

- There are a few ways to prove the convergence of NAG.
- A way is to use a non-trivial technique known as the Nesterov's estimate sequence.
- Consider a sequence of function $\left\{\Phi_k(\boldsymbol{x})\right\}_{k\in\mathbb{N}}$ that
  - $\Phi_k(\boldsymbol{x})$ has a general structure with "parameters" varies with iteration k.
  - $\Phi_k(\boldsymbol{x})$ is based on f
  - $\Phi_k(\boldsymbol{x})$ is m-strongly convex
- $\Phi_k(\boldsymbol{x})$ can be defined as

$$\begin{aligned}\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x}-\boldsymbol{x}_0\|_2^2 \\ \Phi_{k+1}(\boldsymbol{x}) &:= \left(1-\frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle\nabla f(\boldsymbol{x}_k), \boldsymbol{x}-\boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x}-\boldsymbol{x}_k\|_2^2\right)\end{aligned}$$

Details of the theory of Nesterov's estimating sequence.

Understanding Nesterov's estimate sequence

$$\Phi_0(\boldsymbol{x}) \quad := \quad f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$$

$$\Phi_{k+1}(\boldsymbol{x}) \quad := \quad \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k \rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)$$

- $\Phi_k(\boldsymbol{x})$ is based on f
- $\Phi_k(\boldsymbol{x})$ is m-strongly convex
- $\Phi_k(\boldsymbol{x})$ varies with iteration k.
- We can see Φ_{k+1} is in the form $\Phi_{k+1} = (1-\lambda)a + \lambda b$.
  - Φ_{k+1} is a convex combination of Φ_k and the 2nd-order Taylor approximation of f at $\boldsymbol{x}_k$.
  - $Q = 1 \iff$ the level sets of f is circular: Φ_{k+1} is more like the Taylor approximation

    In fact by definition of NAG, if $Q = 1$, there is no acceleration and NAG reduces to GD.

    In this case GD should solve the optimization problem in 1 step. Details.
  - $Q \gg 1 \iff$ the level sets of f is elliptic: Φ_{k+1} is more like previous Φ_k

The derivatives of Nesterov's estimating sequence

$$\begin{aligned}\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x}-\boldsymbol{x}_0\|_2^2 \\ \Phi_{k+1}(\boldsymbol{x}) &:= \left(1-\frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}-\boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x}-\boldsymbol{x}_k\|_2^2\right)\end{aligned}$$

- With respected to $\boldsymbol{x}$, the gradient and Hessian are

$$\begin{aligned}\nabla\Phi_0(\boldsymbol{x}) &= m(\boldsymbol{x}-\boldsymbol{x}_0) && (1)\\ \nabla^2\Phi_0(\boldsymbol{x}) &= m\boldsymbol{I}_n && (2)\\ \nabla\Phi_{k+1}(\boldsymbol{x}) &= \left(1-\frac{1}{\sqrt{Q}}\right)\nabla\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\Big(\nabla f(\boldsymbol{x}_k) + m(\boldsymbol{x}-\boldsymbol{x}_k)\Big) && (3)\\ \nabla^2\Phi_{k+1}(\boldsymbol{x}) &= \left(1-\frac{1}{\sqrt{Q}}\right)\nabla^2\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}m\boldsymbol{I}_n && (4)\end{aligned}$$

- In other words,
  - Φ_{k+1} is a convex combination of Φ_k and the 2nd-order Taylor approximation of f at $\boldsymbol{x}_k$.
  - $\nabla\Phi_{k+1}(\boldsymbol{x})$ is a convex combination of $\nabla\Phi_k(\boldsymbol{x})$ and $\nabla f(\boldsymbol{x}_k) + m(\boldsymbol{x}-\boldsymbol{x}_k)$.
  - $\nabla^2\Phi_{k+1}(\boldsymbol{x})$ is a convex combination of $\nabla^2\Phi_k(\boldsymbol{x})$ and $m\boldsymbol{I}_n$.
    In fact we are going to show $\nabla^2\Phi_{k+1}(\boldsymbol{x}) = m\boldsymbol{I}_n$ in Lemma 2.
  - In fact the derivatives of Φ_k plays an important role in the whole proof.

$\Phi_k(\boldsymbol{x})$ with $k = 0, 1$

$$\Phi_{k+1}(\boldsymbol{x}) := \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)$$

$f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2 \;\leq\; f(\boldsymbol{x}) \;\forall \boldsymbol{x}, \boldsymbol{x}_k$ — f is m-strongly cvx

$$\begin{aligned}
\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 \\
\Phi_1(\boldsymbol{x}) &:= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_0(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_0) + \langle \nabla f(\boldsymbol{x}_0), \boldsymbol{x} - \boldsymbol{x}_0\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2\right) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_0(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_0) + \langle \nabla f(\boldsymbol{x}_0), \boldsymbol{x} - \boldsymbol{x}_0\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2\right) - f(\boldsymbol{x}) \\
&\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_0(\boldsymbol{x}) + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}) - f(\boldsymbol{x}) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_0(\boldsymbol{x}) - \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{x}) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right)
\end{aligned}$$

$\Phi_k(\boldsymbol{x})$ with $k = 2$

$$\Phi_{k+1}(\boldsymbol{x}) := \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)$$

$$f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2 \;\leq\; f(\boldsymbol{x}) \;\forall \boldsymbol{x}, \boldsymbol{x}_k$$

f is m-strongly cvx

$$\begin{aligned}
\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 \\
\Phi_1(\boldsymbol{x}) &\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right) \\
\Phi_2(\boldsymbol{x}) &:= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_1(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_1) + \langle \nabla f(\boldsymbol{x}_1), \boldsymbol{x} - \boldsymbol{x}_1\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_1\|_2^2\right) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_1(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_1) + \langle \nabla f(\boldsymbol{x}_1), \boldsymbol{x} - \boldsymbol{x}_1\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_1\|_2^2\right) - f(\boldsymbol{x}) \\
&\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_1(\boldsymbol{x}) + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}) - f(\boldsymbol{x}) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_1(\boldsymbol{x}) - \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{x}) \\
&= f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\left(\Phi_1(\boldsymbol{x}) - f(\boldsymbol{x})\right) \\
&\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\left(1 - \frac{1}{\sqrt{Q}}\right)\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right) \;=\; f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)^2\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right)
\end{aligned}$$

Lemma 1

$$\Phi_{k+1}(\boldsymbol{x}) := \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)$$

$f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2 \;\leq\; f(\boldsymbol{x}) \;\forall \boldsymbol{x}, \boldsymbol{x}_k$ $\quad$ f is m-strongly cvx

$$\begin{aligned}
\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 \\
\Phi_1(\boldsymbol{x}) &\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right) \\
\Phi_2(\boldsymbol{x}) &\leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)^2\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right)
\end{aligned}$$

Lemma 1 For all $k \in \mathbb{N} = \{1, 2, \ldots\}$,

$$\Phi_k(\boldsymbol{x}) \leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)^k\left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right).$$

Proof by induction

- Based case is already proved.
- For case $k+1$, repeat the procedure on deriving Φ_2 and make use of the induction hypothesis.

Lemma 2 $\nabla^2 \Phi_k(\boldsymbol{x}) = m\boldsymbol{I}_n$

$$
\begin{aligned}
\Phi_0(\boldsymbol{x}) &:= f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 \\
\Phi_{k+1}(\boldsymbol{x}) &:= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right)
\end{aligned}
$$

Proof by induction

- **Base case** $k = 0$
  $\nabla^2 \Phi_0(\boldsymbol{x}) = m\boldsymbol{I}_n$ by definition.

- **Induction Hypothesis** $\nabla^2 \Phi_k(\boldsymbol{x}) = m\boldsymbol{I}_n$

- **Case** $k + 1$

$$
\begin{aligned}
\Phi_{k+1}(\boldsymbol{x}) &= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right) && \text{by definition} \\
\nabla^2 \Phi_{k+1}(\boldsymbol{x}) &= \left(1 - \frac{1}{\sqrt{Q}}\right)\nabla^2 \Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}} m\boldsymbol{I}_n \\
&= \left(1 - \frac{1}{\sqrt{Q}}\right) m\boldsymbol{I}_n + \frac{1}{\sqrt{Q}} m\boldsymbol{I}_n && \text{induction hypothesis} \\
&= m\boldsymbol{I}_n \quad \square
\end{aligned}
$$

Lemma 3 $f(\boldsymbol{y}_k) \leq \Phi_k^* \coloneqq \min_{\boldsymbol{x}\in\mathbb{R}^n} \Phi_k(\boldsymbol{x})$ ... 1/7

$\Phi_0(\boldsymbol{x})$	$\coloneqq$	$f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$	estimate seq.
$\boldsymbol{x}_0$	$=$	$\boldsymbol{y}_0$	NAG def.
$\boldsymbol{y}_{k+1}$	$=$	$\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)$	NAG def.
$f(\boldsymbol{a}) - f(\boldsymbol{b})$	$\leq$	$\langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b}\rangle + \frac{L}{2}\|\boldsymbol{a} - \boldsymbol{b}\|_2^2$	L-smooth

Proof by induction

- **Base case** $k = 0$
  $\Phi_0^* = \min_{\boldsymbol{x}\in\mathbb{R}^n} \Phi_0(\boldsymbol{x}_0) = \min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 = f(\boldsymbol{x}_0) = f(\boldsymbol{y}_0)$
- **Induction Hypothesis** $f(\boldsymbol{y}_k) \leq \Phi_k^*$
- **Case** $k+1$ Consider $f(\boldsymbol{y}_{k+1})$ and L-smoothness of f

$$
\begin{aligned}
f(\boldsymbol{y}_{k+1}) &\leq f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{y}_{k+1} - \boldsymbol{x}_k\rangle + \frac{L}{2}\|\boldsymbol{y}_{k+1} - \boldsymbol{x}_k\|_2^2 \\
&= f(\boldsymbol{x}_k) + \left\langle \nabla f(\boldsymbol{x}_k),\, \frac{-\nabla f(\boldsymbol{x}_k)}{L}\right\rangle + \frac{L}{2}\left\|\frac{-\nabla f(\boldsymbol{x}_k)}{L}\right\|_2^2 \quad \text{NAG update} \\
&= f(\boldsymbol{x}_k) - \frac{1}{L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \frac{1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 \\
&= f(\boldsymbol{x}_k) - \frac{1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2
\end{aligned}
$$

Now for shorthand notation we will let $g \coloneqq \frac{1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2$, we have $f(\boldsymbol{y}_{k+1}) \leq f(\boldsymbol{x}_k) - g$.

Lemma 3 ... 2/7

$$\begin{array}{lcll} f(\boldsymbol{y}_k) & \geq & f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{y}_k - \boldsymbol{x}_k \rangle & f \text{ convex} \\ f(\boldsymbol{y}_k) & \leq & \Phi_k^* & \text{Induction Hypothesis} \end{array}$$

- From $f(\boldsymbol{y}_{k+1}) \leq f(\boldsymbol{x}_k) - g$, two tricky steps to create $\left(1 - \frac{1}{\sqrt{Q}}\right)$

$$\begin{aligned} f(\boldsymbol{y}_{k+1}) &\leq f(\boldsymbol{x}_k) - \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} - g \\ &= \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{x}_k) + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} - g \\ &= \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{x}_k) - \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{y}_k) + \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{y}_k) + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} - g \\ &= \left(1 - \frac{1}{\sqrt{Q}}\right) \left(f(\boldsymbol{x}_k) - f(\boldsymbol{y}_k)\right) + \left(1 - \frac{1}{\sqrt{Q}}\right) f(\boldsymbol{y}_k) + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} - g \\ &\leq \left(1 - \frac{1}{\sqrt{Q}}\right) \left(f(\boldsymbol{x}_k) - f(\boldsymbol{y}_k)\right) + \left(1 - \frac{1}{\sqrt{Q}}\right) \Phi_k^* + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) - g \qquad \text{induction hypothesis} \\ &\leq \left(1 - \frac{1}{\sqrt{Q}}\right) \left\langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k \right\rangle + \left(1 - \frac{1}{\sqrt{Q}}\right) \Phi_k^* + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) - g \qquad f \text{ convex} \end{aligned}$$

$$f(\boldsymbol{y}_{k+1}) \leq \left(1 - \frac{1}{\sqrt{Q}}\right) \left\langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k \right\rangle + \left(1 - \frac{1}{\sqrt{Q}}\right) \Phi_k^* + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) - g \qquad \text{(now we have)}$$

- Recall our goal is to show $f(\boldsymbol{y}_{k+1}) \leq \Phi_{k+1}^*$, we can try to show

$$\left(1 - \frac{1}{\sqrt{Q}}\right) \left\langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k \right\rangle + \left(1 - \frac{1}{\sqrt{Q}}\right) \Phi_k^* + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) - g \leq \Phi_{k+1}^*. \qquad \text{(what we want to prove)}$$

This is what we are going to do in the next 4 - 5 slides.

Lemma 3 ... 3/7

- Now consider $\Phi_k(\boldsymbol{x})$. Lemma 2 $\nabla^2\Phi_k(\boldsymbol{x}) = m\boldsymbol{I}_n$ implies $\Phi_k(\boldsymbol{x}) = \Phi_k^* + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{\nu}_k\|_2^2$ for some $\boldsymbol{\nu}_k \in \mathbb{R}^n$ implies
  1. $\nabla\Phi_k(\boldsymbol{x}) = m(\boldsymbol{x} - \boldsymbol{\nu}_k)$
  2. Φ_k is minimized at $\boldsymbol{\nu}_k$, which implies $\nabla\Phi_k(\boldsymbol{\nu}_k) = 0$
  3. Points 1,2 work for all k, including $k+1$
  4. From $\Phi_0(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$, $\boldsymbol{\nu}_0 = \boldsymbol{x}_0$

- By definition of $\Phi_{k+1}(\boldsymbol{x})$ in Nesterov's estimate sequence

$$
\begin{aligned}
\Phi_{k+1}(\boldsymbol{x}) &= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle\nabla f(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k\rangle + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{x}_k\|_2^2\right) \\
\nabla\Phi_{k+1}(\boldsymbol{x}) &= \left(1 - \frac{1}{\sqrt{Q}}\right)\nabla\Phi_k(\boldsymbol{x}) + \frac{1}{\sqrt{Q}}\left(\nabla f(\boldsymbol{x}_k) + m(\boldsymbol{x} - \boldsymbol{x}_k)\right) \\
&= \left(1 - \frac{1}{\sqrt{Q}}\right)m(\boldsymbol{x} - \boldsymbol{\nu}_k) + \frac{1}{\sqrt{Q}}\left(\nabla f(\boldsymbol{x}_k) + m(\boldsymbol{x} - \boldsymbol{x}_k)\right) \\
\nabla\Phi_{k+1}(\boldsymbol{\nu}_{k+1}) &= \left(1 - \frac{1}{\sqrt{Q}}\right)m(\boldsymbol{\nu}_{k+1} - \boldsymbol{\nu}_k) + \frac{1}{\sqrt{Q}}\left(\nabla f(\boldsymbol{x}_k) + m(\boldsymbol{\nu}_{k+1} - \boldsymbol{x}_k)\right) \\
&= \boldsymbol{0} \qquad \text{(2) \& (3) gives } \nabla\Phi_{k+1}(\boldsymbol{\nu}_{k+1}) = \boldsymbol{0}
\end{aligned}
$$

Lemma 3 ... 4/7 (just some algebra)

$$\boxed{\left(1-\frac{1}{\sqrt{Q}}\right)m(\boldsymbol{\nu}_{k+1}-\boldsymbol{\nu}_k)+\frac{1}{\sqrt{Q}}\left(\nabla f(\boldsymbol{x}_k)+m(\boldsymbol{\nu}_{k+1}-\boldsymbol{x}_k)\right)\;=\;\mathbf{0}}$$

$$\left(1-\frac{1}{\sqrt{Q}}\right)(\boldsymbol{\nu}_{k+1}-\boldsymbol{\nu}_k)+\frac{1}{\sqrt{Q}}\left(\frac{\nabla f(\boldsymbol{x}_k)}{m}+(\boldsymbol{\nu}_{k+1}-\boldsymbol{x}_k)\right) \;=\; \mathbf{0}$$

$$\iff \quad \left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_{k+1}-\left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k+\frac{1}{\sqrt{Q}}\boldsymbol{\nu}_{k+1}+\frac{1}{\sqrt{Q}}\left(\frac{\nabla f(\boldsymbol{x}_k)}{m}-\boldsymbol{x}_k\right) \;=\; \mathbf{0}$$

Now

$$\boldsymbol{\nu}_{k+1} = \left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k+\frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k-\frac{\nabla f(\boldsymbol{x}_k)}{m}\right) \tag{5}$$

$$\iff \quad -\boldsymbol{\nu}_{k+1} = -\left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k-\frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k-\frac{\nabla f(\boldsymbol{x}_k)}{m}\right)$$

$$\iff \quad \boldsymbol{x}_k-\boldsymbol{\nu}_{k+1} = \boldsymbol{x}_k-\left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k-\frac{1}{\sqrt{Q}}\boldsymbol{x}_k+\frac{1}{\sqrt{Q}}\frac{\nabla f(\boldsymbol{x}_k)}{m}$$

$$= \left(1-\frac{1}{\sqrt{Q}}\right)\left(\boldsymbol{x}_k-\boldsymbol{\nu}_k\right)+\frac{\nabla f(\boldsymbol{x}_k)}{m\sqrt{Q}}$$

$$\iff \quad \|\boldsymbol{x}_k-\boldsymbol{\nu}_{k+1}\|_2^2 = \left(1-\frac{1}{\sqrt{Q}}\right)^2\|\boldsymbol{x}_k-\boldsymbol{\nu}_k\|_2^2+2\left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle\nabla f(\boldsymbol{x}_k),\,\boldsymbol{x}_k-\boldsymbol{\nu}_k\rangle}{m\sqrt{Q}}+\frac{\|\nabla f(\boldsymbol{x}_k)\|_2^2}{m^2Q}$$

Lemma 3 ... 5/7

$$\|\boldsymbol{x}_k - \boldsymbol{\nu}_{k+1}\|_2^2 = \left(1 - \frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 + 2\left(1 - \frac{1}{\sqrt{Q}}\right) \frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k \rangle}{m\sqrt{Q}} + \frac{\|\nabla f(\boldsymbol{x}_k)\|_2^2}{m^2 Q}$$

- Now consider $\Phi_{k+1}(\boldsymbol{x})$ evaluate at $\boldsymbol{x}_k$, from in slide 14 we have

$$\begin{aligned}
\Phi_{k+1}(\boldsymbol{x}_k) &= \Phi^*_{k+1} + \tfrac{m}{2}\|\boldsymbol{x}_k - \boldsymbol{\nu}_{k+1}\|_2^2 \\
&= \Phi^*_{k+1} + \frac{m}{2}\left(1 - \frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 + \left(1 - \frac{1}{\sqrt{Q}}\right) \frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k \rangle}{\sqrt{Q}} + \frac{\|\nabla f(\boldsymbol{x}_k)\|_2^2}{2mQ} \\
&= \Phi^*_{k+1} + \frac{m}{2}\left(1 - \frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 + \left(1 - \frac{1}{\sqrt{Q}}\right) \frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k \rangle}{\sqrt{Q}} + g \quad (*)
\end{aligned}$$

by using the fact $mQ = L$ and $g = \frac{1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2$.

- By definition of $\Phi_{k+1}(\boldsymbol{x})$ from page 5, $\Phi_{k+1}(\boldsymbol{x}_k)$ is

$$\begin{aligned}
\Phi_{k+1}(\boldsymbol{x}_k) &= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}_k) + \frac{1}{\sqrt{Q}}\left(f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \underbrace{\boldsymbol{x}_k - \boldsymbol{x}_k}_{=\mathbf{0}} \rangle + \frac{m}{2}\|\underbrace{\boldsymbol{x}_k - \boldsymbol{x}_k}_{=\mathbf{0}}\|_2^2\right) \\
&= \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}_k) + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) \quad (**)
\end{aligned}$$

- $(*) = (**)$ gives

$$\Phi^*_{k+1} + \frac{m}{2}\left(1 - \frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 + \left(1 - \frac{1}{\sqrt{Q}}\right) \frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k \rangle}{\sqrt{Q}} + g = \left(1 - \frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}_k) + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k)$$

Lemma 3 ... 6/7

$$\Phi^*_{k+1} = -\frac{m}{2}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 - \left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k\rangle}{\sqrt{Q}} - g + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}_k) + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k)$$

By $\Phi_k(\boldsymbol{x}) = \Phi^*_k + \frac{m}{2}\|\boldsymbol{x} - \boldsymbol{\nu}_k\|_2^2$ (slide 14)

$$\left(1-\frac{1}{\sqrt{Q}}\right)\Phi_k(\boldsymbol{x}_k) \;=\; \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k + \left(1-\frac{1}{\sqrt{Q}}\right)\frac{m}{2}\|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2$$

Hence

$$\Phi^*_{k+1} \;=\; -\frac{m}{2}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 - \left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k\rangle}{\sqrt{Q}} - g + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k + \left(1-\frac{1}{\sqrt{Q}}\right)\frac{m}{2}\|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}}$$

Simplify the term

$$\Phi^*_{k+1} \;=\; \frac{m}{2\sqrt{Q}}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 - \left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k\rangle}{\sqrt{Q}} + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k - g + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}}$$

To proceed, we need lemma 4.

Lemma 4 $\boldsymbol{\nu}_k - \boldsymbol{x}_k = \sqrt{Q}(\boldsymbol{x}_k - \boldsymbol{y}_k)$

$$
\begin{array}{rcll}
Q & = & \frac{L}{m} & \text{def of } Q \\
\boldsymbol{y}_{k+1} & = & \boldsymbol{x}_k - \frac{\nabla f(\boldsymbol{x}_k)}{L} & \text{NAG def (1)} \\
\boldsymbol{x}_{k+1} & = & \left(1 + \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\right)\boldsymbol{y}_{k+1} - \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\boldsymbol{y}_k & \text{NAG def (2)}
\end{array}
$$

Proof by induction

- **Base case** $k = 0$ is true by $\boldsymbol{x}_0 = \boldsymbol{y}_0$ hence $\boldsymbol{\nu}_0 = \boldsymbol{x}_0$.
- **Induction hypothesis** $\boldsymbol{\nu}_k - \boldsymbol{x}_k = \sqrt{Q}(\boldsymbol{x}_k - \boldsymbol{y}_k)$
- **Case** $k+1$

$$
\begin{aligned}
\boldsymbol{\nu}_{k+1} &\overset{(5)}{=} \left(1 - \frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k + \frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k - \frac{\nabla f(\boldsymbol{x}_k)}{m}\right) \\
&= \left(1 - \frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k + \frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k - \frac{Q\nabla f(\boldsymbol{x}_k)}{L}\right) && \text{def of } Q \\
\boldsymbol{\nu}_{k+1} - \boldsymbol{x}_{k+1} &= \left(1 - \frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k + \frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k - \frac{Q\nabla f(\boldsymbol{x}_k)}{L}\right) - \boldsymbol{x}_{k+1} \\
&= \left(1 - \frac{1}{\sqrt{Q}}\right)\left(\boldsymbol{x}_k + \sqrt{Q}(\boldsymbol{x}_k - \boldsymbol{y}_k)\right) + \frac{1}{\sqrt{Q}}\boldsymbol{x}_k - \sqrt{Q}\frac{\nabla f(\boldsymbol{x}_k)}{L} - \boldsymbol{x}_{k+1} && \text{induction hypothesis} \\
&= \sqrt{Q}\left(\boldsymbol{x}_k - \frac{\nabla f(\boldsymbol{x}_k)}{L}\right) - \left(\sqrt{Q} - 1\right)\boldsymbol{y}_k - \boldsymbol{x}_{k+1} \\
&= \sqrt{Q}\boldsymbol{y}_{k+1} + \left(\sqrt{Q} + 1\right)\boldsymbol{x}_{k+1} - 2\sqrt{Q}\boldsymbol{y}_{k+1} - \boldsymbol{x}_{k+1} && \text{NAG def (1) NAG def (2)} \\
&= \sqrt{Q}(\boldsymbol{x}_{k+1} - \boldsymbol{y}_{k+1}) \quad \square
\end{aligned}
$$

Lemma 3 ... 7/7

Lemma 4 $\boldsymbol{\nu}_k - \boldsymbol{x}_k = \sqrt{Q}(\boldsymbol{x}_k - \boldsymbol{y}_k)$

The proof of Lemma 3 stops at

$$\Phi^*_{k+1} = \frac{m}{2\sqrt{Q}}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 - \left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k\rangle}{\sqrt{Q}} + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k - g + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}}$$

By lemma 4 we have

$$\begin{aligned}\Phi^*_{k+1} &= \frac{m}{2\sqrt{Q}}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{\nu}_k\|_2^2 - \left(1-\frac{1}{\sqrt{Q}}\right)\frac{\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{\nu}_k\rangle}{\sqrt{Q}} + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k - g + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}} \\ &= \frac{m\sqrt{Q}}{2}\left(1-\frac{1}{\sqrt{Q}}\right)^2 \|\boldsymbol{x}_k - \boldsymbol{y}_k\|_2^2 + \left(1-\frac{1}{\sqrt{Q}}\right)\langle \nabla f(\boldsymbol{x}_k),\, \boldsymbol{x}_k - \boldsymbol{y}_k\rangle + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k - g + \frac{f(\boldsymbol{x}_k)}{\sqrt{Q}}\end{aligned}$$

Recall (slide 13)

$$f(\boldsymbol{y}_{k+1}) \le \left(1-\frac{1}{\sqrt{Q}}\right)\left\langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k\right\rangle + \left(1-\frac{1}{\sqrt{Q}}\right)\Phi^*_k + \frac{1}{\sqrt{Q}} f(\boldsymbol{x}_k) - g \qquad \text{(now we have)}$$

By $a = \Phi^*_{k+1} = \underbrace{\quad}_{\ge 0} + \quad \ge \quad \overset{\text{now we have}}{\ge} f(\boldsymbol{y}_{k+1})$, we have proved for the case $k+1$ that $f(\boldsymbol{y}_{k+1}) \le \Phi^*_{k+1}$.

' By induction, Lemma 3 is now proved. $\square$

Proving NAG convergence rate

Lemma 1 $\Phi_{k+1}(\boldsymbol{x}) \leq f(\boldsymbol{x}) + \left(1 - \frac{1}{\sqrt{Q}}\right)^k \left(\Phi_0(\boldsymbol{x}) - f(\boldsymbol{x})\right) \ \forall k$

Lemma 3 $f(\boldsymbol{y}_k) \leq \Phi_k^* \ \forall k$

f L-smooth $f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b} \rangle + \frac{L}{2}\|\boldsymbol{a} - \boldsymbol{b}\|_2^2$

$\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$

- **Theorem** $f(\boldsymbol{y}_k) - f^* \leq \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 e^{\frac{-k}{\sqrt{Q}}}$

- **Proof**

$$
\begin{aligned}
f(\boldsymbol{y}_k) - f^* &\leq \Phi_k(\boldsymbol{x}^*) - f^* && \text{lemma 3} \\
&\leq f(\boldsymbol{x}^*) + \left(1 - \tfrac{1}{\sqrt{Q}}\right)^k \left(\Phi_0(\boldsymbol{x}^*) - f(\boldsymbol{x}^*)\right) - f^* && \text{lemma 1} \\
&= \left(\Phi_0(\boldsymbol{x}^*) - f^*\right) \left(1 - \tfrac{1}{\sqrt{Q}}\right)^k && f(\boldsymbol{x}^*) = f^* \\
&= \left(f(\boldsymbol{x}_0) - f^* + \tfrac{m}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2\right) \left(1 - \tfrac{1}{\sqrt{Q}}\right)^k && \text{Def. of } \Phi_0(\boldsymbol{x}) \\
&\leq \left(\langle \nabla f(\boldsymbol{x}^*), \boldsymbol{x}_0 - \boldsymbol{x}^* \rangle + \tfrac{L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 + \tfrac{m}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2\right) \left(1 - \tfrac{1}{\sqrt{Q}}\right)^k && f \text{ L-smooth} \\
&\leq \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \left(1 + (-\tfrac{1}{\sqrt{Q}})\right)^k && \nabla f(\boldsymbol{x}^*) = \boldsymbol{0} \\
&\leq \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \left(\exp(-\tfrac{1}{\sqrt{Q}})\right)^k && 1 + x \leq e^x \\
&= \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \exp\left(\frac{-k}{\sqrt{Q}}\right)
\end{aligned}
$$

Discussion

- If we stop the algorithm when ϵ-accuracy is achieved

$$\frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \exp\left(\frac{-k}{\sqrt{Q}}\right) \quad \leq \quad \epsilon.$$

  Re-arrange

$$k \quad \geq \quad \sqrt{Q}\ln\frac{1}{\epsilon} + \text{constant}.$$

  I.e. it takes $\mathcal{O}\left(\sqrt{Q}\ln\frac{1}{\epsilon}\right)$ steps for NAG to converges.

- Compared to GD with rate $\mathcal{O}\left(Q\ln\frac{1}{\epsilon}\right)$, the improvement $Q \to \sqrt{Q}$ is significant as m can be viewed as regularization parameter in various machine learning model (norm regularized) and $\frac{1}{m}$ can be as large as sample size. Here the number of step reduced from sample size to $\sqrt{\text{sample size}}$.

Last page - summary

- For unconstrained smooth strongly-convex problem $\min_{x \in \mathbb{R}^n} f(\boldsymbol{x})$, with $f : \mathbb{R}^n \to \mathbb{R}$ being L-smooth and m-strongly convex, the NAG algorithm iterates the following :

$$\boldsymbol{y}_{k+1} = \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k), \qquad \boldsymbol{x}_{k+1} = \left(1 - \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\right)\boldsymbol{y}_{k+1} + \frac{\sqrt{Q}-1}{\sqrt{Q}+1}\boldsymbol{y}_k, \qquad Q = \frac{L}{m}$$

with initial point $\boldsymbol{x}_0 = \boldsymbol{y}_0 \in \mathbb{R}^n$, will produce a sequences $\left\{f(\boldsymbol{y}_k)\right\}_{k\in\mathbb{N}}$ that

$$f(\boldsymbol{y}_k) - f^* \;\leq\; \frac{m+L}{2}\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2 \exp\left(\frac{-k}{\sqrt{Q}}\right).$$

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