Discover acceleration of gradient descent

Daniil Merkulov

Optimization methods. MIPT

Coordinate shift

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$$
\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_{++}.
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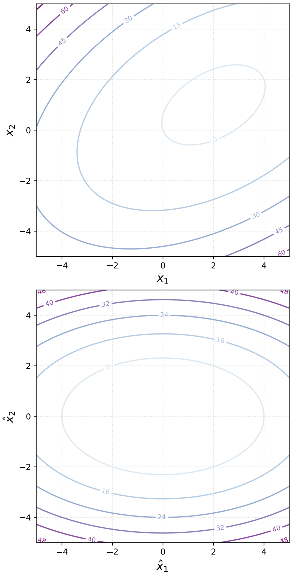

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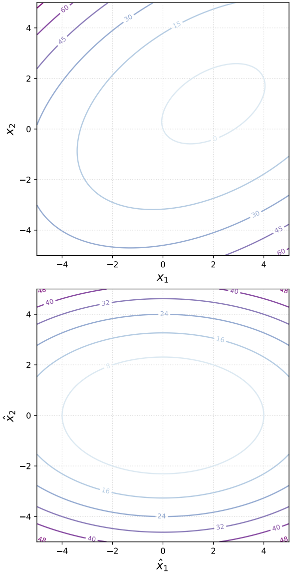

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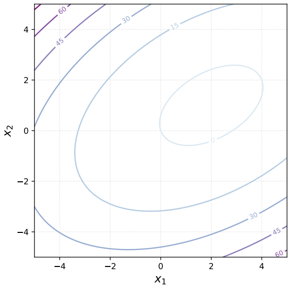
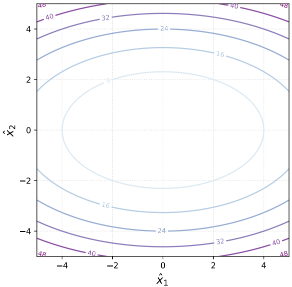
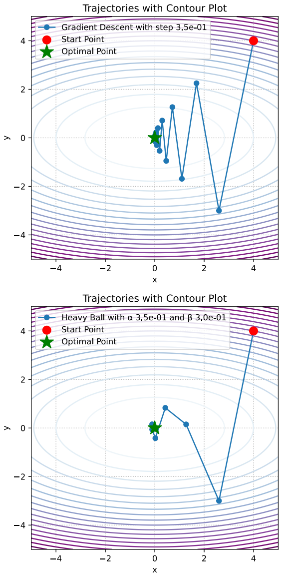
- Let's show, that we can switch coordinates in order to make an analysis a little bit easier. Let $\hat{x} = Q^T(x - x^*)$, where x^* is the minimum point of initial function, defined by $Ax^* = b$. At the same time $x = Q\hat{x} + x^*$.

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





Polyak Heavy ball method



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

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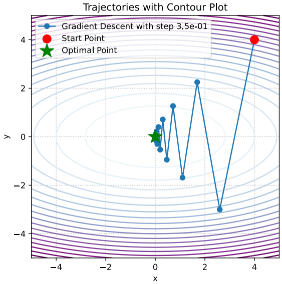

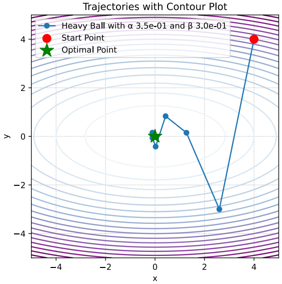

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Which is in our case is

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

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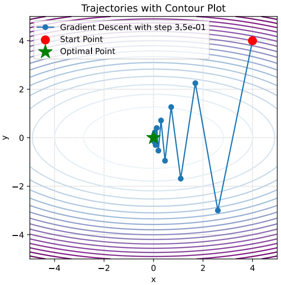

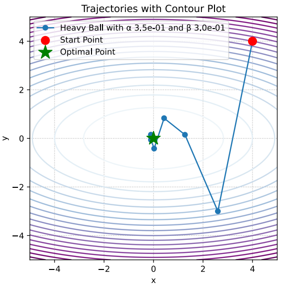

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This can be rewritten as a follows

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

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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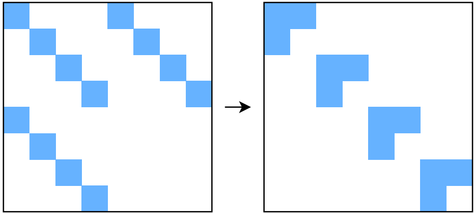

Figure 1: Illustration of matrix M rearrangement

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

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

$$\alpha^*, \beta^* = \arg\min_{\alpha,\beta} \max_{\lambda \in [\mu, L]} \rho(M) \quad \alpha^* = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \beta^* = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} \right)^2.$$

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:

$$\lambda^M_1, \lambda^M_2 = \lambda \left(\begin{bmatrix} 1 - \alpha\lambda_i + \beta & -\beta \\ 1 & 0 \end{bmatrix} \right) = \frac{1 + \beta - \alpha\lambda_i \pm \sqrt{(1 + \beta - \alpha\lambda_i)^2 - 4\beta}}{2}.$$

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. $\beta \geq (1 - \sqrt{\alpha\lambda_i})^2$.

$$\text{Re}(\lambda^M_1) = \frac{L + \mu - 2\lambda_i}{(\sqrt{L} + \sqrt{\mu})^2}; \quad \text{Im}(\lambda^M_1) = \frac{\pm 2\sqrt{(L - \lambda_i)(\lambda_i - \mu)}}{(\sqrt{L} + \sqrt{\mu})^2}; \quad |\lambda^M_1| = \frac{L - \mu}{(\sqrt{L} + \sqrt{\mu})^2}.$$

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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- 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

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

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

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

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

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

- 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 $f_k - f^* \leq \mathcal{O}\left(\frac{1}{k}\right)$

Nesterov's Accelerated Gradient Descent (NAGD)

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

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

$$\begin{aligned}
&\text{Gradient update} & \boldsymbol{y}_{k+1} &= \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) & (1)\\
&\text{Extrapolation} & \boldsymbol{x}_{k+1} &= (1-\gamma_k)\boldsymbol{y}_{k+1} + \gamma_k \boldsymbol{y}_k & (2)\\
&\text{Extrapolation weight} & \gamma_k &= \frac{1-\lambda_k}{\lambda_{k+1}} & (3)\\
&\text{Extrapolation weight} & \lambda_k &= \frac{1+\sqrt{1+4\lambda_{k-1}^2}}{2} & (4)
\end{aligned}$$

  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

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

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

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

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

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

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

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

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

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

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

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

- 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**

$$
\begin{aligned}
\boldsymbol{y}_{k+1} &= \boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k) && (1)\\
f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* &\le \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{x}^*\rangle. && (8)\\
f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f(\boldsymbol{y}_k) &\le \frac{-1}{2L}\|\nabla f(\boldsymbol{x}_k)\|_2^2 + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{x}_k - \boldsymbol{y}_k\rangle. && (9)
\end{aligned}
$$

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

$$
\begin{aligned}
f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) &\overset{(1)}{=} f(\boldsymbol{y}_{k+1}) && (10)\\
f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* &\overset{(10),\delta_k}{=} \delta_{k+1} && (11)\\
f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f(\boldsymbol{y}_k) &= f\Big(\boldsymbol{x}_k - \frac{1}{L}\nabla f(\boldsymbol{x}_k)\Big) - f^* - \Big(f(\boldsymbol{y}_k) - f^*\Big)\\
&= \delta_{k+1} - \delta_k && (12)\\
\nabla f(\boldsymbol{x}_k) &\overset{(1)}{=} -L(\boldsymbol{y}_{k+1} - \boldsymbol{x}_k) && (13)\\
\|\nabla f(\boldsymbol{x}_k)\|_2^2 &\overset{(13)}{=} L^2\|\boldsymbol{y}_{k+1} - \boldsymbol{x}_k\|_2^2 && (14)
\end{aligned}
$$

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

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

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

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

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

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

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

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

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

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

- (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

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

Proof 4/6

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

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

- 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).

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

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

- Using this (17) becomes

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

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

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

Proof ... 5/6

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

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 $k=n$

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

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

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

Therefore $\delta_K \leq \dfrac{L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{2\lambda_{K-1}^2}$ 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 $\begin{cases} \text{complicated} \\ \text{highly-involved} \\ \text{non-intuitive} \end{cases}$ 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:

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

the sequences $\{f(\boldsymbol{y}_k)\}_{k\in\mathbb{N}}$ 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

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

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

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 $f(\boldsymbol{y}_k) \leq \Phi_k^* := \min\limits_{x \in \mathbb{R}^n} \Phi_k(\boldsymbol{x})$

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 $\dfrac{\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\|}{\|\boldsymbol{x} - \boldsymbol{y}\|} \leq L$
  - $(\forall \boldsymbol{a} \in \operatorname{dom} f)(\forall \boldsymbol{b} \in \operatorname{dom} f)\Big\{ f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \big\langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b} \big\rangle + \dfrac{L}{2}\|\boldsymbol{a} - \boldsymbol{b}\|_2^2 \Big\}$
- $f : \mathbb{R}^n \to \mathbb{R}$ is m-strongly convex — the global minima of $\mathcal{P}$ is unique
  - f is convex — all local minima of $\mathcal{P}$ are global minima
    - $(\forall \boldsymbol{x} \in \operatorname{dom} f)(\forall \boldsymbol{y} \in \operatorname{dom} f)\Big\{ f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \big\langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \big\rangle \Big\}$
  - 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)

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

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

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

- **If f is L-smooth and m-strongly convex**, $f_k - f^* \le \mathcal{O}\left(\exp \frac{-k}{Q}\right)$ 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)

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

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

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)

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

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

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 $\{\Phi_k(\boldsymbol{x})\}_{k\in\mathbb{N}}$ 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

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

- $\Phi_k(\boldsymbol{x})$ 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

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

- 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 $k = 0, 1$

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

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

f is m-strongly cvx

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

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

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

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

f is m-strongly cvx

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

Lemma 1

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

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

f is m-strongly cvx

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

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

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

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

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

Proof by induction

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

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

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

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

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

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

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

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

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

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

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

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

Now

$$\begin{aligned}
\boldsymbol{\nu}_{k+1} &= \left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k+\frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k-\frac{\nabla f(\boldsymbol{x}_k)}{m}\right) \qquad (5) \\
\iff \quad -\boldsymbol{\nu}_{k+1} &= -\left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k-\frac{1}{\sqrt{Q}}\left(\boldsymbol{x}_k-\frac{\nabla f(\boldsymbol{x}_k)}{m}\right) \\
\iff \quad \boldsymbol{x}_k-\boldsymbol{\nu}_{k+1} &= \boldsymbol{x}_k-\left(1-\frac{1}{\sqrt{Q}}\right)\boldsymbol{\nu}_k-\frac{1}{\sqrt{Q}}\boldsymbol{x}_k+\frac{1}{\sqrt{Q}}\frac{\nabla f(\boldsymbol{x}_k)}{m} \\
&= \left(1-\frac{1}{\sqrt{Q}}\right)\Big(\boldsymbol{x}_k-\boldsymbol{\nu}_k\Big)+\frac{\nabla f(\boldsymbol{x}_k)}{m\sqrt{Q}} \\
\iff \quad \|\boldsymbol{x}_k-\boldsymbol{\nu}_{k+1}\|_2^2 &= \left(1-\frac{1}{\sqrt{Q}}\right)^2\|\boldsymbol{x}_k-\boldsymbol{\nu}_k\|_2^2+2\left(1-\frac{1}{\sqrt{Q}}\right)\frac{\big\langle\nabla f(\boldsymbol{x}_k),\,\boldsymbol{x}_k-\boldsymbol{\nu}_k\big\rangle}{m\sqrt{Q}}+\frac{\|\nabla f(\boldsymbol{x}_k)\|_2^2}{m^2Q}
\end{aligned}$$

Lemma 3 ... 5/7

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

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

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

  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

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

- $(*) = (**)$ 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

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

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

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

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.

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

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

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

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

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 $a = \Phi_{k+1}^* = \underbrace{\square}_{\ge 0} + \square \ge \square \overset{\text{now we have}}{\ge} f(\boldsymbol{y}_{k+1})$, 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. □

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 $f(\boldsymbol{a}) - f(\boldsymbol{b}) \leq \langle \nabla f(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b} \rangle + \frac{L}{2} \|\boldsymbol{a} - \boldsymbol{b}\|_2^2$
$\nabla f(\boldsymbol{x}^*) = \mathbf{0}$

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

- **Proof**

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

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 $\big\{f(\boldsymbol{y}_k)\big\}_{k \in \mathbb{N}}$ 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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