Iterative Algorithms in Optimization, Variational Analysis and Fixed Point Theory

Unit 03: Second order in space and time.

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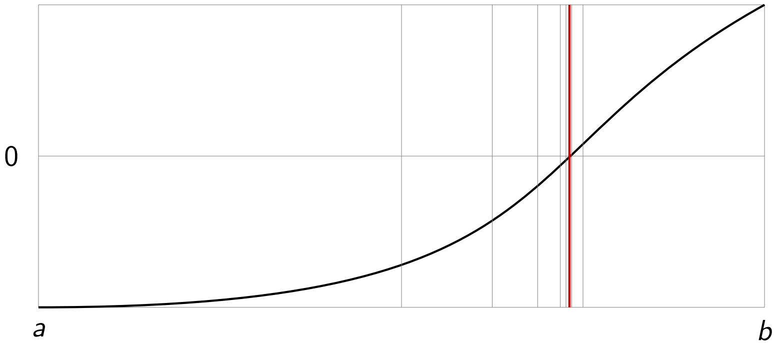
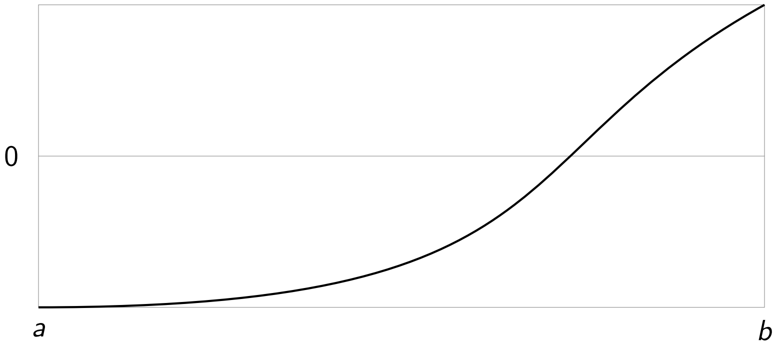
Recall the bisection method to solve $g(x) = 0$



Let us use information about the function



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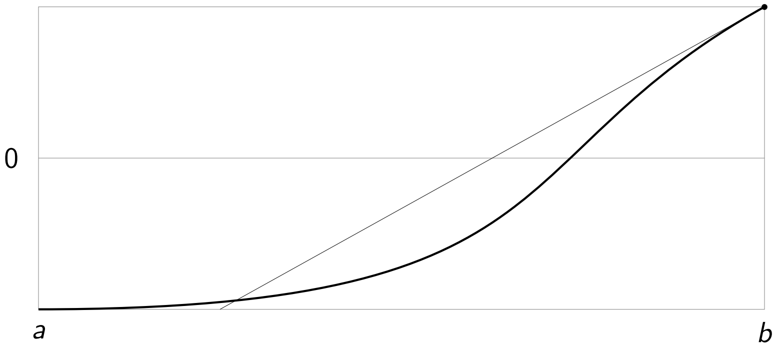

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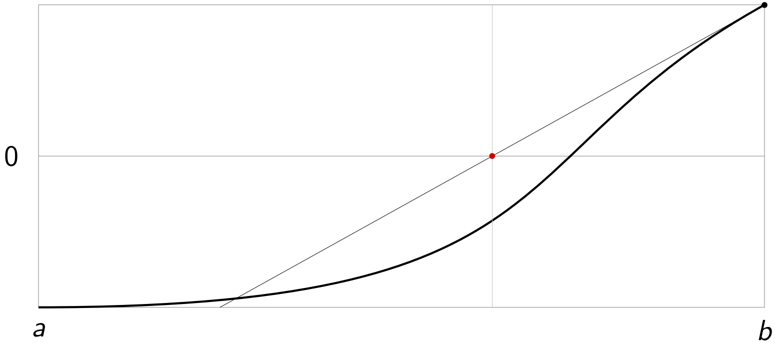

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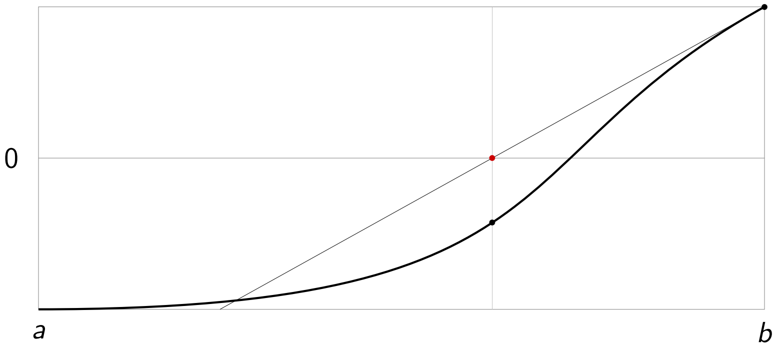

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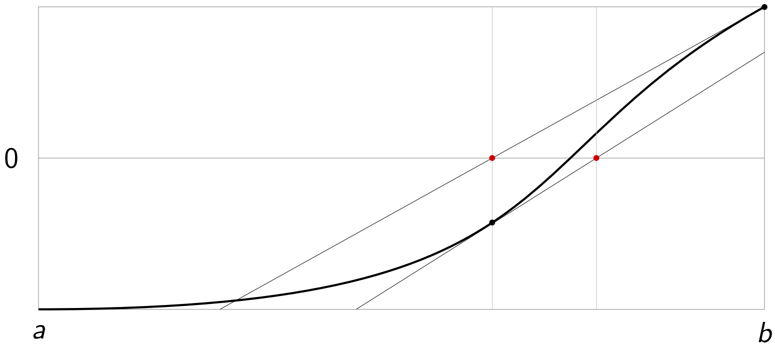

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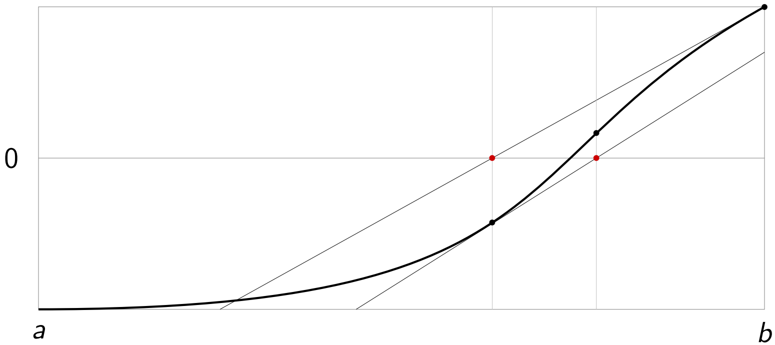

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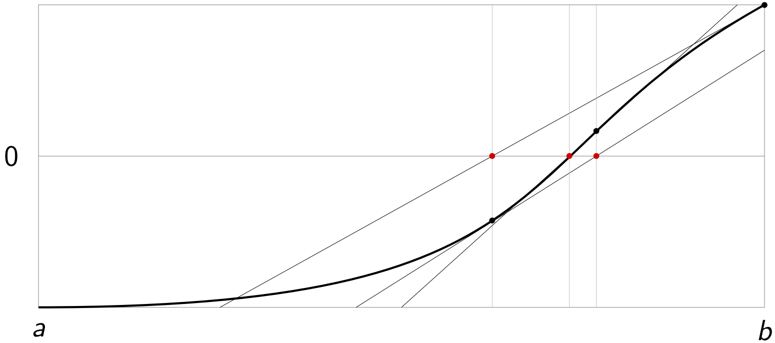

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$g : \mathbb{R} \to \mathbb{R}$ differentiable

- Start with x_0 and compute $g(x_0)$ and $g'(x_0)$.

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- If $g'(x_0) \neq 0$, then $x_1 = x_0 - \frac{g(x_0)}{g'(x_0)}$.
- Repeat the procedure to find $x_2, x_3 \ldots$ by

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)}$$

if $g'(x_k) \neq 0$.

Newton's Method

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$$x_{k+1} = x_k - \left[DG(x_k)\right]^{-1} G(x_k).$$

We expect x_k to converge to some $\hat{x}$ such that $G(\hat{x}) = 0$.

Newton's Method in optimization

If $G = \nabla f$, this is

$$x_{k+1} = x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k),$$

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Since the solution $\hat{x}$ satisfies $A^T(A\hat{x} - b) = 0$, we must have $x_1 = \hat{x}$.

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Since the solution $\hat{x}$ satisfies $A^T(A\hat{x} - b) = 0$, we must have $x_1 = \hat{x}$. One iteration of Newton's Method is equivalent to solving the problem.

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

- If f is $L-$smooth, $\|\nabla^2 f(x)d\| \leq L\|d\|$ for all $x, d \in \mathbb{R}^N$.

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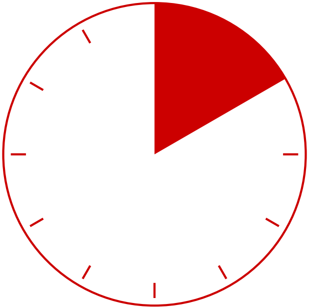
- If f is strongly convex, then $-\left[\nabla^2 f(x)\right]^{-1} \nabla f(x)$ is a descent direction for f at x. Which numbers are descent step sizes?

Break



Convergence of Newton's method

$x_{k+1} = x_k - [DG(x_k)]^{-1}\, G(x_k)$

Theorem

Consider $G : \mathbb{R}^N \to \mathbb{R}^N$ *and* $\hat{x} \in \mathbb{R}^N$ *such that* $G(\hat{x}) = 0$.

Suppose $\|DG(x) - DG(y)\| \le L\|x - y\|$ *and* $\|DG(x)^{-1}\| \le M$ *for all* x, y *in a neighborhood of* $\hat{x}$.

Then, there is $\delta > 0$ *such that if* $\|x_0 - \hat{x}\| < \delta$, *then*

$$\|x_{k+1} - \hat{x}\| \le \frac{LM}{2}\|x_k - \hat{x}\|^2$$

for all $k \ge 0$, *and so*

$$\|x_k - \hat{x}\| \le Cr^{2^k}$$

for some $C > 0$, $r \in (0,1)$ *and all* $k \ge 0$.

Avoid the cost of $\nabla^2 f(x_k)^{-1}$

Define $x_{k+1} = x_k - \alpha_k D_k \nabla f(x_k)$, where

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One simple heuristic is periodic evaluation: Choose $p \in \mathbb{N}$ and define

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Another idea is to update D_k to D_{k+1} keeping the essence of Newton's method, but using first order information only.

Quasi-Newton methods

Newton's method is based on the fact that

$$\nabla f(x_{k+1}) \sim \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k),$$

which implies

$$\nabla^2 f(x_k)^{-1}\left[\nabla f(x_{k+1}) - \nabla f(x_k)\right] \sim x_{k+1} - x_k.$$

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D_{k+1} will be symmetric, close to D_k, and satisfy the secant condition:

$$D_{k+1} \left[\nabla f(x_{k+1}) - \nabla f(x_k) \right] = x_{k+1} - x_k.$$

BFGS: Broyden, Fletcher, Goldfarb and Shanno (1970)

At iteration k, use x_k, $\nabla f(x_k)$ and D_k to compute

$$x_{k+1} = x_k - \alpha_k D_k \nabla f(x_k), \quad \text{with } \alpha_k \text{ given by line search.}$$

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Then compute $\nabla f(x_{k+1})$, $g_k = \nabla f(x_{k+1}) - \nabla f(x_k)$, $s_k = x_{k+1} - x_k$, and

$$D_{k+1} = D_k + \left(\frac{g_k^T s_k + g_k^T D_k g_k}{(g_k^T s_k)^2} \right) s_k s_k^T + \frac{1}{g_k^T s_k} \left(D_k g_k s_k^T + \left(D_k g_k s_k^T \right)^T \right),$$

which minimizes the Frobenius distance to D_k, subject to the constraints.

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Theorem

Let $f : \mathbb{R}^N \to \mathbb{R}$ be μ-strongly convex and L-smooth, and let D_0 be positive definite. Then, x_n converges to the minimizer of f.
It does so in at most N steps if f is quadratic.

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Momentum, inertia, acceleration

$x_{n+1} = x_n - \alpha_n \nabla f(x_n)$ is equivalent to

$$-\frac{x_{n+1} - x_n}{\alpha_n} = \nabla f(x_n),$$

which is an approximation of the steepest descent evolution equation

$$-\dot{x}(t) = \nabla f\big(x(t)\big).$$

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Other dynamics are related to minimization of potentials. For example,

$$m\ddot{x}(t) + \gamma(t)\dot{x}(t) + \nabla f\big(x(t)\big) = 0.$$

Discretization

We discretize

$$m\ddot{x}(t) + \gamma(t)\dot{x}(t) + \nabla f\big(x(t)\big) = 0$$

to obtain

$$m\,\frac{x_{k+1} - 2x_k + x_{k-1}}{h_k^2} + \gamma_k\,\frac{x_k - x_{k-1}}{h_k} + \nabla f(y_k) = 0.$$

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Equivalently,

$$x_{k+1} = x_k + \beta_k\,(x_k - x_{k-1}) - \alpha_k\,\nabla f(y_k),$$

with $\alpha_k = \frac{h_k^2}{m}$ and $\beta_k = 1 - \frac{\gamma_k h_k}{m}$.

Two popular choices

Polyak's heavy ball (1964)

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

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Nesterov's extrapolation (1983)

$$\left\{ \begin{array}{rcl} y_k & = & x_k + \beta_k\,(x_k - x_{k-1}) \\ x_{k+1} & = & y_k - \alpha_k\,\nabla f(y_k). \end{array} \right.$$

Quadratic case:

$$f(x) = f^* + \frac{1}{2}(x - x^*)^T H(x - x^*).$$

Remark

f is L-smooth and μ-strongly convex if, and only if, $\sigma(H) \subset [\mu, L]$.

The Heavy Ball method

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

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The Heavy Ball method is equivalent to

$$\begin{pmatrix} x_{k+1} \\ x_k \end{pmatrix} = \begin{pmatrix} 1 + \beta - \alpha H & -\beta \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_k \\ x_{k-1} \end{pmatrix}.$$

The convergence rate depends on the eigenvalues of that matrix

$$\begin{pmatrix} 1+\beta-\alpha\lambda & -\beta \\ 1 & 0 \end{pmatrix}, \qquad \text{for} \qquad \lambda \in [\mu, L].$$

Proposition

If $\alpha L \geq 2(1+\beta)$, there is a matrix H, with $\sigma(H) \subset [\mu, L]$, for which the Heavy Ball does not converge for any initial condition.

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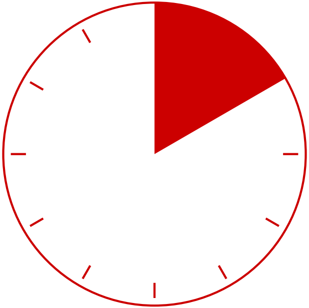
Proposition

The best uniform convergence rate is

$$\rho^* = \frac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}, \quad \textit{obtained when} \quad \beta^* = (\rho^*)^2 \textit{ and } \alpha^* = \frac{2(1+\beta^*)}{L+\mu}.$$

Break



Nesterov's extrapolation

Standard formulation

$$\begin{cases} y_k &= x_k + \beta_k (x_k - x_{k-1}) \\ x_{k+1} &= y_k - \alpha_k \nabla f(y_k). \end{cases}$$

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Alternative description

$$y_{k+1} = y_k - \alpha_k \nabla f(y_k) + \beta_k(y_k - y_{k-1}) - \alpha_k\beta_k\big(\nabla f(y_k) - \nabla f(y_{k-1})\big).$$

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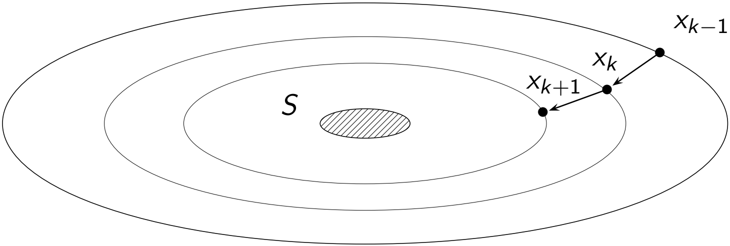
High-resolution differential equation

$$\ddot{y}(t) + A(t)\dot{x}(t) + B(t)\nabla^2 f\big(y(t)\big)\dot{y}(t) + C(t)\nabla f\big(y(t)\big) = 0.$$

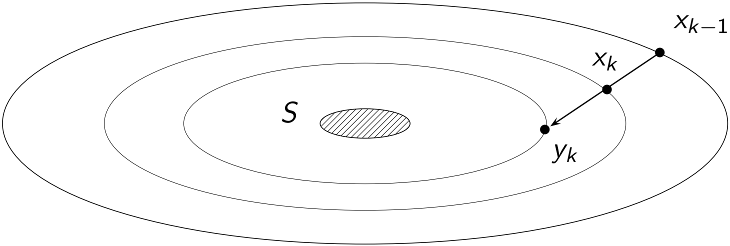
Nesterov's extrapolation

The main idea is the following: Instead of doing this



Nesterov's extrapolation

Better try this



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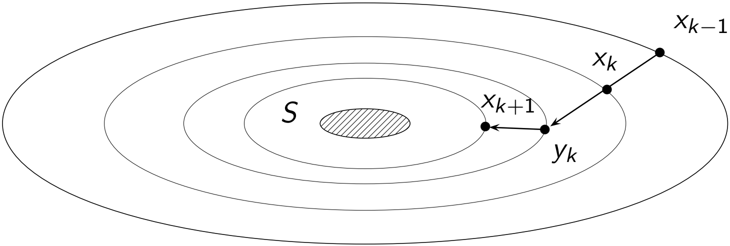

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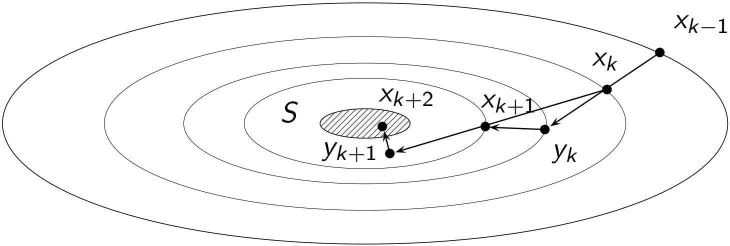

Convergence of Nesterov's method

Theorem

Let $f : \mathbb{R}^N \to \mathbb{R}$ be an L-smooth convex function with minimizers, and let (x_k, y_k) be generated by Nesterov's method with convenient α_k, β_k.

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- *Then,* $f(x_k) - \min(f) \leq \dfrac{L\,\mathrm{dist}(x_0, S)^2}{(k+1)^2}$ *for all* $k \geq 1$. *In addition,* $\lim_{k\to\infty} k^2\big(f(x_k) - \min(f)\big) = 0.$

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- *If, moreover,* f *is* μ*-strongly convex, then*
  $$f(x_k) - \min(f) \leq L\,\mathrm{dist}(x_0, S)^2 \left(1 - \sqrt{\frac{\mu}{L}}\right)^k \text{ for all } k \geq 1.$$

$$\alpha_k \equiv \frac{1}{L}, \quad \beta_k \equiv \frac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}$$