

Gradient Descent



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$$h = -\frac{f'(x)}{\|f'(x)\|_2}$$

gives the direction of the **steepest local** decreasing of the function f. The result of this method is

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

Let's consider the following ODE, which is referred to as the Gradient Flow equation.

$$\frac{dx}{dt} = -f'(x(t)) \tag{GF}$$

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From here we get the expression for x_{k+1}

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 $f \rightarrow \min$

 $f \to \min_{x,y,z}$ Gradient Descent

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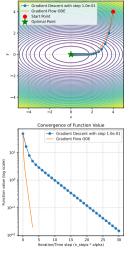
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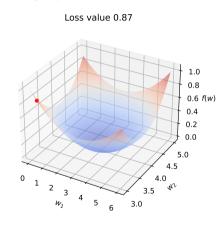
Trajectories with Contour Plot

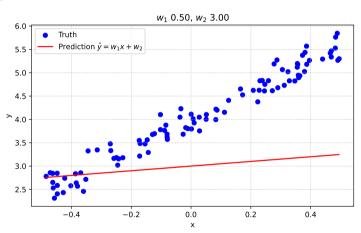
Figure 1: Gradient flow trajectory

Gradient Descent

Convergence of Gradient Descent algorithm

Heavily depends on the choice of the learning rate α :







Exact line search aka steepest descent

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}^+} f(x_{k+1}) = \arg\min_{\alpha \in \mathbb{R}^+} f(x_k - \alpha \nabla f(x_k))$$

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot. An interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

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Optimality conditions:

$$\nabla f(x_{k+1})^{\top} \nabla f(x_k) = 0$$

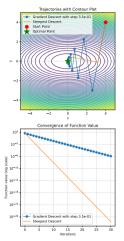


Figure 2: Steepest Descent

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Strongly convex quadratics



Consider the following quadratic optimization problem:

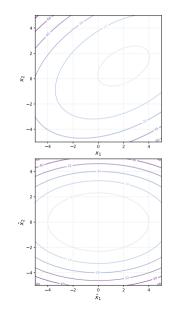
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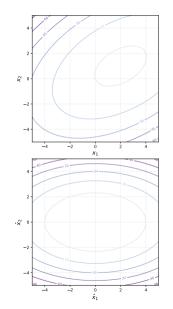
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$$A = Q\Lambda Q^T$$



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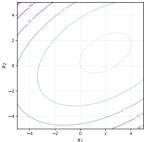
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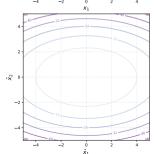
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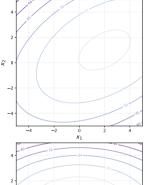
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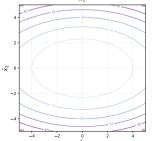
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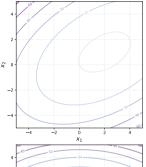
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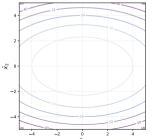
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$$= \frac{1}{2} \hat{x}^T Q^T A Q \hat{x} + (x^*)^T A Q \hat{x} + \frac{1}{2} (x^*)^T A (x^*)^T - b^T Q \hat{x} - b^T x^*$$





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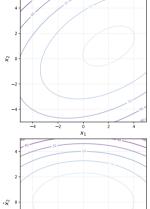
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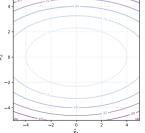
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$$= \frac{1}{2} \hat{x}^T \Lambda \hat{x}$$





Strongly convex quadratics

Now we can work with the function $f(x)=\frac{1}{2}x^T\Lambda x$ with $x^*=0$ without loss of generality (drop the hat from the \hat{x})

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 $f \to \min_{x,y,z}$ Strongly convex quadratics

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Let's use constant stepsize $\alpha^k=\alpha.$ Convergence condition:

$$\rho(\alpha) = \max_{i} |1 - \alpha \lambda_{(i)}| < 1$$

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$$x^{k+1} = x^k - \alpha^k \nabla f(x^k) = x^k - \alpha^k \Lambda x^k$$
$$= (I - \alpha^k \Lambda) x^k$$
$$x^{k+1} = (1 - \alpha^k \Lambda) x^k, \text{ For } i \text{-th coording}$$

$$x_{(i)}^{k+1}=(1-lpha^k\lambda_{(i)})x_{(i)}^k$$
 For i -th coordinate
$$x_{(i)}^{k+1}=(1-lpha^k\lambda_{(i)})^kx_{(i)}^0$$

Let's use constant stepsize $\alpha^k = \alpha$. Convergence

condition: $\rho(\alpha) = \max |1 - \alpha \lambda_{(i)}| < 1$

Person have that
$$\lambda = u > 0$$
 $\lambda = I > u$

Remember, that
$$\lambda_{\min} = \mu > 0, \lambda_{\max} = L \ge \mu.$$

 $|1 - \alpha \mu| < 1 \qquad \qquad |1 - \alpha L| < 1$

$$\begin{array}{ll} -1<1-\alpha\mu<1 & -1<1-\alpha L<1 \\ \alpha<\frac{2}{\mu} & \alpha\mu>0 & \alpha<\frac{2}{L} & \alpha L>0 \\ \alpha<\frac{2}{T} \text{ is needed for convergence.} \end{array}$$

 $= (I - \alpha^k \Lambda) x^k$

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 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)}) x_{(i)}^k$ For *i*-th coordinate

 $|1-\alpha\mu|<1$ $|1-\alpha L|<1$ $-1<1-\alpha L<1$

$$\alpha<\frac{2}{\mu} \qquad \alpha\mu>0 \qquad \qquad \alpha<\frac{2}{L} \qquad \alpha L>0$$

$$\alpha<\frac{2}{L} \text{ is needed for convergence}.$$

Now we would like to tune α to choose the best (lowest) convergence rate

$$\rho^* = \min_{\alpha} \rho(\alpha)$$

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 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})^k x_{(i)}^0$

convergence rate

Remember, that
$$\lambda_{\min} = \mu > 0, \lambda_{\max} = L \geq \mu.$$

$$|1 - \alpha \mu| < 1$$
 $|1 - \alpha L| < 1$

 $\rho(\alpha) = \max|1 - \alpha\lambda_{(i)}| < 1$

Let's use constant stepsize $\alpha^k = \alpha$. Convergence

$$-1 < 1 - \alpha \mu < 1$$

$$\alpha < \frac{2}{\mu} \quad \alpha \mu > 0$$

$$-1 < 1 - \alpha L < 1$$

$$\alpha < \frac{2}{L} \quad \alpha L > 0$$

$$= \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_{i} |1 - \alpha \lambda_{(i)}|$$

Now we would like to tune α to choose the best (lowest)

$$\rho^* = \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_{i} |1 - \alpha \lambda_{(i)}|$$

$$\alpha L < 1$$
 $\alpha L > 0$

 $\alpha < \frac{2}{L}$ is needed for convergence.

condition:

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 $x_{(i)}^{k+1} = (1 - \alpha^k \lambda_{(i)})^k x_{(i)}^0$

Let's use constant stepsize
$$\alpha^k=\alpha$$
. Convergence condition:
$$\rho(\alpha)=\max_i|1-\alpha\lambda_{(i)}|<1$$

$$\rho(\alpha) = \max_{i} |1 - \alpha \lambda_{(i)}| < 1$$

Remember, that
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$$\rho(\alpha) = \max_i |1 - \alpha \lambda_{(i)}| < 1$$

Let's use constant stepsize $\alpha^k = \alpha$. Convergence

Remember, that $\lambda_{\min} = \mu > 0, \lambda_{\max} = L > \mu$.

$$< 1$$
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$$\rho^* = \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_{i} |1 - \alpha \lambda_{(i)}|$$
$$= \min_{\alpha} \{|1 - \alpha \mu|, |1 - \alpha L|\}$$
$$\alpha^* : 1 - \alpha^* \mu = \alpha^* L - 1$$

$$= \alpha L - 1$$

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$$f \to \min_{x,y,z}$$
 Strongly convex quadratics

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convergence rate

 $\rho^* = \min_{\alpha} \rho(\alpha) = \min_{\alpha} \max_{i} |1 - \alpha \lambda_{(i)}|$ $= \min \left\{ |1 - \alpha \mu|, |1 - \alpha L| \right\}$

$$\alpha^*: 1 - \alpha^* \mu = \alpha^* L - 1$$

$$\alpha^* = \frac{2}{\mu + L} \quad \rho^* = \frac{L - \mu}{L + \mu}$$

$$\rho^* = \frac{L - L}{L + L}$$

$$=\frac{L-\mu}{L+\mu}$$

$$-\frac{1}{L+\mu}$$

Now we would like to tune α to choose the best (lowest)

$$+\mu$$

$$\vdash \mu$$
 $k+1$

$$x^{k+1} = \left(\frac{L-\mu}{L+\mu}\right)^k x^0 \quad f(x^{k+1}) = \left(\frac{L-\mu}{L+\mu}\right)^{2k} f(x^0)$$

$$f o \min$$
 Strongly convey guar

So, we have a linear convergence in the domain with rate $\frac{\kappa-1}{\kappa+1}=1-\frac{2}{\kappa+1}$, where $\kappa=\frac{L}{\mu}$ is sometimes called *condition number* of the quadratic problem.

κ	ho	Iterations to decrease domain gap $10\ \mathrm{times}$	Iterations to decrease function gap $10\ \mathrm{times}$
1.1	0.05	1	1
2	0.33	3	2
5	0.67	6	3
10	0.82	12	6
50	0.96	58	29
100	0.98	116	58
500	0.996	576	288
1000	0.998	1152	576



Polyak-Lojasiewicz smooth case



Polyak-Lojasiewicz condition. Linear convergence of gradient descent without convexity

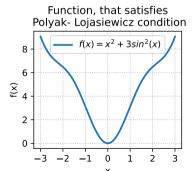
PL inequality holds if the following condition is satisfied for some $\mu > 0$,

$$\|\nabla f(x)\|^2 \ge 2\mu(f(x) - f^*) \quad \forall x$$

It is interesting, that the Gradient Descent algorithm might converge linearly even without convexity.

The following functions satisfy the PL condition but are not convex. Link to the code

$$f(x) = x^2 + 3\sin^2(x)$$



Polyak-Loiasiewicz smooth case



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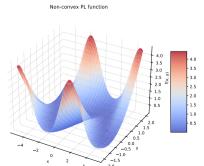
Function, that satisfies
Polyak- Lojasiewicz condition

8

6 $x = x^2 + 3sin^2(x)$ 0

-3 -2 -1 0 1 2 3

$$f(x,y) = \frac{(y - \sin x)^2}{2}$$



i Theorem

Consider the Problem

$$f(x) \to \min_{x \in \mathbb{R}^d}$$

and assume that f is μ -Polyak-Lojasiewicz and L-smooth, for some $L \geq \mu > 0$.

Consider $(x^k)_{k\in\mathbb{N}}$ a sequence generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0 < \alpha \leq \frac{1}{T}$. Then:

$$f(x^k) - f^* \le (1 - \alpha \mu)^k (f(x^0) - f^*).$$



$$f(x^{k+1}) \leq f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2$$

$$f(x^{k+1}) \le f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2$$
$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

$$f(x^{k+1}) \le f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2$$

$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

$$= f(x^k) - \frac{\alpha}{2} (2 - L\alpha) \|\nabla f(x^k)\|^2$$

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$$\le f(x^k) - \frac{\alpha}{2} \|\nabla f(x^k)\|^2,$$

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We can use L-smoothness, together with the update rule of the algorithm, to write

$$f(x^{k+1}) \le f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L}{2} \|x^{k+1} - x^k\|^2$$

$$= f(x^k) - \alpha \|\nabla f(x^k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x^k)\|^2$$

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where in the last inequality we used our hypothesis on the stepsize that $\alpha L \leq 1$.

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where in the last inequality we used our hypothesis on the stepsize that $\alpha L \leq 1$.

We can now use the Polyak-Loiasiewicz property to write:

$$f(x^{k+1}) \le f(x^k) - \alpha \mu (f(x^k) - f^*).$$

The conclusion follows after subtracting f^* on both sides of this inequality and using recursion.

1 Theorem

If a function f(x) is differentiable and μ -strongly convex, then it is a PL function.

Proof

By first order strong convexity criterion:

$$f(y) \ge f(x) + \nabla f(x)^{T} (y - x) + \frac{\mu}{2} ||y - x||_{2}^{2}$$

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||_2^2$$

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Polyak-Loiasiewicz smooth case

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$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||_2^2 =$$

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$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||_2^2 =$$

$$= \left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T} (x - x^{*}) =$$

$$= \frac{1}{2} \left(\frac{2}{\sqrt{\mu}} \nabla f(x)^{T} - \sqrt{\mu} (x^{*} - x) \right)^{T} \sqrt{\mu} (x - x^{*}) =$$

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Let $a = \frac{1}{\sqrt{\mu}} \nabla f(x)$ and $b = \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x)$

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||_2^2$$
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$$= \left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T}(x - x^{*}) =$$

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$$f(y) \ge f(x) + \nabla f(x)^{T} (y - x) + \frac{\mu}{2} ||y - x||_{2}^{2}$$

Putting $y = x^*$:

$$f(x^*) \ge f(x) + \nabla f(x)^T (x^* - x) + \frac{\mu}{2} ||x^* - x||_2^2$$
$$f(x) - f(x^*) \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x^* - x||_2^2 =$$

$$= \left(\nabla f(x)^{T} - \frac{\mu}{2}(x^{*} - x)\right)^{T}(x - x^{*}) =$$

$$= \frac{1}{2} \left(\frac{2}{\sqrt{\mu}} \nabla f(x)^{T} - \sqrt{\mu}(x^{*} - x)\right)^{T} \sqrt{\mu}(x - x^{*}) =$$

Let $a = \frac{1}{\sqrt{\mu}} \nabla f(x)$ and $b = \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}}\nabla f(x)$

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$$f(x) - f(x^*) \le \frac{1}{2} \left(\frac{1}{\mu} \|\nabla f(x)\|_2^2 - \left\| \sqrt{\mu}(x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x) \right\|_2^2 \right)$$



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which is exactly the PL condition. It means, that we already have linear convergence proof for any strongly convex function.

Smooth convex case





Smooth convex case

i Theorem

Consider the Problem

$$f(x) \to \min_{x \in \mathbb{R}^d}$$

and assume that f is convex and L-smooth, for some L > 0.

Let $(x^k)_{k\in\mathbb{N}}$ be the sequence of iterates generated by the gradient descent constant stepsize algorithm, with a stepsize satisfying $0<\alpha\leq \frac{1}{L}$. Then, for all $x^*\in \operatorname{argmin} f$, for all $k\in\mathbb{N}$ we have that

$$f(x^k) - f^* \le \frac{\|x^0 - x^*\|^2}{2\alpha k}.$$



• As it was before, we first use smoothness:

$$f(x^{k+1}) \leq f(x^{k}) + \langle \nabla f(x^{k}), x^{k+1} - x^{k} \rangle + \frac{L}{2} \|x^{k+1} - x^{k}\|^{2}$$

$$= f(x^{k}) - \alpha \|\nabla f(x^{k})\|^{2} + \frac{L\alpha^{2}}{2} \|\nabla f(x^{k})\|^{2}$$

$$= f(x^{k}) - \frac{\alpha}{2} (2 - L\alpha) \|\nabla f(x^{k})\|^{2}$$

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$$= f(x^{k+1}) \geq \frac{1}{2} \|\nabla f(x^{k})\|^{2} \text{ if } \alpha \leq \frac{1}{2}$$
(1)

$$f(x^k) - f(x^{k+1}) \ge \frac{1}{2L} \|\nabla f(x^k)\|^2 \text{ if } \alpha \le \frac{1}{L}$$

Typically, for the convergent gradient descent algorithm the higher the learning rate the faster the convergence. That is why we often will use $\alpha = \frac{1}{4}$.

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 $f \to \min_{x,y,z}$ Smooth convex case

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 $f \to \min_{x,y,z}$ Smooth convex case

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 $f \to \min_{x,y,z}$ Smooth convex case

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• Now suppose, that the last line is defined for some index i and we sum over $i \in [0, k-1]$. Almost all summands will vanish due to the telescopic nature of the sum:

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 $2\alpha \sum (f(x^{i+1}) - f^*) \le ||x^0 - x^*||_2^2 - ||x^k - x^*||_2^2$

$$f \to \min_{x,y,z}$$
 Smooth convex case

(3)

Now we put Equation 2 to Equation 1:

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 $f \to \min_{x,y,z}$ Smooth convex case

(3)

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$$2\alpha k f(x^k) - 2\alpha k f^* \le 2\alpha \sum_{i=1}^{k-1} \left(f(x^{i+1}) - f^* \right) \le ||x^0 - x^*||_2^2$$



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$$f(x^k) - f^* \le \frac{\|x^0 - x^*\|_2^2}{2\alpha k} \le \frac{L\|x^0 - x^*\|_2^2}{2k}$$

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