

ORF522 – Linear and Nonlinear Optimization

11. Gradient descent

Today's lecture

[Chapter 1 and 2, ILCO][Chapter 9, CO][Chapter 5, FMO]

Gradient descent algorithms

- Optimization algorithms and convergence rates
- Gradient descent analysis (fixed-step size)
 - quadratic functions,
 - smooth and strongly convex functions
 - smooth functions

Optimization algorithms and convergence rates

Iterative solution idea

1. Start from initial point x^0
2. Generate sequence $\{x^k\}$ by applying an operator

$$x^{k+1} = T(x^k)$$

3. Converge to fixed-point $x^* = T(x^*)$ for which **necessary optimality conditions** hold

Note: typically, we have $f(x^{k+1}) \leq f(x^k)$

Convergence rates

Rank methods by how fast they converge

Error function $e(x) \geq 0$ such that $e(x^*) = 0$

- Cost function distance: $e(x) = f(x) - f(x^*)$
- Solution distance: $e(x) = \|x - x^*\|_2$

Convergence rate

A sequence converges with order p and factor c if

$$\lim_{k \rightarrow \infty} \frac{e(x^{k+1})}{e(x^k)^p} < c$$

Convergence rates types

Linear convergence (geometric) ($c \in (0, 1)$)

$$e(x^{k+1}) \leq ce(x^k)$$

Examples

$$e(x^k) = 0.6^k$$

Sublinear convergence (slower than linear)

$$e(x^{k+1}) \leq \frac{M}{(k+1)^q}, \quad \text{with } q = 0.5, 1, 2, \dots$$

$$e(x^k) = \frac{1}{\sqrt{k}}$$

Superlinear convergence (faster than linear)

If it converges linearly $p = 1$ for any factor $c \in (0, 1)$

$$e(x^k) = \frac{1}{k^k}$$

Quadratic convergence (c can be > 1)

$$e(x^{k+1}) \leq ce(x^k)^2$$

$$e(x^k) = 0.9^{(2^k)}$$

Convergence rates

Number of iterations

Solve inequality for k

Example: linear convergence ($c \in (0, 1)$)

$$e(x^{k+1}) \leq ce(x^k)$$

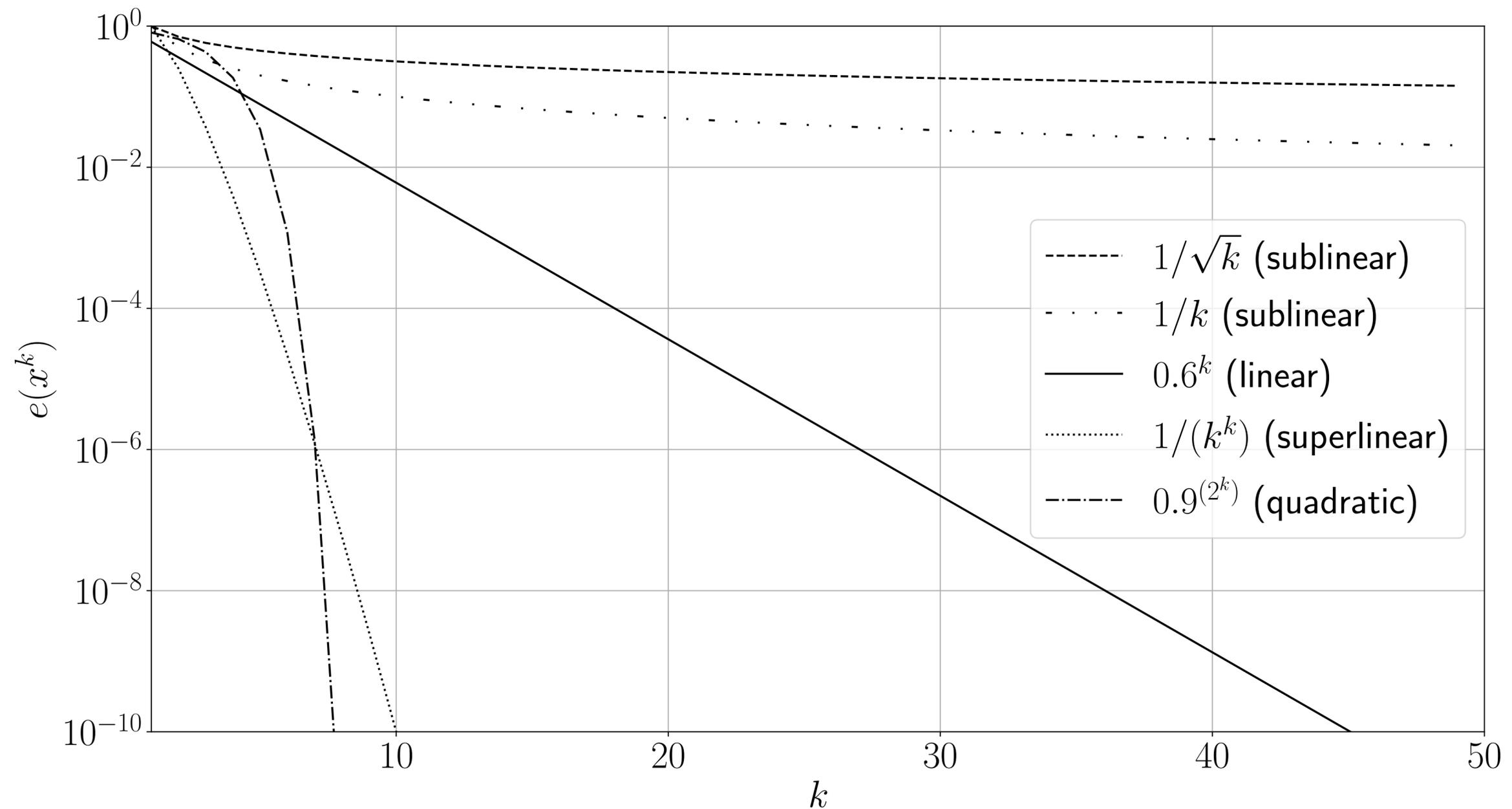
$$e(x^{k+1}) \leq \epsilon \iff c^k e(x^0) \leq \epsilon \iff k \geq O(\log(1/\epsilon))$$

Example: sublinear convergence

$$e(x^{k+1}) \leq \frac{M}{k+1} \implies k \geq O(1/\epsilon)$$

Convergence rates

Examples



Optimization methods overview

Zero order. They rely only on $f(x)$. Not possible to evaluate the curvature. Extremely slow.

Examples: Random search, genetic algorithms, particle swarm optimization, simulated annealing, etc.

First order. They use $f(x)$ and $\nabla f(x)$ or $\partial f(x)$. Inexpensive iterations make them extremely popular in large-scale optimization and machine learning

(our focus)

Examples: Gradient descent, stochastic gradient descent, coordinate descent, proximal algorithms, ADMM.

Second order. They use $f(x)$, $\nabla f(x)$ and $\nabla^2 f(x)$. Expensive iterations but very fast convergence

Examples: Newton method, interior-point methods.

Iterative descent algorithms

Problem setup

Unconstrained smooth optimization

minimize $f(x)$ $x \in \mathbf{R}^n$ f is differentiable

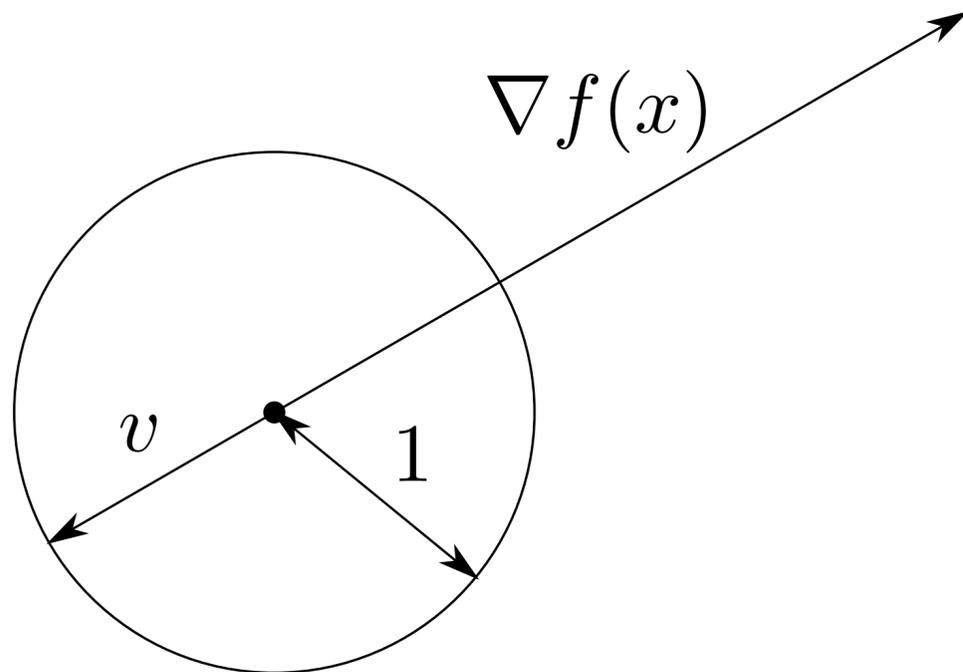
Gradient descent scheme

- Pick descent direction d^k , i.e., $\nabla f(x^k)^T d^k < 0$
- Pick step size t_k
- $x^{k+1} = x^k + t^k d^k, \quad k = 0, 1, \dots$

Gradient descent

[Cauchy 1847]

Choose $d_k = -\nabla f(x^k)$



Interpretation: steepest descent (Cauchy-Schwarz)

$$v = \operatorname{argmin}_{\|v\|_2 \leq 1} \nabla f(x)^T v = -\frac{\nabla f(x)}{\|\nabla f(x)\|_2} \longrightarrow d = v \|\nabla f(x)\|_2$$

Iterations

$$x^{k+1} = x^k - t_k \nabla f(x^k), \quad k = 0, 1, \dots$$

(very cheap)

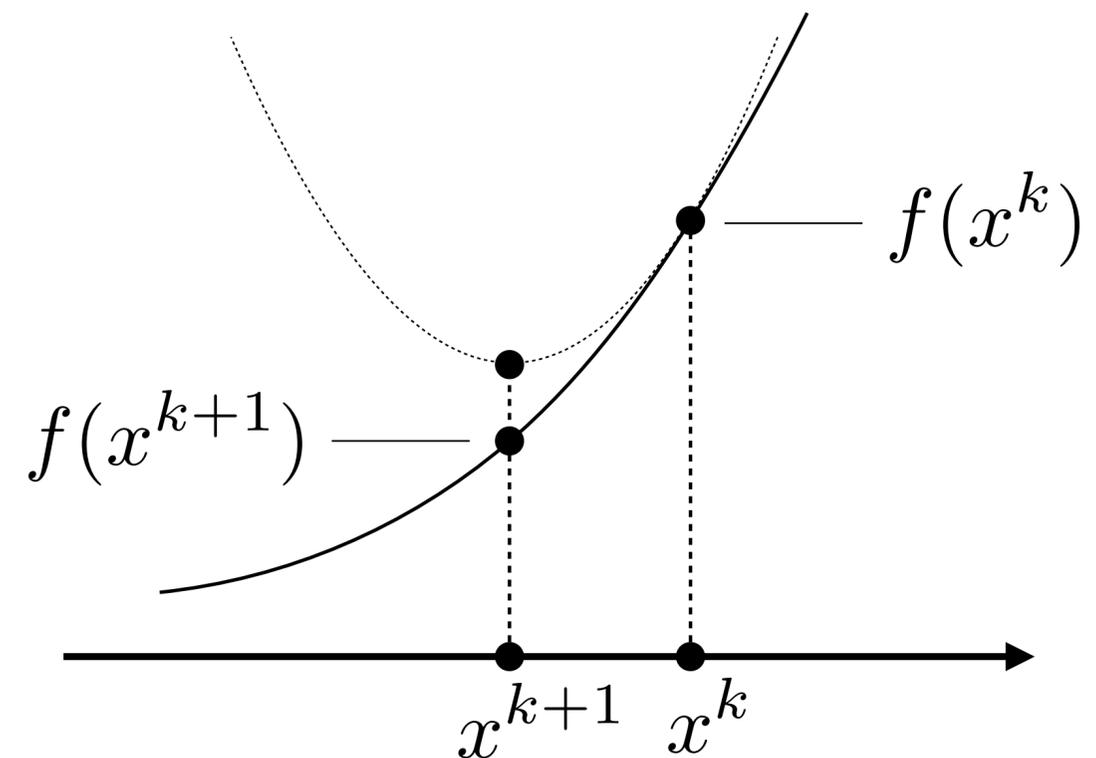
Quadratic function interpretation

Quadratic approximation, replacing Hessian $\nabla^2 f(x^k)$ with $\frac{1}{t_k} I$

$$x^{k+1} = \underset{y}{\operatorname{argmin}} f(x^k) + \nabla f(x^k)^T (y - x^k) + \frac{1}{2t_k} \|y - x^k\|_2^2 \quad (\text{proximity to } x^k)$$

Set gradient with respect to y to 0...

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

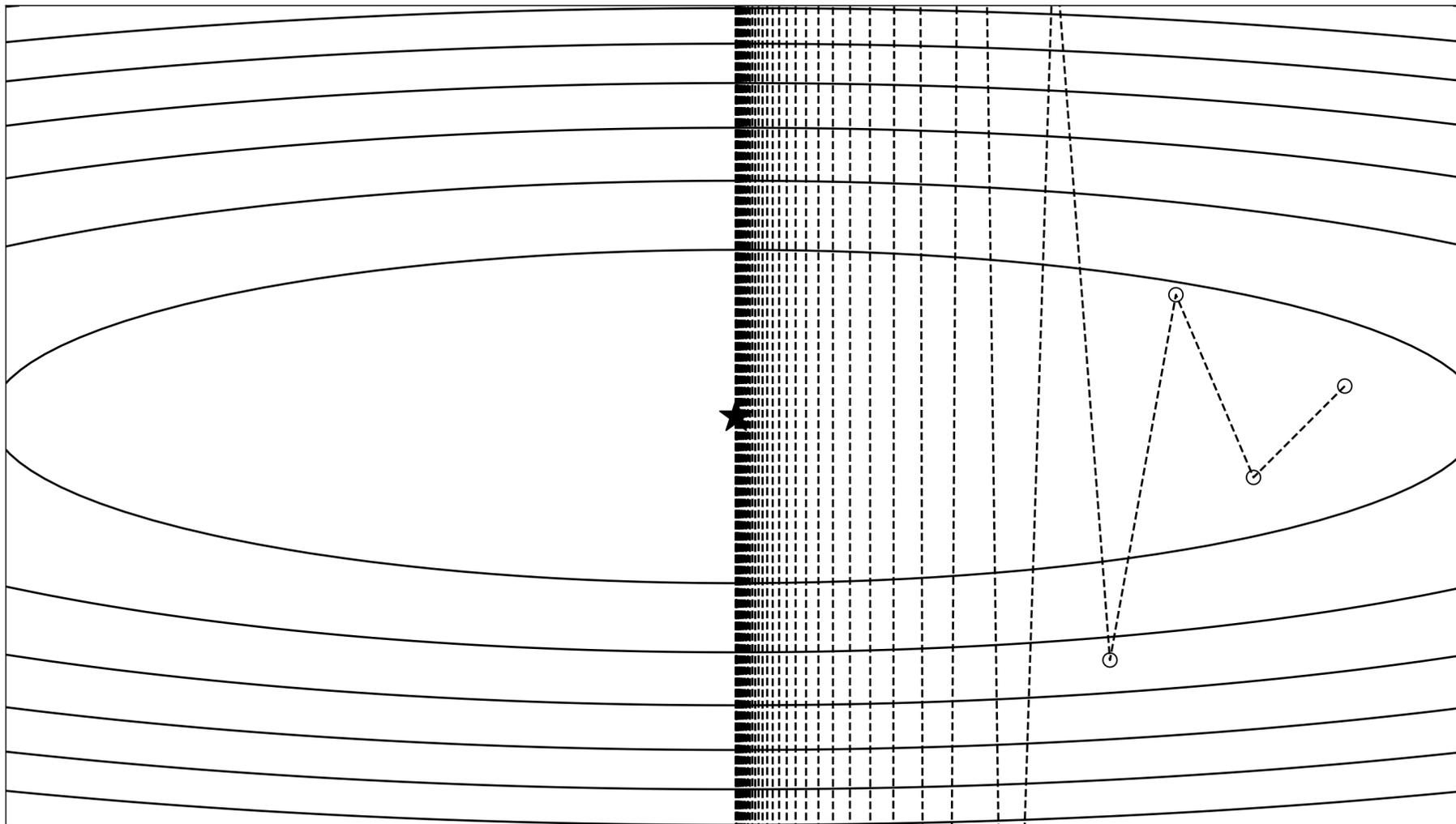


Fixed step size choice

$$t_k = t \text{ for all } k = 0, 1, \dots$$

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$x^0 = (20, 1)$$
$$t = 0.15$$



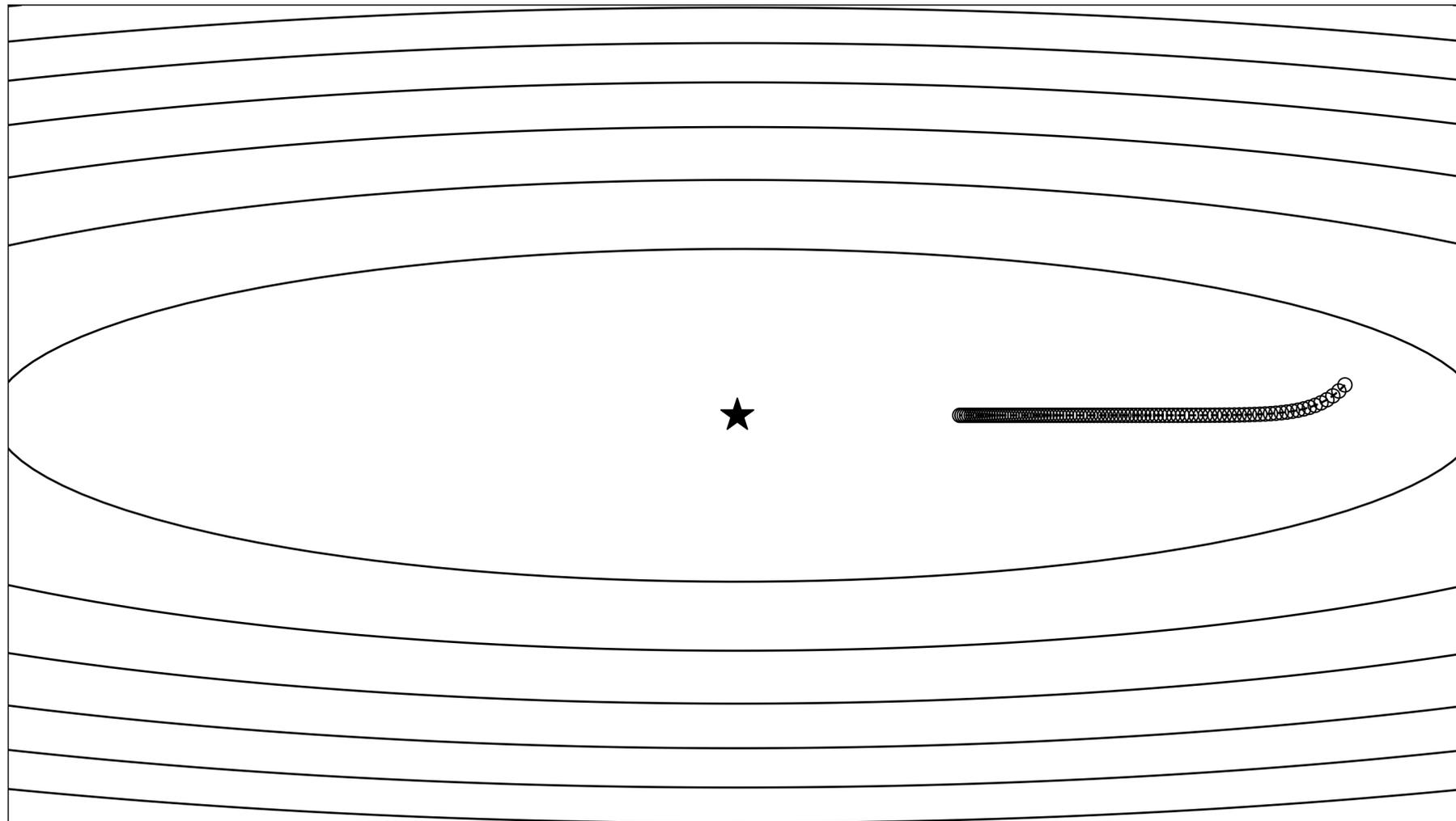
It diverges

Fixed step size choice

$$t_k = t \text{ for all } k = 0, 1, \dots$$

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$x^0 = (20, 1)$$
$$t = 0.01$$



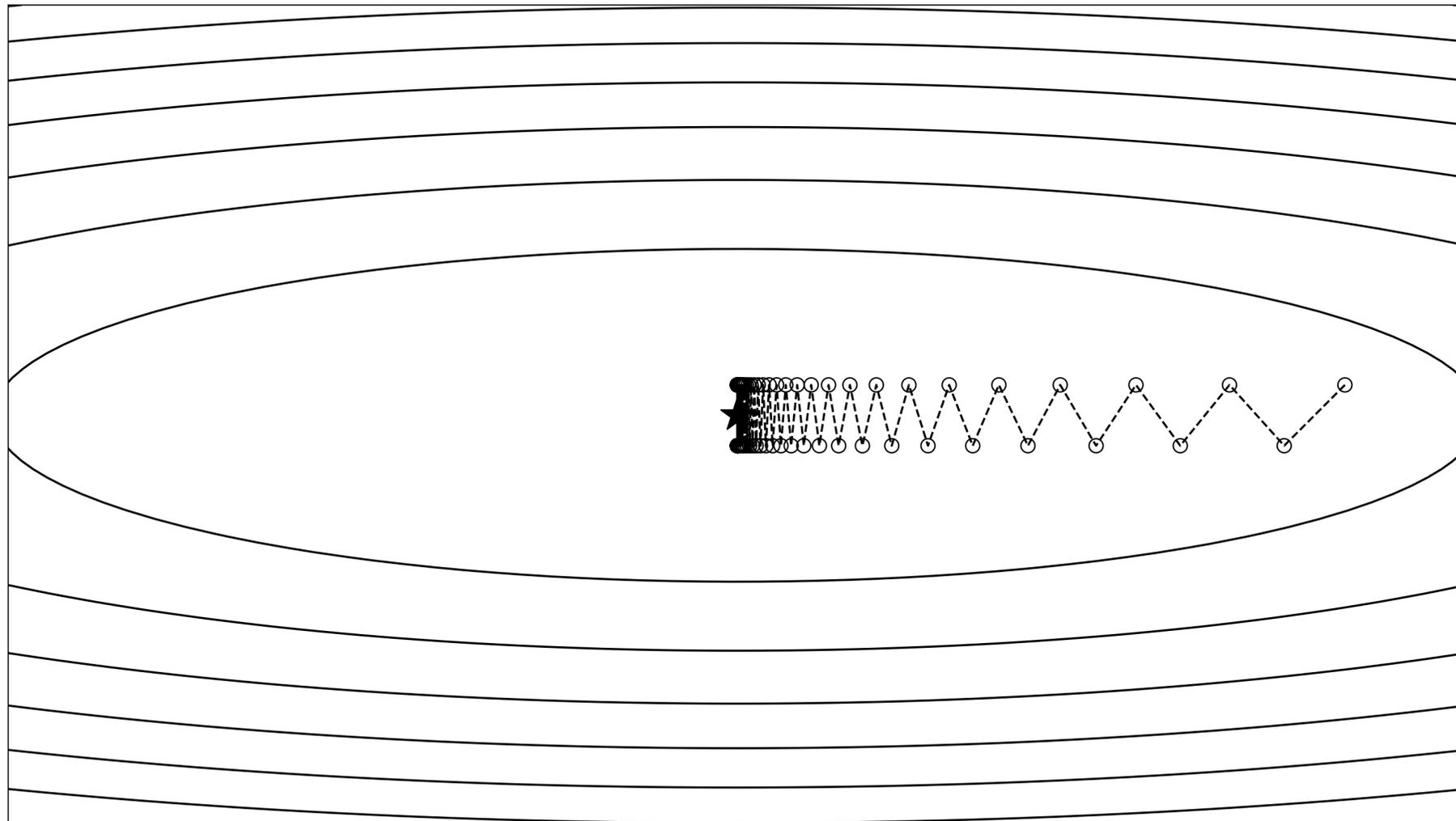
too slow

Fixed step size choice

$$t_k = t \text{ for all } k = 0, 1, \dots$$

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$x^0 = (20, 1)$$
$$t = 0.10$$



it oscillates

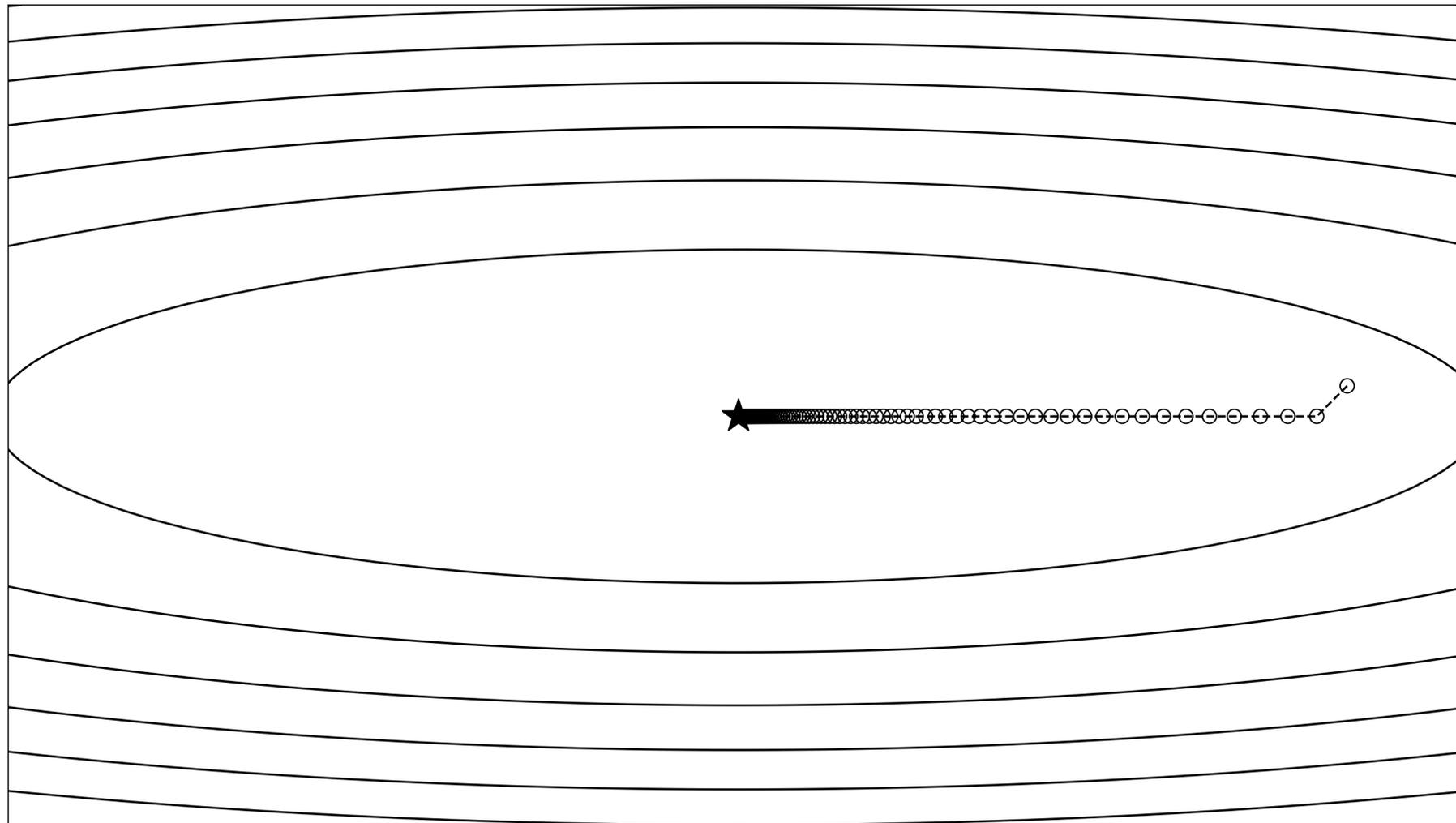
Fixed step size choice

$$t_k = t \text{ for all } k = 0, 1, \dots$$

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$x^0 = (20, 1)$$

$$t = 0.05$$



just right!

It converges in 149 iterations

How do we find the best one?

Quadratic optimization

Quadratic optimization

$$\text{minimize } f(x) = \frac{1}{2}(x - x^*)^T P(x - x^*)$$

where $P \succ 0$

$$\nabla f(x) = P(x - x^*)$$

Study behavior of

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

Remarks

- Always possible to write QPs in this form
- Important for smooth nonlinear programming. Close to x^* , $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ dominates other terms of the Taylor expansion.

Quadratic optimization convergence

Theorem

If $t_k = t = \frac{2}{\lambda_{\min}(P) + \lambda_{\max}(P)}$, then

$$\|x^k - x^*\|_2 \leq \left(\frac{\text{cond}(P) - 1}{\text{cond}(P) + 1} \right)^k \|x^0 - x^*\|_2$$

Remarks

- Linear (geometric) convergence rate: $O(\log(1/\epsilon))$ iterations
- It depends on the **condition number** of P : $\text{cond}(P) = \frac{\lambda_{\max}(P)}{\lambda_{\min}(P)}$

Quadratic optimization convergence

Proof

Rewrite iterations using $\nabla f(x^k) = P(x^k - x^*)$

$$x^{k+1} - x^* = x^k - x^* - t\nabla f(x^k) = (I - tP)(x^k - x^*)$$

Therefore $\|x^{k+1} - x^*\|_2 \leq \|I - tP\|_2 \|x^k - x^*\|_2$

Let's rewrite $\|I - tP\|_2$:

Matrix norm: $\|M\|_2 = \max_i |\lambda_i(M)|$

Decomposition: $I - tP = U \text{diag}(\mathbf{1} - t\lambda) U^T$ where $P = U \text{diag}(\lambda) U^T$

Therefore, $\|I - tP\|_2 = \max_i |1 - t\lambda_i(P)|$

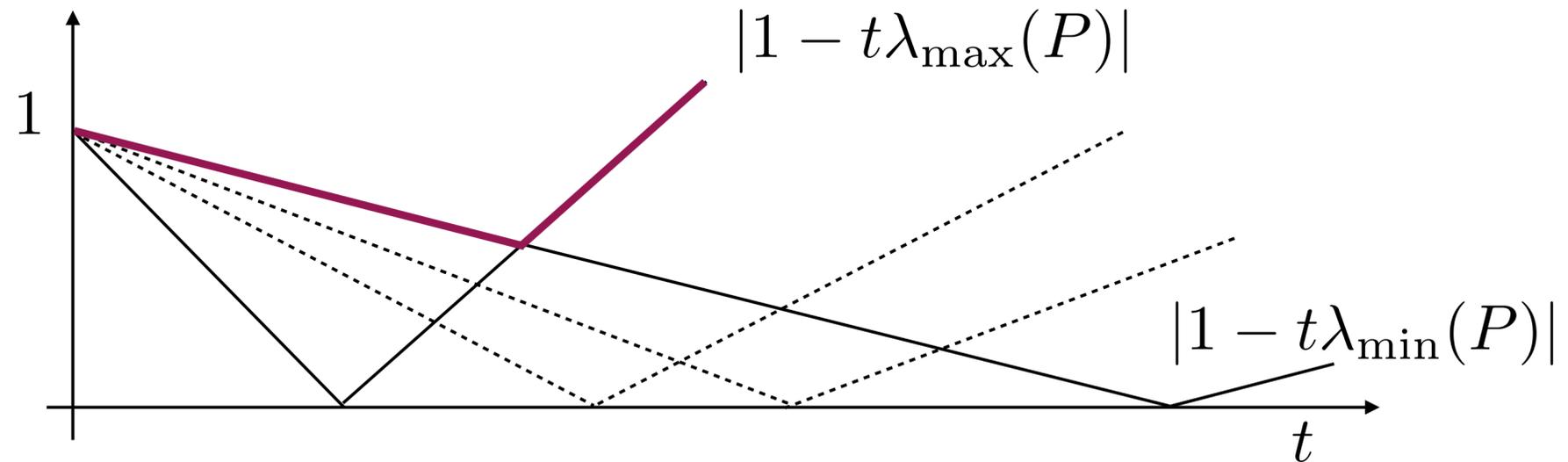
Quadratic optimization convergence

Proof (continued)

$$\|I - tP\|_2 = \max_i |1 - t\lambda_i(P)|$$

$$= \max\{|1 - t\lambda_{\max}(P)|, |1 - t\lambda_{\min}(P)|\}$$

$$= \max\{1 - t\lambda_{\min}(P), -1 + t\lambda_{\max}(P)\}$$



To have the fastest convergence, we want to minimize

$$\min_t \|I - tP\|_2 = \min_t \max\{1 - t\lambda_{\min}(P), -1 + t\lambda_{\max}(P)\}$$

Minimum achieved when

$$1 - t\lambda_{\min}(P) = -1 + t\lambda_{\max}(P) \quad \implies \quad t = \frac{2}{\lambda_{\max}(P) + \lambda_{\min}(P)}$$

Quadratic optimization convergence

Proof (continued)

$$\|x^{k+1} - x^*\|_2 \leq \|I - tP\|_2 \|x^k - x^*\|_2$$

with $t = \frac{2}{\lambda_{\max}(P) + \lambda_{\min}(P)}$ we have

$$\|I - tP\|_2 = 1 - t\lambda_{\min}(P) = \frac{\lambda_{\max}(P) - \lambda_{\min}(P)}{\lambda_{\max}(P) + \lambda_{\min}(P)} = \left(\frac{\mathbf{cond}(P) - 1}{\mathbf{cond}(P) + 1} \right)$$

Apply the inequality recursively to get the result



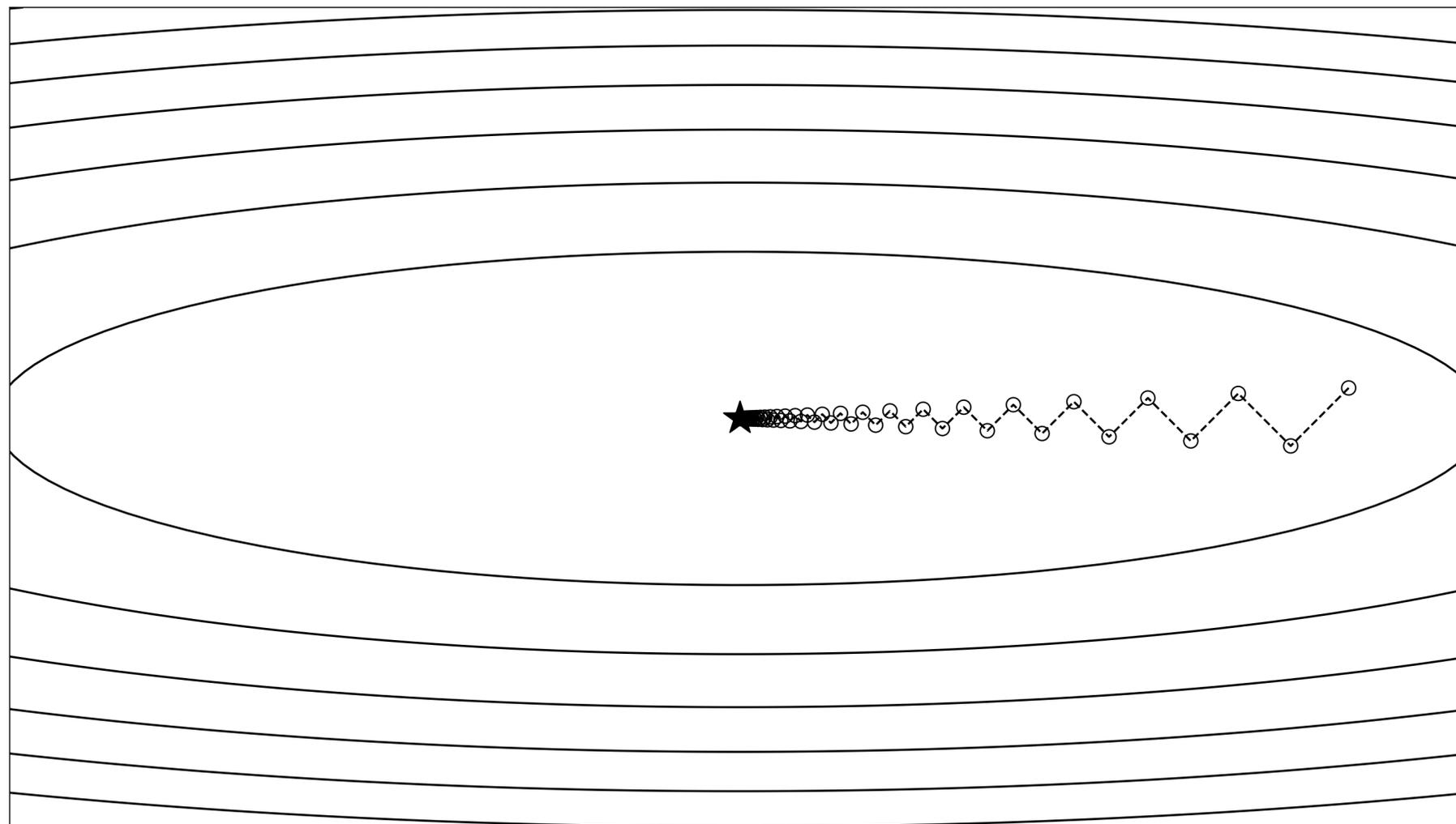
Optimal fixed step size

$$t_k = t \text{ for all } k = 0, 1, \dots$$

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$x^0 = (20, 1)$$

$$t = 2/(1 + 20) = 0.0952$$



Optimal step size

It converges in 80 iterations

When does it converge?

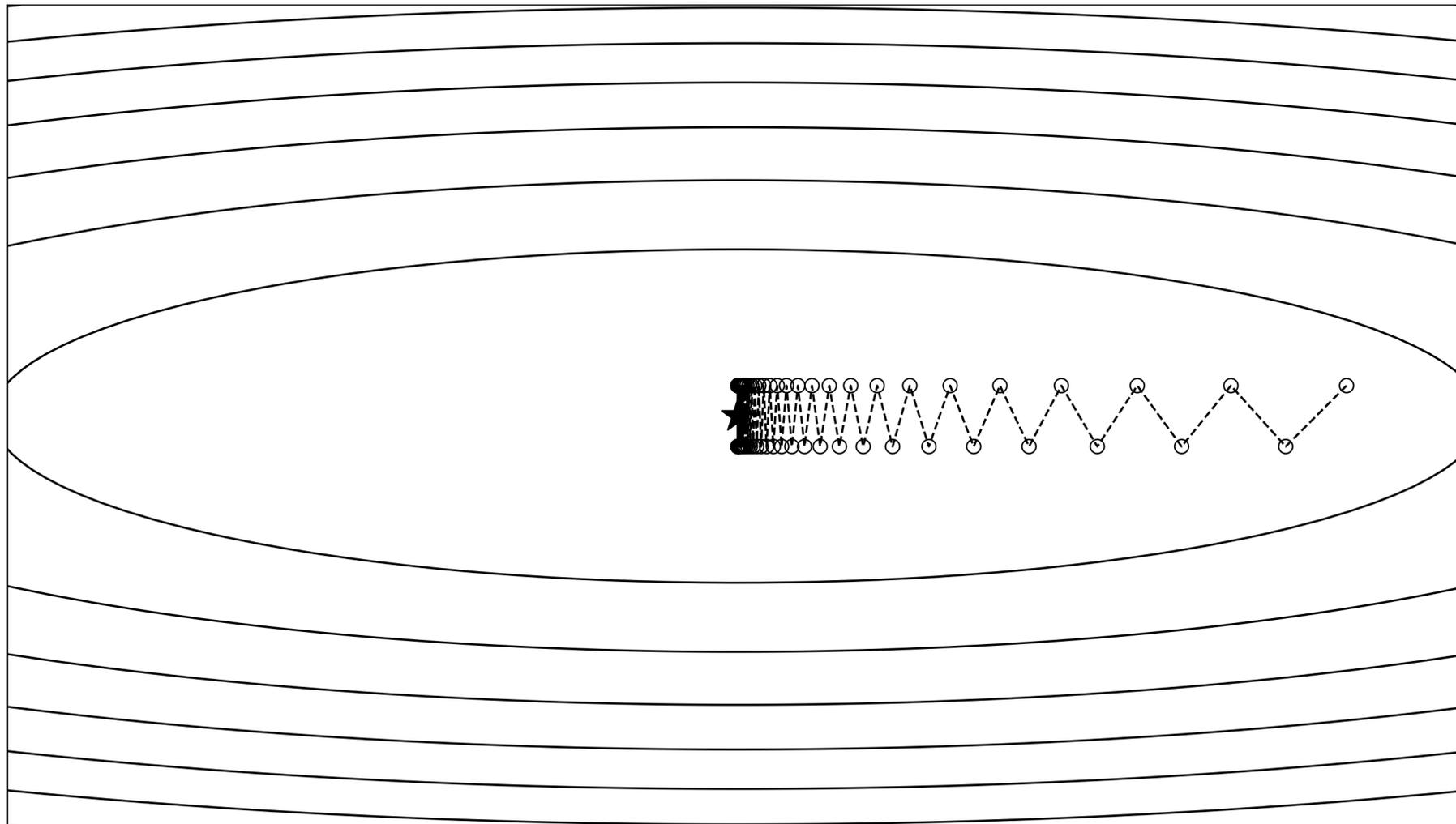
Iterations

$$\|x^k - x^*\|_2 \leq c^k \|x^0 - x^*\|_2$$

Contraction factor

$$c = \|I - tP\|_2 = \max\{1 - t\lambda_{\min}(P), -1 + t\lambda_{\max}(P)\}$$

If $t < 2/\lambda_{\max}(P)$ then $c < 1$



Oscillating case

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$t = 0.1 = 2/20 = 2/\lambda_{\max}(P)$$

Step size ranges

- If $t < 0.1$, it converges
- If $t = 0.1$, it oscillates
- If $t > 0.1$, it diverges

Strongly convex and smooth problems

Gradient monotonicity for convex functions

A differentiable function f is convex if and only if $\text{dom } f$ is convex and

$$(\nabla f(x) - \nabla f(y))^T (x - y) \geq 0, \quad \forall x, y \in \text{dom } f$$

i.e., the gradient is a **monotone mapping**.

Proof

(\Rightarrow) Combine $f(y) \geq f(x) + \nabla f(x)^T (y - x)$ and $f(x) \geq f(y) + \nabla f(y)^T (x - y)$

(\Leftarrow) Let $g(t) = f(x + t(y - x))$. Then, $\nabla g(t) \geq \nabla g(0)$, $\forall t \geq 0, t \in \text{dom } g$ with

$$\nabla g(t) = \nabla f(x + t(y - x))^T (y - x)$$

Hence, $f(y) = g(1) = g(0) + \int_0^1 \nabla g(t) dt \geq g(0) + \nabla g(0) = f(x) + \nabla f(x)^T (y - x)$

(first-order condition for convexity) ■

Smooth functions

Function f is L -smooth with parameter $L > 0$ if

$$f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} \|x - y\|_2^2, \quad \forall x, y \in \mathbf{dom} f$$

equivalent characterizations

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2 \quad \forall x, y \in \mathbf{dom} f \quad (\text{Lipschitz continuous gradient})$$

$$\nabla^2 f(x) \preceq LI, \quad \forall x \in \mathbf{dom} f$$

Strongly convex functions

A function f is μ -strongly convex if

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} \|x - y\|_2^2, \quad \forall x, y \in \mathbf{dom} f$$

equivalent characterizations

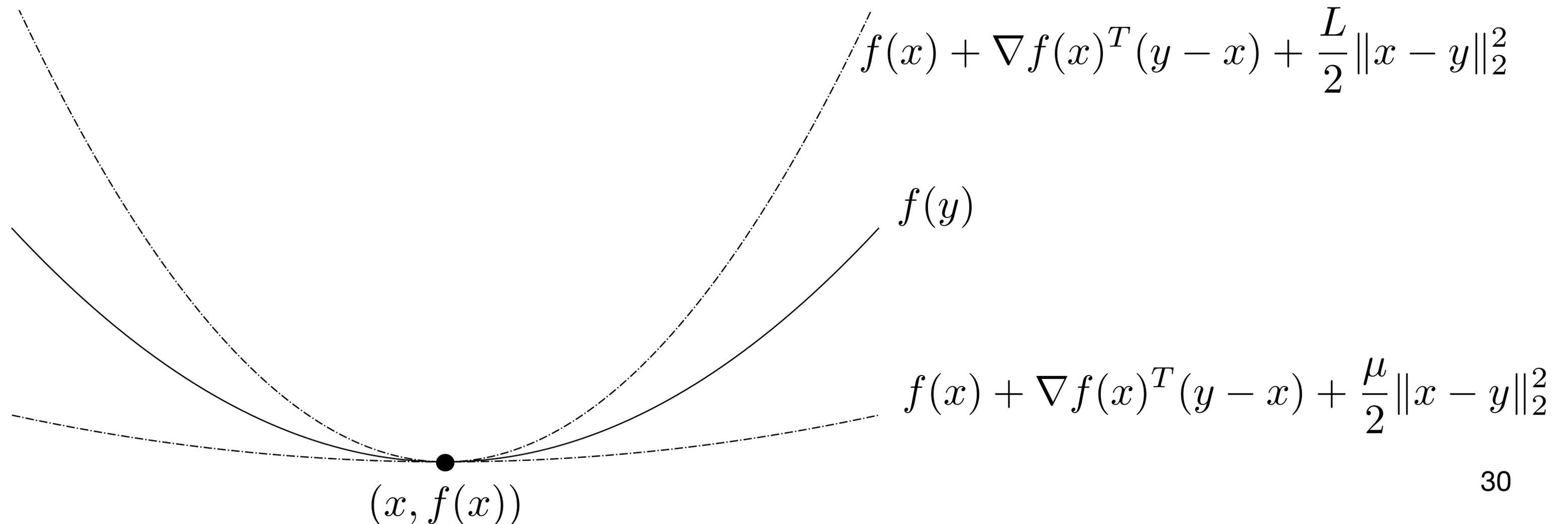
$$(\nabla f(x) - \nabla f(y))^T (x - y) \geq \mu \|x - y\|^2, \quad \forall x, y \in \mathbf{dom} f \quad (\text{strongly monotone gradient})$$

$$\nabla^2 f(x) \succeq \mu I, \quad \forall x \in \mathbf{dom} f$$

Strongly convex and smooth functions

f is μ -strongly convex and L -smooth if

$$0 \preceq \mu I \preceq \nabla^2 f(x) \preceq LI, \quad \forall x$$



Strongly convex and smooth convergence

Theorem

Let f be μ -strongly convex and L -smooth. If $t = \frac{2}{\mu + L}$, then

$$\|x^k - x^*\|_2 \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^k \|x^0 - x^*\|_2$$

where $\kappa = L/\mu$ is the **condition number**

Remarks

- **Linear (geometric) convergence rate** $O(\log(1/\epsilon))$ iterations
- **Generalizes quadratic problems** where
 $t = 2/(\lambda_{\max}(P) + \lambda_{\min}(P))$, $\text{cond}(P)$ instead of κ
- **Dimension-free contraction factor**, if κ does not depend on n

Strongly convex and smooth convergence

Proof Fundamental

theorem of calculus: $\nabla f(x^k) = \nabla f(x^k) - \underbrace{\nabla f(x^*)}_{=0} = \int_{x^*}^{x^k} \nabla^2 f(x_\tau) dx_\tau$

x^k $x_\tau = x^* + \tau(x^k - x^*)$ x^*

$$= \left(\int_0^1 \nabla^2 f(x_\tau) d\tau \right) (x^k - x^*)$$

Therefore, $\|x^{k+1} - x^*\|_2 = \|x^k - x^* - t\nabla f(x^k)\|_2$

$$= \left\| \left(\int_0^1 (I - t\nabla^2 f(x_\tau)) d\tau \right) (x^k - x^*) \right\|_2$$

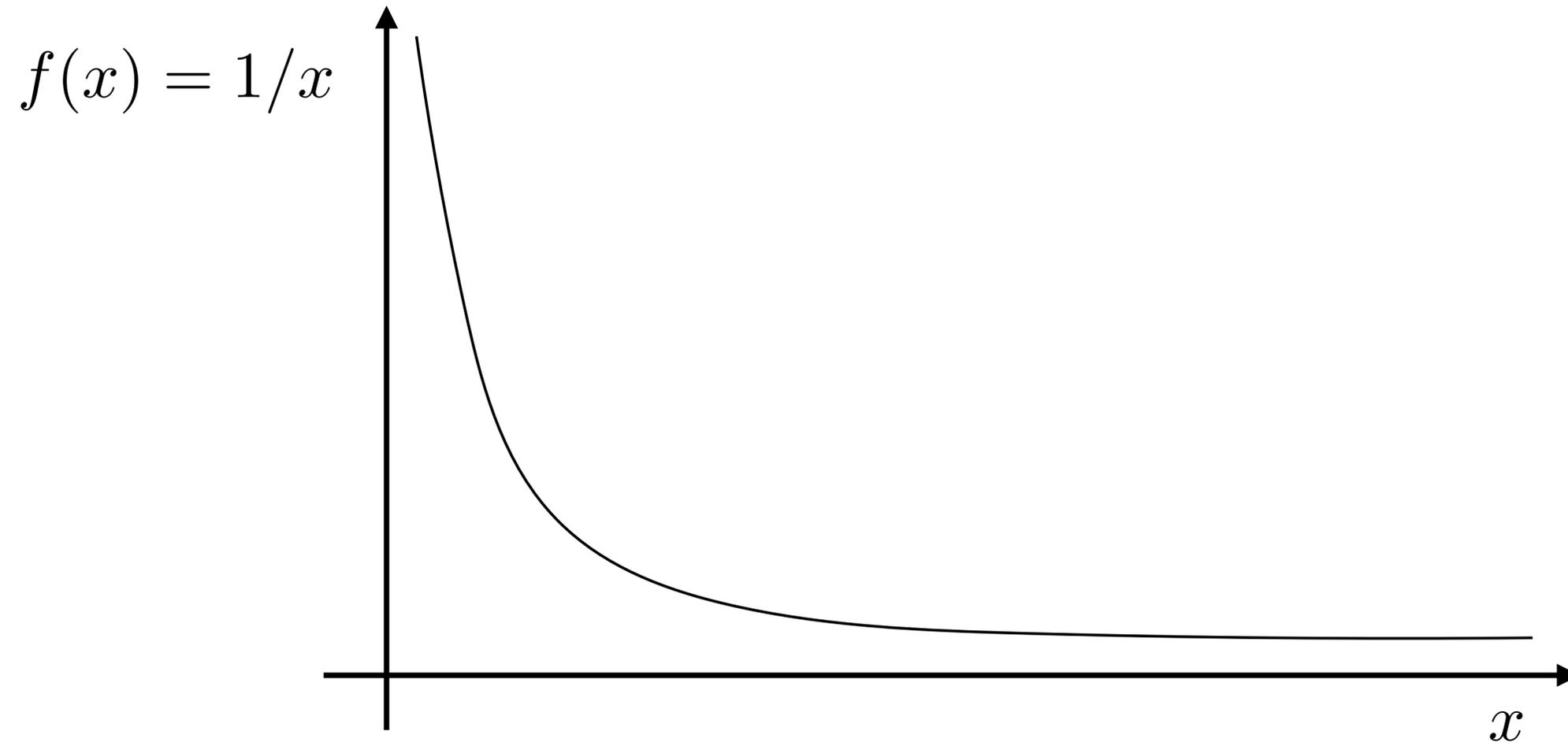
$$\leq \max_{0 \leq \tau \leq 1} \|I - t\nabla^2 f(x_\tau)\|_2 \|x^k - x^*\|_2$$

$$\leq \frac{L - \mu}{L + \mu} \|x^k - x^*\|_2 \quad (\text{similar to quadratic})$$

Apply the inequality recursively to get the result ■

Dropping strong convexity

Many functions are not strongly convex



Without strong convexity, the optimal solution might be very far ($x^* = \infty$) but the objective value very close

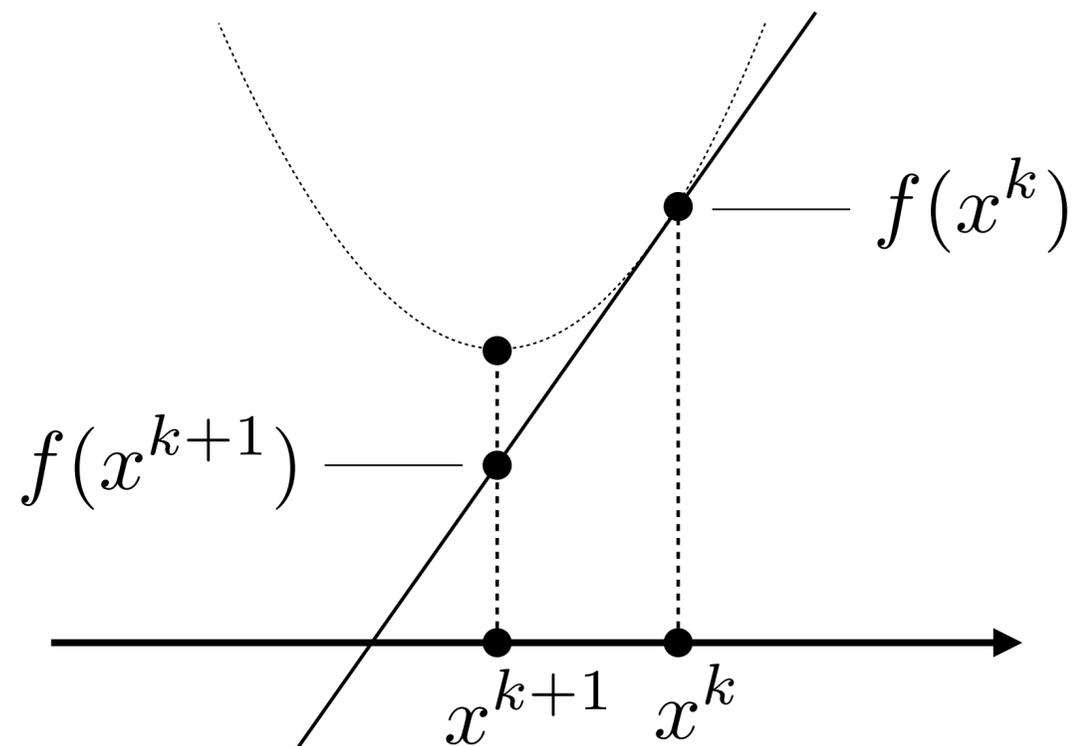
Focus on objective error $f(x^k) - f(x^*)$ instead of variable error $\|x^k - x^*\|_2$

Null growth directions without strong convexity

Hessian $\nabla^2 f(x)$ has some null growth directions (it can even be 0)

Gradient descent interpretation: replace $\nabla^2 f(x^k)$ with $\frac{1}{t_k} I$

$$x^{k+1} = \operatorname{argmin}_y f(x^k) + \nabla f(x^k)^T (y - x^k) + \frac{1}{2t_k} \|y - x^k\|_2^2$$



How to pick a quadratic approximation?

Use L -Lipschitz smoothness

Convergence for smooth functions

Theorem

Let f be L -smooth. If $t < 1/L$ then gradient descent satisfies

$$f(x^k) - f(x^*) \leq \frac{\|x^0 - x^*\|_2^2}{2tk}$$

Sublinear convergence rate $O(1/\epsilon)$ iterations (can be very slow!)

Convergence for smooth functions

Proof

Use L -Lipschitz constant

$$f(x^{k+1}) \leq f(x^k) + \nabla f(x^k)^T (x^{k+1} - x^k) + \frac{L}{2} \|x^k - x^{k+1}\|_2^2$$

Plug in iterate $x^{k+1} = x^k - t\nabla f(x^k)$ in right-hand side

$$f(x^{k+1}) \leq f(x^k) - \left(1 - \frac{Lt}{2}\right) t \|\nabla f(x^k)\|_2^2$$

Take $0 < t \leq 1/L$ we get $2 - Lt \geq 1$ and

$$f(x^{k+1}) \leq f(x^k) - \frac{t}{2} \|\nabla f(x^k)\|_2^2 \quad \text{(non increasing cost)}$$

Note: non-increasing for any $t > 0$ such that $\left(1 - \frac{Lt}{2}\right) t > 0 \Rightarrow t \in (0, 2/L)$

Convergence for smooth functions

Proof (continued)

Convexity of f implies $f(x^k) \leq f(x^*) + \nabla f(x^k)^T (x^k - x^*)$

Therefore, we rewrite $f(x^{k+1}) \leq f(x^k) - \frac{t}{2} \|\nabla f(x^k)\|_2^2$ as

$$\begin{aligned} f(x^{k+1}) - f(x^*) &\leq \nabla f(x^k)^T (x^k - x^*) - \frac{t}{2} \|\nabla f(x^k)\|_2^2 \\ &= \frac{1}{2t} (\|x^k - x^*\|_2^2 - \|x^k - x^* - t\nabla f(x^k)\|_2^2) \\ &= \frac{1}{2t} (\|x^k - x^*\|_2^2 - \|x^{k+1} - x^*\|_2^2) \end{aligned}$$

Convergence for smooth functions

Proof (continued)

Summing over the iterations with $i = 1, \dots, k$

$$\begin{aligned}\sum_{i=1}^k (f(x^i) - f(x^*)) &\leq \frac{1}{2t} \sum_{i=1}^k (\|x^{i-1} - x^*\|_2^2 - \|x^i - x^*\|_2^2) \\ &= \frac{1}{2t} (\|x^0 - x^*\|_2^2 - \|x^k - x^*\|_2^2) \\ &\leq \frac{1}{2t} \|x^0 - x^*\|_2^2\end{aligned}$$

Since $f(x^k)$ is non-increasing, we have

$$f(x^k) - f(x^*) \leq \frac{1}{k} \sum_{i=1}^k (f(x^i) - f(x^*)) \leq \frac{1}{2kt} \|x^0 - x^*\|_2^2 \quad \blacksquare$$

Issues with computing the optimal step size

Quadratic programs

The rule $t = 2/(\lambda_{\max}(P) + \lambda_{\min}(P))$ can be **very expensive to compute**

It relies on eigendecomposition of P (iterative factorizations...)

Smooth and strongly convex functions

Very hard to estimate μ and L in general

Can we select a good step-size as we go?

Gradient descent

Today, we learned to:

- **Classify** optimization algorithms (zero, first, second-order)
- **Derive and recognize** convergence rates
- **Analyze** gradient descent complexity under smoothness and strong convexity (linear convergence, fast!)
- **Analyze** gradient descent complexity under only smoothness (sublinear convergence, slow!)

Next lecture

- Line search
- Subgradient methods