Gradient Methods III: Convergence Speed

Ruoyu Sun

Questions for Last Time

- Q1: You use GD with constant stepsize to solve an unconstrained differentiable optimization problem, but it doesn't converge.
 - 1) What are the possible reasons?
 - (i)
 - (ii)
 - 2) How to make it work?
- ▶ **Q2** You use GD with diminishing stepsize to solve a problem. Recall the conditions $\sum_r \alpha_r = \infty$ and $\alpha_r \to 0$.

This time, you set a lower bound 0.01; e.g., $\alpha_r = 1/r + 0.01$.

Will this algorithm converge?

▶ **Q3** Use GD to solve $\min_x x^6$. How to ensure your algorithm will convergence to stationary points?



Questions for Last Time

- Q1: You use GD with constant stepsize to solve an unconstrained differentiable optimization problem, but it doesn't converge.
 - 1) What are the possible reasons?

Answer: (i) This is a maximization problem.

- (ii) The objective is not L-smooth for any L.
- (iii) The stepsize is set to too large.
- 2) How to make it work?

Answer: For (i), switch to gradient ascent. For (ii), try line search rules. For (iii), tune down stepsize.

▶ **Q2** You use GD with diminishing stepsize to minimize $f(\mathbf{x})$. Recall the conditions $\sum_{r} \alpha_r = \infty$ and $\alpha_r \to 0$.

This time, you set a lower bound 0.01 and use $\alpha_r = 1/r + 0.01$.

Will this algorithm converge?

Answer: Depending on the Lipschitz-smoothness. If f is L-smooth with L < 2/0.01 = 200, then the algorithm converges to stationary points.

▶ **Q3** Use GD to solve $\min_x x^6$. How to ensure your algorithm will convergence to stationary points?

Answer: Use line search, such as Armijor rule.



Today

- Convergence Rate Analysis of GD
- After today's course, you will be able to
 - Describe the convergence rate of GD for strongly convex, convex and nonconvex problems
 - Analyze the convergence rate for quadratic problems
 Optional: Analyze the convergence rate of strongly convex problems
 - Explain why preprocessing data is useful
- ▶ **Advanced**: Analyzing a problem starting from simple cases.

Outline

Applying Gradient Descent to Regression

Convergence Rate Analysis for Quadratic Functions

Results for Strongly Convex, Convex, Nonconvex Functions



What is Convergence Rate Analysis

Goal: find an " ϵ -approximate solution":

- ► For convex functions: ϵ -optimal solution in $\{\mathbf{x}_{\epsilon} \mid f(\mathbf{x}_{\epsilon}) f^* \leq \epsilon\}$
- ► For nonconvex functions: consider ϵ -stationary solution in $\{\mathbf{x}_{\epsilon} \mid \|\nabla f(\mathbf{x}_{\epsilon})\| \leq \epsilon\}$

Convergence Rate:

- 1. Measures the number of iterations required to get an ϵ -approximate solution'
- Important measure for evaluating algorithms in big data applications
- Question: What determines the convergence rate?

Convergence v.s. Convergence Speed Analysis

Convergence (convergence to stat-pt or global-min)

- 1. Sanity check
- 2. Minimal requirement of any reasonable algorithm

Convergence speed.

- Asymptotic convergence rate: local analysis, assuming already close to a solution
 - 1. characterize algorithm behavior when # of iterations go to infinity
 - 2. Linear rate/Superlinear rate/Sublinear rate
- Non-asymptotic convergence rate (Iteration complexity)
 - 1. Describes global behavior of the algorithm
 - 2. Focus of today

Illustration



Figure: What Determines Convergence Rate?

- ► How steep the mountain is (environment; formulation)
- ► Route you pick; your speed (your choice; algorithm)

Toy Example in Regression: Data

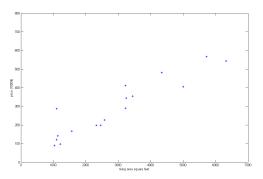
Let's take a look at a simple example in predicting the house price giving the living areas

Living Area ($feet^2$)	Price (1000\$)
5719	567
3241	345
1139	141
1572	167
1101	287
2576	227
:	i i

Let's build a linear regression model and use GD to solve the problem

Toy Example in Regression: Optimization Problem

- ▶ Data points $x_1, ..., x_n$ (total of n = 17 data points)
- Construct the regression model: variables w_1 (slope), w_0 (intercept); P=2
- ▶ Data matrix $X \in \mathbb{R}^{2 \times 17}$ $(P \times n)$; first row the area data, second row all 1
- ▶ True output $y \in \mathbb{R}^{17 \times 1}$ ($n \times 1$): housing price.
- Solve the following problem $\min \frac{1}{2} ||X^T w y||^2$



Toy Example in Regression: First Try

- ▶ First Try: Scale the data so that all the areas are multiplied by 0.01, and all the prices are multiplied by 0.1 scaling the data
- ▶ Run GD for 1000 iterations; initial w = (10, 50)

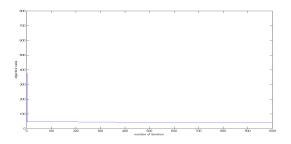


Figure: The decrease of objective function

Error seems quite large.

First try: fitting

- Final fitting: far from optimum.
- So the issue is "not converged yet"

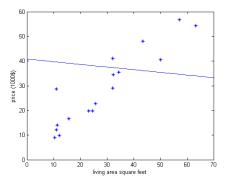


Figure: The final fitting.

Eigenvalues of XX^T ($P \times P$, i.e., 2×2) are 0.0004 and 1.856. Hessian is ill-conditioned!

Toy Example in Regression: Second Try

- ➤ **Second Try**: Scale the data so that all the areas are multiplied by 0.0001, and all the prices are multiplied by 0.1 scaling the data
- ► Run GD for 1000 iterations; initial (10, 50)

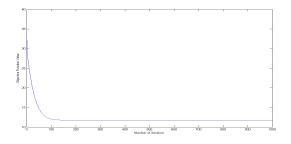


Figure: The decrease of objective function

Why does it work now?

Eigenvalues of XX^T are 0.4 and 18.45. Hessian is well-conditioned!

Second try: fitting

Final fitting:

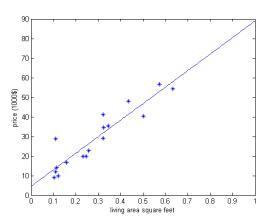


Figure: The final fitting.

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Data Preprocessing: Normalization

- ill-conditioning: the condition number is very large
- Can arise when the variables are scaled incoherently Example:
 - 1. feature 1: area, unit m^2 , nominal value 120
 - 2. featuer 2: age, unit "day", nominal value 6000
 - 3. feature 3: # of bedrooms, nominal value 3
- "Data preprocessing": preprocess the data so that the data matrix has a better property (e.g. better condition number)
 - Suppose $X = [x[1], x[2], \dots, x[n]] \in \mathbb{R}^{d \times n}$
 - Each column represents a sample
 - Each row represents a feature
 - Normalization: Scale each row so that each row has unit norm
- Claim:(informal) Normalizing data can reduce condition number (in most cases), which makes GD faster.



Data Preprocessing: Centering

Example: Predict which university to get in:

- feature 1: score, $X_1^T = [630, 650, 640, 660]$
- ► After normalization: (0.488, 0.503, 0.496, 0.511); quite close

Centering: substract each entry by the mean of all data

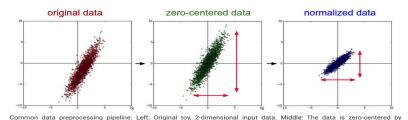
$$\mathsf{E.g.}\ X_1^T = [630, 650, 640, 660]$$

- ▶ After centering: -15, -5, 5, 15.
- ► Further after normalization: -0.67, -0.22, 0.22, 0.67

Claim (informal): Centering can also reduce condition number (in most cases), which makes GD faster.

Exercise: compare matrix with entries in Unif[0,1] and matrix with entries in Unif[-0.5,0.5]

Data preprocessing: Figure Illustration



subtracting the mean in each dimension. The data cloud is now centered around the origin. Right: Each dimension is additionally scaled by its standard deviation. The red lines indicate the extent of the data - they are of unequal length in the middle, but of equal length on the right.

Figure: Data preprocessing pipeline. Source: Stanford CS231n course notes.

Story

- Story: When I learned Torch, 1st "trick": scale data properly.
 It looks magical first; one day, I realize it should be explainable by optimization theory
 - Step 1: Scaling data is reducing condition number
 - Step 2: Condition number is critical for convergence speed
- Quora: When does logistic regression not converge?

Top Answer: Common reasons:

- 1. Code/Optimization method has bug.
- 2. Learning rate too large
- 3. Feature not normalized (values of different features have totally different scale, just ran into today).



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Analysis of 2-dim Example

- ▶ Start from simple case $\min_{x_1,x_2} \frac{1}{2}(Lx_1^2 + x_2^2)$.
- ► GD: $x^+ = x \alpha \begin{pmatrix} Lx_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} (1 \alpha L)x_1 \\ (1 \alpha)x_2 \end{pmatrix}$
- ▶ Pick stepsize $\alpha = 1/L$, then

$$x_1^+ = 0$$

 $x_2^+ = (1 - \frac{1}{L})x_2$

▶ Convergence speed depends on $|1 - \frac{1}{L}|$



Analysis of Quadratic Problems: Diagonal Case

- Next, consider $\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \mathbf{x}^T Q \mathbf{x}$. For simplicity, assume Q is symmetric positive-definite.

Diagonal case: $Q = diag(\lambda_1, \dots, \lambda_n)$, $\lambda_1 \ge \dots \ge \lambda_n$.

$$\mathbf{x}^{+} = \begin{pmatrix} I - \alpha \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} = \begin{pmatrix} (1 - \alpha \lambda_1) x_1 \\ (1 - \alpha \lambda_2) x_2 \\ \dots \\ (1 - \alpha \lambda_n) x_n \end{pmatrix}$$

We get independent sequences $x_i^+ = (1 - \alpha \lambda_i) x_i, i = 1, \dots, n$. Convergence speed of $\{x_i^r\}_{r=0}^{\infty}$ depends on $|1 - \alpha \lambda_i|$.

Claim:
$$\frac{\|x^r\|}{\|x^0\|} \leq \max_{i \in [n]} |1 - \alpha \lambda_i|^r$$
.

General Convex Quadratic Problem

- ▶ What about general quadratic problem $\min_{\mathbf{x}} \mathbf{x}^T Q \mathbf{x} + 2 \mathbf{b}^T \mathbf{x}$?

Suppose x^* is one optimal solution, then it satisfies $\mathbf{x}^* = \mathbf{x}^* - \alpha(Q\mathbf{x} + \mathbf{b})$.

Then
$$\mathbf{x}^+ - \mathbf{x}^* = (\mathbf{x} - \mathbf{x}^*) - \alpha Q(\mathbf{x} - \mathbf{x}^*) = (I - \alpha Q)(\mathbf{x} - \mathbf{x}^*).$$

Eigenvalues of $I - \alpha Q$ are $1 - \alpha \lambda_i, i = 1, 2, \dots, n$.

Thus $\|\mathbf{x}^+ - \mathbf{x}^*\| \le \max_i |1 - \alpha \lambda_i| \|\mathbf{x} - \mathbf{x}^*\|$.

Claim:
$$\frac{\|\mathbf{x}^r - \mathbf{x}^*\|}{\|\mathbf{x}^0 - \mathbf{x}^*\|} \le \max_{i \in [n]} |1 - \alpha \lambda_i|^r$$
.

Corollary: If stepsize $\alpha = 1/\lambda_1$, then $\frac{\|\mathbf{x}^r - \mathbf{x}^*\|}{\|\mathbf{x}^0 - \mathbf{x}^*\|} \le (1 - \frac{\lambda_n}{\lambda_1})^r$.

Analysis chain: diagonal → pure quadratic → quadratic plus linear term.

Result for Quadratic Case

Thm 1a (strongly convex quadratic): Suppose Q is symmetric PD (positive-definite). Consider solving

$$\min_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w}) \triangleq 0.5 \mathbf{w}^T Q \mathbf{w} + \mathbf{b}^T \mathbf{w} + \mathbf{c}.$$

Suppose GD with stepsize 1/L, where $L=\lambda_{\max}(Q)$, generates a sequence $\{\mathbf{w}_r\}$. Then

$$\|w_{r+1} - w^*\|^2 \le \left(1 - \frac{1}{\kappa}\right) \|w_r - w^*\|^2,$$
 (1)

where the condition number $\kappa = \lambda_{\max}(Q)/\lambda_{\min}(Q)$.

Normalization and Preconditioning

- ▶ What is the effect of normalization? Assume $X^T = [X_1, \dots, X_d]$
- Linear regression $||X_1w_1 + \cdots + X_dw_d \mathbf{b}||^2$. Convergence speed depends on $\kappa(XX^T)$.
- Scale each row X_i^T by $\gamma_i=1/\|X_i\|, i=1,\ldots,d.$ Equivalent to: Change matrix X to $\hat{X}=\Gamma X$ For this $\hat{X}\hat{X}^T=\Gamma XX^T\Gamma^T$, all of its diagonal entries are 1
- ► Convergence speed now depends on $\kappa(\hat{X}\hat{X}^T)$
 - e.g. X = [100, 0; 0, 1], what is \hat{X} ?
- ► Called Jacobi preconditioning in numerical linear algebra.
 - ▶ Does it improve condition number always? Open question; mentioned in R. Sun, Y. Ye, Worst case complexity of Cyclic Coordinate Descent: O(n²) Gap with Randomized Version. MP 2019.



Why Data Preprocessing is Useful?

Claim: (informal) Normalizing data can reduce condition number (in most cases), which makes GD faster, which makes GD faster.

- Part I: In linear regression, normalizing data is called Jacobi preconditioning, which likely improves condition number (but no proof yet)
- ▶ Part II: In linear regression, smaller condition number implies faster convergence (Thm 1)

Claim:(informal) Centering can reduce condition number (in most cases), which makes GD faster, which makes GD faster.

Part I: centering reduces condition number. No aware of a proof; but likely true for most cases

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Result for Strongly Convex Functions

For a twice-differentiable function f, we say it is L-smooth and μ -strongly-convex iff

$$LI \succeq \nabla^2 f(\mathbf{w}) \succeq \mu I, \quad \forall \mathbf{w}.$$
 (2)

Theorem 1b (strongly convex): Suppose a twice-differentiable function f is L-smooth and μ -strongly convex, and \mathbf{w}^* is a global minimum. Then GD with stepsize 1/L generates a sequence $\{\mathbf{w}_r\}$ that satisfies

$$\|\mathbf{w}_{r+1} - \mathbf{w}^*\|^2 \le \left(1 - \frac{1}{\kappa}\right) \|\mathbf{w}_r - \mathbf{w}^*\|^2,$$
 (3)

where $\kappa = L/\mu$.

- ► Remark 1: The assumption can be weakend to continuously differentiable function with *L*-Lipschitz gradient and is *μ*-strongly convex.
- ▶ **Remark 2**: Best stepsize is $2/(L + \mu)$, with rate $1 2/(\kappa + 1)$.



Proof of Theorem 1b

By the fundamental theorem of calculus, we have

$$\nabla f(\mathbf{w}_r) = \nabla f(\mathbf{w}_r) - \underbrace{\nabla f(\mathbf{w}^*)}_{0} = \int_{t=0}^{1} \nabla^2 f(\mathbf{v}(t))(\mathbf{w}_r - \mathbf{w}^*) dt$$

where $\mathbf{v}(t) = \mathbf{w}_r + t(\mathbf{w}^* - \mathbf{w}_r)$.

Then we have

$$\begin{aligned} \|\mathbf{w}_{r+1} - \mathbf{w}^*\| &= \|\mathbf{w}_r - \mathbf{w}^* - \alpha \nabla f(\mathbf{w}_r)\| \\ &= \|\mathbf{w}_r - \mathbf{w}^* - \int_{t=0}^1 \nabla^2 f(\mathbf{v}(t))(\mathbf{w}_r - \mathbf{w}^*) dt \| \\ &= \|\int_{t=0}^1 [I - \alpha \nabla^2 f(\mathbf{v}(t))](\mathbf{w}_r - \mathbf{w}^*) dt \| \\ &\leq (1 - \frac{\mu}{L}) \|\mathbf{w}_r - \mathbf{w}^*\|. \end{aligned}$$

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Alternative Proof for Strongly Convex Case (reading)

Proof: Theorem 2.1.11 in [Nesterov,2013] states that

$$\langle w - w^*, \nabla f(w) \rangle \ge \frac{\mu L}{\mu + L} \|w - w^*\|^2 + \frac{1}{\mu + L} \|\nabla f(w)\|^2.$$
 (4)

Then we have

$$||w_{r+1} - w^*||^2 = ||w_r - \eta \nabla F(w_r) - w^*||^2$$

$$= ||w_r - w^*||^2 + \eta^2 ||\nabla F(w_r)||^2 - 2\eta \langle w_r - w^*, \nabla F(w_r) \rangle$$

$$\leq \left(1 - 2\eta \frac{\mu L}{\mu + L}\right) ||w_r - w^*||^2 + \eta \left(\eta - \frac{2}{\mu + L}\right) ||\nabla F(w_r)||^2$$

$$\leq \left(1 - 2\eta \frac{\mu L}{\mu + L}\right) ||w_r - w^*||^2.$$

Plugging in $\eta = 1/L$, we obtain the desired result. \square

[Nesterov'2013]: Introductory Lectures on Convex Optimization.

Remark: This proof looks simple, but requires a non-trivial lemma (4). It can be relaxed a bit: $\langle w-w^*, \nabla f(w) \rangle \geq \frac{\mu}{2} \|w-w^*\|^2 + \frac{1}{2L} \|\nabla f(w)\|^2$. Then using $\eta=1/L$, can obtain rate $1-\frac{1}{\kappa}$, which is only slightly worse than Thm 1.

Result for Convex Functions

Theorem 2: Suppose f is a convex function with Lipschitz gradient, i.e.,

$$0 \leq \nabla^2 f(\mathbf{x}) \leq LI, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

Consider $\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$. Suppose GD with stepsize 1/L generates a sequence \mathbf{x}^r , then for any optimal solution \mathbf{x}^* , we have

$$e_T \triangleq f(\mathbf{x}^T) - f(\mathbf{x}^*) \le \frac{2L}{T} ||\mathbf{x}^0 - \mathbf{x}^*||^2.$$

Remark 1: This is called "sublinear rate" O(1/T).

Error of linear rate: 1, 0.1, 0.01, 0.001, ...

Error of sublinear rate O(1/T): $1, 1/2, 1/3, \dots, 1/10, \dots, 1/100, \dots$

▶ Remark 2: For most convex problems in practice, they achieve linear rate [Luo,Tseng'92], due to a deeper reason not covered here



Non-convex Functions

Theorem 3: Suppose $F(\mathbf{w})$ is differentiable and L-smooth. Consider GD with stepsize 1/L. Then

$$\min_{0 \le r \le T} \{ \|\nabla F(\mathbf{w}^r)\| \} \le \sqrt{\frac{2L(F(\mathbf{w}^0) - F^*)}{T}}.$$

Corollary 2 Under the same conditions as Theorem 2, when $T \geq \frac{2L(F(\mathbf{w}^0) - F^*)}{\epsilon^2}$, we have $\min_{0 \leq r \leq T} \{\|\nabla F(\mathbf{w}^r)\|\} \leq \epsilon$.

This is sub-linear convergence with rate $O(1/\sqrt{T})$.

Proof for Nonconvex Case I (reading)

Descent lemma: If F(w) is L-smooth, then

$$F(v) \le F(w) + \langle \nabla F(w), v - w \rangle + \frac{L}{2} \|w - v\|^2, \quad \forall w, v.$$
 (5)

Proof of Thm. 2: Step 1 (sufficient descent): GD method makes significant progress in each iteration.

$$F(w_{r+1}) - F(w_r) \le \langle \nabla F(w_r), w_{r+1} - w_r \rangle + \frac{L}{2} \|w_{r+1} - w_r\|^2$$
 (6a)

$$= -\frac{1}{L} \|\nabla F(w_r)\|^2 + \frac{L}{2} \|w_{r+1} - w_r\|^2$$
 (6b)

$$\leq -\frac{1}{2L} \|\nabla F(w_r)\|^2 \tag{6c}$$

where (6a) is by the L-smoothness of F (by the descent lemma); (6b) and (6c) are due to the identity $w_{r+1}-w_r=-\frac{1}{L}\nabla f(w_r)$.



Proof for Nonconvex Case II (reading)

Step 2: Telescope sum. Take the sum for r = 0, 1, 2, ..., T, we have

$$F(w_{T+1}) - F(w_0) \le -\frac{1}{2L} \sum_{r=0}^{T} \|\nabla F(w_r)\|^2.$$

$$\Longrightarrow \frac{T}{2L} \min_{0 \le r \le T} \{\|\nabla F(w_r)\|^2\} \le \frac{1}{2L} \sum_{r=0}^{T} \|\nabla F(w_r)\|^2 \le F(w_0) - F(w_{T+1}) \le F(w_0) - F^*$$

$$\Longrightarrow \min_{0 \le r \le T} \{\|\nabla F(w_r)\|^2\} \le \frac{2L(F(w_0) - F^*)}{T}.$$
(7)

Transform Rate to Number of Iterations

Iteration complexity of strongly convex functions:

- ► How many iterations needed for $e(\mathbf{x}^r) = \|\mathbf{x}^r \mathbf{x}^*\|$ to reach below ϵ ?
- We know $e(\mathbf{x}^r)/e(\mathbf{x}^0) \leq \beta^r$, where $\beta = 1 1/\kappa$. To make sure $e(\mathbf{x}^r)/e(\mathbf{x}^0) \leq \epsilon$, we only need , $\beta^r \leq \epsilon \Leftarrow r \ln \beta \leq \ln \epsilon$

$$\Leftrightarrow r\ln\frac{1}{\beta} \geq \ln\frac{1}{\epsilon} \Leftrightarrow r \geq \frac{1}{\ln\frac{1}{\beta}}\ln\frac{1}{\epsilon} = \frac{1}{\ln\frac{1}{1-1/\kappa}}\ln\frac{1}{\epsilon}$$

For large κ , # of iterations

$$r \succsim \kappa \ln \frac{1}{\epsilon}$$

Iteration complexity of convex functions: $r \geq \frac{2LD_0^2}{\epsilon}$ iterations are enough to make sure $f(\mathbf{x}^r) - f^* \leq \epsilon$

Iteration complexity of nonconvex functions: $r \geq \frac{2L(F(\mathbf{x}^0) - F^*)}{\epsilon^2}$, we have $\min_{0 \leq t \leq r} \{ \|\nabla F(\mathbf{x}^t)\| \} \leq \epsilon$.



Discussion

- Practical lessons: what do we learn from these results?
- If the algorithm fails to converge or converge very slowly, what could be the reasons?
 - ► Bad stepsize choice; bad condition number
- ► How to improve algorithm performance?
 - ► Tune algorithm, e.g., stepsize (can use the help of Hessian info)
 - Modify formulation to get better condition number (data processing; preconditioning methods; etc.)
- How to analyze an algorithm?
 - use simple functions to gain understanding
 - Insights today all come from 2D quadratic functions!
- The main lesson comes from κ -ite-complexity result of strongly convex case; we do not mention insight from convex and nonconvex problems
 - ▶ General insight: even for nonconvex problems, local $\kappa(\nabla^2 f(\mathbf{x}^r))$ could be an informative metric for understanding convergence speed (though no rigorous proof)



Summary

Convergence rate of GD with constant stepsize for three cases:

- **Strongly convex**: $O(\kappa \log \frac{1}{\epsilon})$ iterations to achieve ϵ -optimal solution
- **Convex**: $O(\frac{L}{\epsilon})$ iterations to achieve ϵ -optimal solution
- **Nonconvex**: $O(\frac{L}{\sqrt{\epsilon}})$ iterations to achieve ϵ -stationary solution

Stepsize choice:

- **Strongly convex**: optimal stepsize $2/(L + \mu)$
- Convex and nonconvex: common stepsize 1/L

A common issue for slow convergence of GD: ill-conditioning

Data preprocessing: in data analysis, always normalize and/or center data!

Improve condition number!