CS498: Algorithmic Engineering

Lecture 10: Convexity, Gradient Descent, & PyTorch.

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Week 05 – 02/19/2026

Outline

Where We Are

Part I (Weeks 1–5): Linear and Integer Programming.

- LPs, duality, simplex, branch-and-bound, modeling.
- Everything was *constrained* optimization over a **polytope**.

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Part II (Weeks 6–8/9): Continuous Optimization.

- Convex optimization, Gradient methods, Non-convex optimization, neural networks, constrained nonlinear optimization.
- We need new tools.

Motivating Example: Which problem is “easy”?

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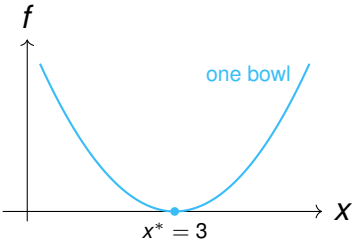

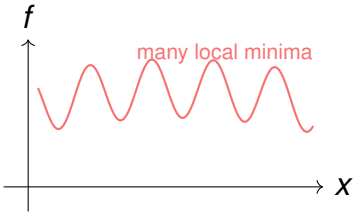

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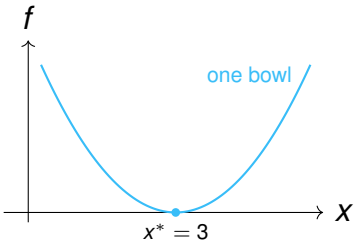

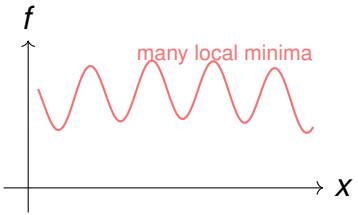

Why does Problem A feel easy? It is **convex**: any local minimum is automatically a global minimum.

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Definition

A set $C \subseteq \mathbb{R}^n$ is **convex** if for every $x, y \in C$ and $\theta \in [0, 1]$:

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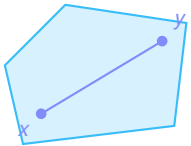
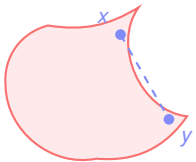


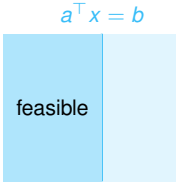
Convex



Non-convex

Examples of Convex Sets

Halfspace: $\{x : a^\top x \leq b\}$



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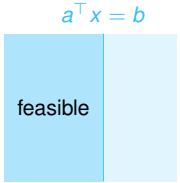

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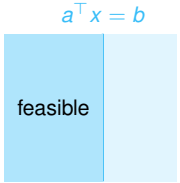
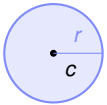


Ball: $\{x : \|x - c\|_2 \leq r\}$



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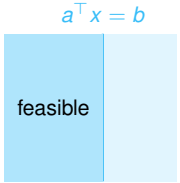

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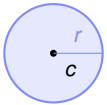

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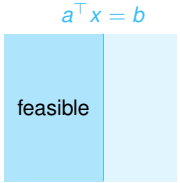

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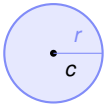

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Connection to Part I

LP feasible regions $\{x : Ax \leq b, x \geq 0\}$ are **polyhedra**, convex sets we already know!

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- Therefore $\theta x + (1 - \theta)y \in C_1 \cap C_2$.

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Why this matters

A polyhedron is the intersection of halfspaces.
Each halfspace is convex. So every LP feasible region is convex.
We have been doing convex optimization all along in Part I.

Convex Functions: Definition

Definition

$f : \mathbb{R}^n \to \mathbb{R}$ is **convex** if for all x, y and $\theta \in [0, 1]$:

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y).$$

f is **concave** if and only if $-f$ is convex.

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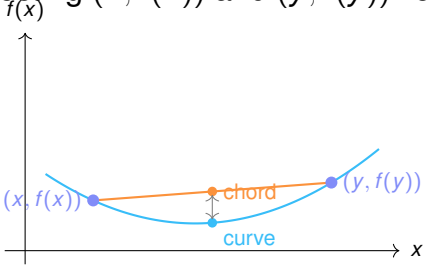
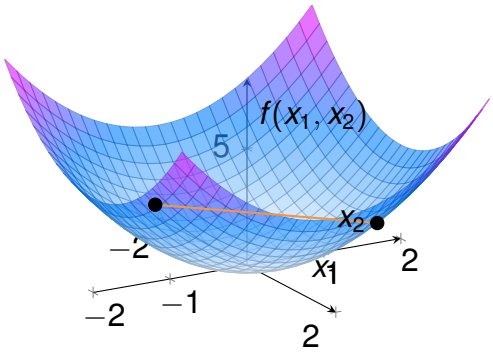


Convex Functions in $\mathbb{R}^2$



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- $f(x) = e^x$ (exponential)
- $f(x) = |x|$ (absolute value)
- $f(\mathbf{x}) = \|\mathbf{x}\|$ (norm)
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Note

Linear functions are both convex and concave.

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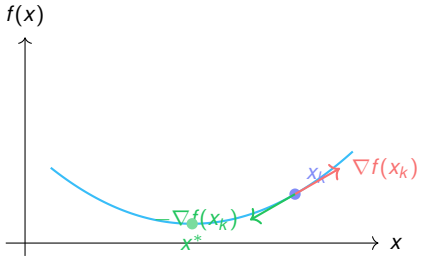

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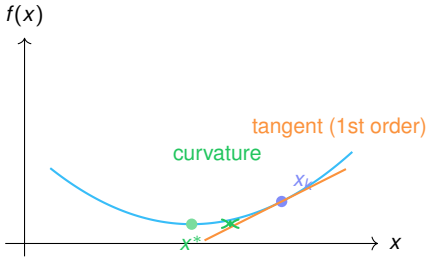

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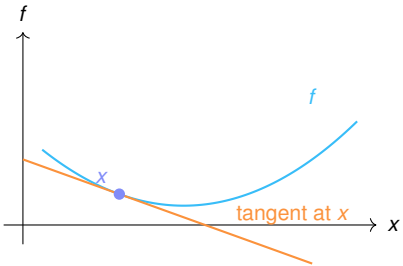

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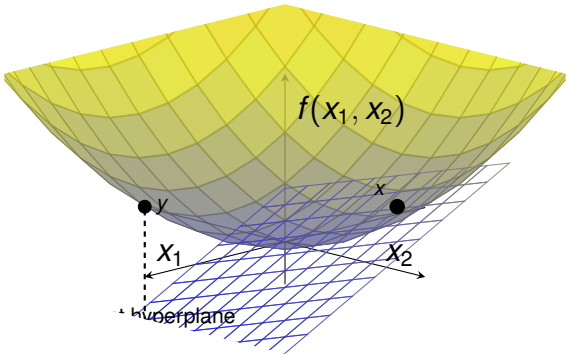

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- **Norms:** all norms $f(\mathbf{x}) = \|\mathbf{x}\|_p$ for $p \geq 1$ are convex.

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- $\|Ax - b\|^2$ convex. $\lambda\|x\|^2$ convex ($\lambda \geq 0$). Sum: **convex.**
- (This is ridge regression. We'll come back here soon.)

The Core Theorem: Local = Global

Theorem (Fundamental Property of Convex Optimization)

Let f be convex and C be a convex set. Then any **local minimum** of

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Consider the segment $x_\theta = \theta x^* + (1-\theta)y \in C$ for $\theta \in [0,1]$.
By convexity:

$$f(x_\theta) \leq \theta f(x^*) + (1-\theta) f(y) < f(x^*)$$

for θ close to 1. This contradicts x^* being a local minimum. $\square$

First-Order Optimality for Unconstrained Convex Problems

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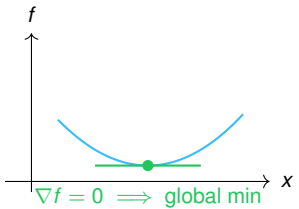

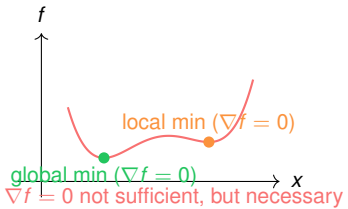

First-Order Optimality in Higher Dimensions

Convex example (2 variables):

$$f(x_1, x_2) = x_1^2 + 2x_2^2$$

$$\nabla f(x) = \begin{bmatrix} 2x_1 \\ 4x_2 \end{bmatrix} \quad \Rightarrow \quad \nabla f(x) = 0 \iff x = (0, 0)$$

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At $(0, 0)$: saddle point.
$\nabla f = 0$ is not sufficient in general.

The Convex Program Hierarchy

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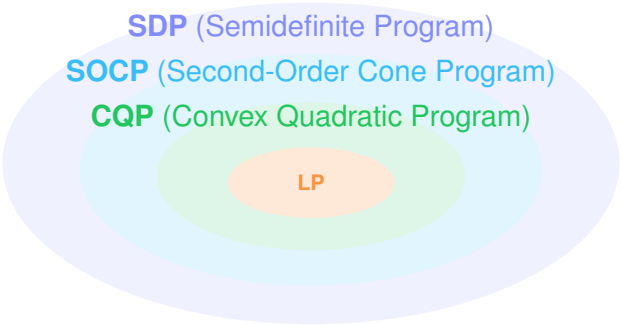

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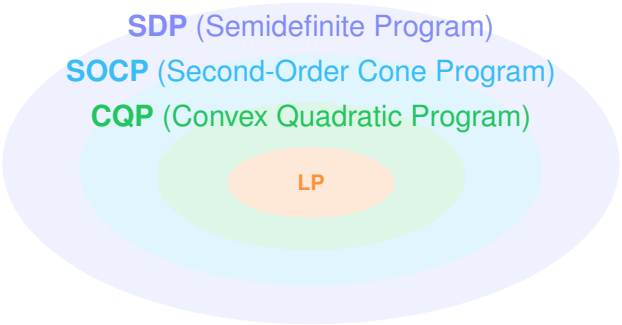

Each layer is **strictly more expressive** than the one inside.
Each layer remains **tractable**: polynomial-time solvable by Ellipsoid Method.

Setup: What Are We Solving?

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We will not assume we can solve $\nabla f(x^*) = 0$ in closed form.

Gradient Descent: The Algorithm

Gradient Descent

Start at some x_0. Repeat:

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

where $\alpha > 0$ is the **step size** (also called *learning rate*).

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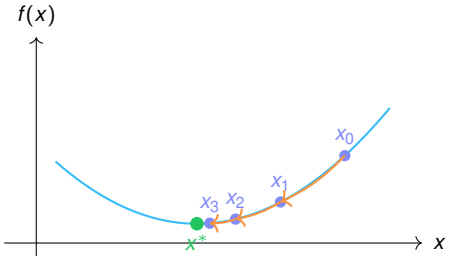
Geometric interpretation: at each step, move in the direction that decreases f most rapidly.



Step Size: The Critical Hyperparameter

The step size α completely controls behavior.

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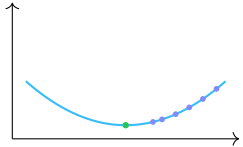

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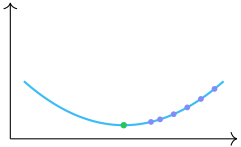

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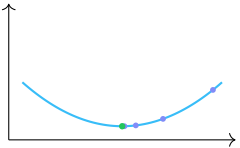

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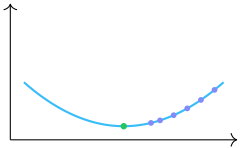

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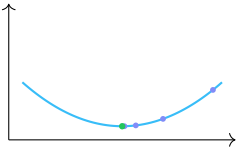

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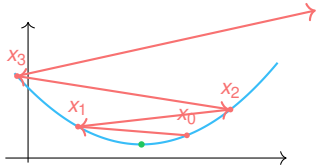

Diverges (oscillations).

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Example, $f(x) = 4x^2$, then $L = 8$ is safe.

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Key Fact

The new Lipschitz constant is $L_g = cL$. **Scaling the function scales the curvature**

One Step Size Can Fail After Scaling

Same step size in both panels: $\alpha = 0.4$

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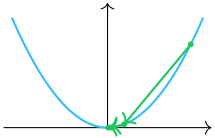

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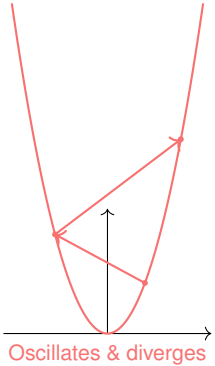

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This guarantees we move downhill without knowing the Lipschitz constant.
More advanced rules (e.g., Armijo, Wolfe) give stronger guarantees, but the core idea is just: **try a step and shrink until it decreases.**

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But actually, $x_1 = x_0 - \frac{1}{8} \cdot 8x_0 = 0$. We find $x_1 = x^* = 0$ in one iteration. The bound here is an upper bound!

Application: Linear Regression Problem

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$$(x_i, y_i), \quad i = 1, \ldots, m$$

Goal: fit a line

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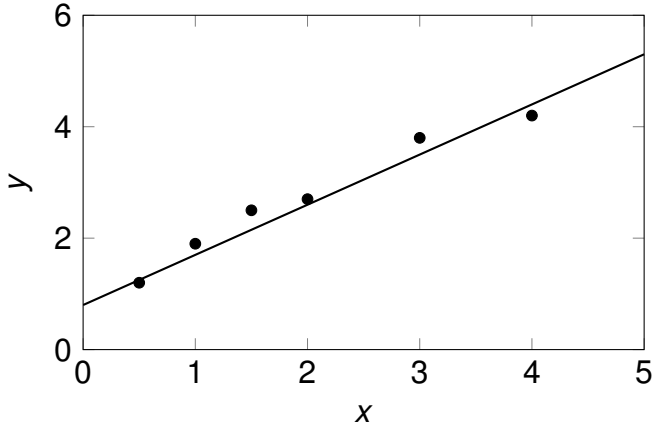
So we minimize squared residuals:

$$\min_{\beta_0, \beta_1} \sum_{i=1}^{m} \left(y_i - (\beta_0 + \beta_1 x_i)\right)^2.$$

Least Squares Fit



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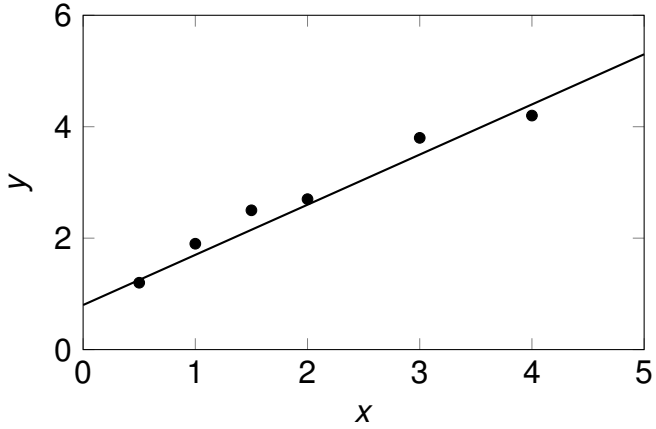

Minimize $\sum_i$(vertical errors)^2.

Matrix Form

Define

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_m \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

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This is the general least squares problem.

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$$\min_{x \in \mathbb{R}^n} \; f(x) = \|Ax - b\|^2.$$

Is f convex?

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Note: Least squares has a closed form soluton of $x^* = (A^T A)^{-1} A^T b$. However, computing it takes $O(n^3)$ which can be slow for large n.

Gradient Descent from Scratch

```python
import numpy as np

def gradient_descent(A, b, alpha=0.01, n_iters=500):
    """
    Least Squares regression via gradient descent.
    Minimizes ||Ax - b||^2
    """
    m, n = A.shape
    x = np.zeros(n)                # x_0 = 0

    for k in range(n_iters):
        grad = 2 * A.T @ (A @ x - b)  # nabla f(x)
        x = x - alpha * grad                        # x_{k+1} = x_k - alpha * grad
    return x
np.random.seed(0)
m, n = 200, 50
A = np.random.randn(m, n)
b = np.random.randn(m)
x_gd = gradient_descent(A, b, alpha=1e-3, n_iters=1000)
```

The Problem with Hand-Derived Gradients

We previously computed ∇f by hand:

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That was easy. Now consider a 3-layer neural network loss function:

$$f(W_1, W_2, W_3) = \frac{1}{m}\sum_{i=1}^{m} \ell(\sigma(W_3\,\sigma(W_2\,\sigma(W_1 x_i + b_1) + b_2) + b_3),\ y_i)\,.$$

Where $\ell(x, y) = (x - y)^2$ and $\sigma(x) = 1/(1 + e^{-x})$.

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- **Tedious.** Pages of chain rule.
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The fix: Automatic Differentiation ("autograd")

Write your loss as code. The framework computes ∇f for you, exactly.

What Is PyTorch?

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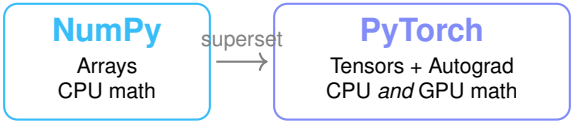

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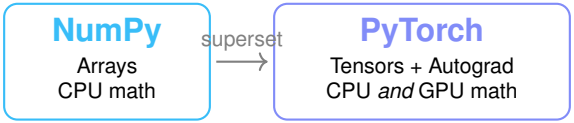

Why do we care?

Gradient descent needs $\nabla f(x)$. PyTorch computes it automatically, so we can focus on *modeling* instead of *calculus*.

PyTorch Tensors: NumPy → PyTorch

```
#!pip install torch
import numpy as np
import torch

# NumPy way
a_np = np.array([1.0, 2.0, 3.0])
b_np = np.array([4.0, 5.0, 6.0])
c_np = a_np @ b_np                      # dot product: 32.0

# PyTorch way (almost identical syntax!)
a_pt = torch.tensor([1.0, 2.0, 3.0])
b_pt = torch.tensor([4.0, 5.0, 6.0])
c_pt = a_pt @ b_pt                      # dot product: tensor(32.)

# Convert between them freely
a_pt = torch.from_numpy(a_np)           # numpy -> torch
a_np = a_pt.numpy()                     # torch -> numpy
```

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Key point

If you know NumPy, you already know 90% of PyTorch's tensor API.
Same operations: `@`, `+`, `*`, `.T`, `reshape`, `sum`, indexing, slicing, ...

The Magic Switch: `requires_grad=True`

The key difference from NumPy: PyTorch tensors can **track their history**.

```
# This tensor will record every operation done to it
x = torch.tensor([2.0, 3.0], requires_grad=True)

# Any computation involving x builds a hidden "computation graph"
y = x[0]**2 + x[1]**2       # y = 4 + 9 = 13
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# One call: compute ALL gradients via chain rule
y.backward()

# Result: dy/dx = [2*x[0], 2*x[1]] = [4, 6]
print(x.grad)                # tensor([4., 6.])
```

Gradient Descent: From Scratch in PyTorch

Let us solve ridge regression: $\min_x \|Ax - b\|^2 + \lambda\|x\|^2$.

```
import torch
torch.manual_seed(0)
m, n = 200, 50
A = torch.randn(m, n)
b = torch.randn(m)
lam = 1.0
x = torch.zeros(n, requires_grad=True)   # x_0 = 0
alpha = 1e-3
```

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alpha = 1e-3

for k in range(100):
    # Forward: compute loss (PyTorch records the graph)
    loss = (A @ x - b) @ (A @ x - b) + lam * (x @ x)

    # Backward: compute gradients
    loss.backward() #Now x.grad has the gradient of loss with respect to x
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    # Update: gradient descent step
    with torch.no_grad():           # don't track this arithmetic
        x -= alpha * x.grad
        x.grad.zero_()              # CRITICAL: clear gradients for next iteration
print(f"Final loss: {loss:.4f}")
```

Two Details That Trip Everyone Up

- Why do we need `with torch.no_grad()`?
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- Why do we need `with torch.no_grad()`?
- Why do we need `x.grad.zero_()`?

These two lines prevent:

1. Tracking *the update itself* (not what we want)
2. Accidentally accumulating gradients across iterations

Gradients Accumulate by Default

```python
import torch

x = torch.tensor(2.0, requires_grad=True)

f1 = x**2
f1.backward()
print(x.grad)   # ?
```

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For $f(x) = x^2$, we expect:

$$\nabla f(x) = 2x = 4$$

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For $f(x) = x^2$, we expect:

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So `x.grad = 4`.

Second Backward Without Zeroing

```
# Second backward pass (without zeroing!)
f2 = x**2
f2.backward()
print(x.grad)   # ?
```

Expected gradient at $x = 2$:

$$2x = 4$$

But PyTorch ADDS it:

$$x.grad = 4 + 4 = 8$$

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But PyTorch ADDS it:

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Key Point

.backward() adds to .grad.

That's why we must reset gradients every iteration with x.grad.zero_().

What If We Forget `with torch.no_grad():`?

```
x = torch.tensor(2.0, requires_grad=True)
f = x**2
f.backward()
#with torch.no_grad(): <-- OOPS
x = x - 0.1 * x.grad
```

Now autograd tracks the update step itself.

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- $x_1 = x_0 - \alpha \cdot 2x_0$ becomes part of the graph
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The update $x \leftarrow x - \alpha \nabla f(x)$ is **bookkeeping**, not part of the model or function.

Rule

Always use `with torch.no_grad():` for parameter updates.

The 3-Line Pattern You Always Write

```
loss.backward()              # compute gradients
with torch.no_grad():
    x -= alpha * x.grad      # update parameters
    x.grad.zero_()           # reset gradients
```

Memorize this pattern. You will write it hundreds of times.