CS498: Algorithmic Engineering

Lecture 11: PyTorch, Ridge Regression & Constrained Optimization Preview.

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Week 06 – 02/24/2026

Outline

Recap: What We Saw Last Time

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y.backward()
print(x.grad)                 # tensor([4., 6.])
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Today: how does this actually work inside? And how do we use it for real optimization?

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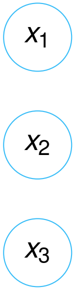

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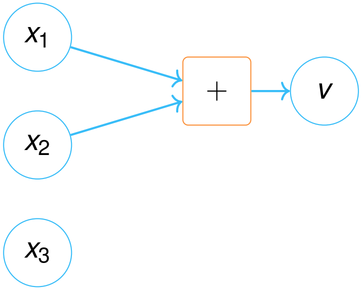

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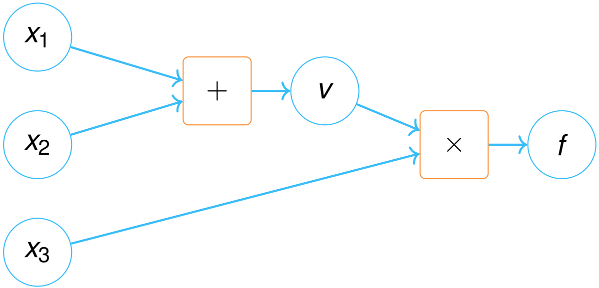

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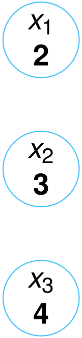
Multiply them. Pass the result upstream. That is **all of backpropagation**.

Concrete Example: Forward Pass (Values)

$f(x_1, x_2, x_3) = (x_1 + x_2) \cdot x_3$ with $x_1 = 2,\ x_2 = 3,\ x_3 = 4.$



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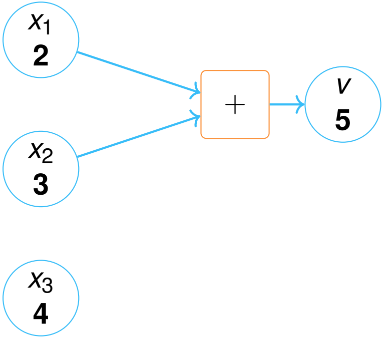

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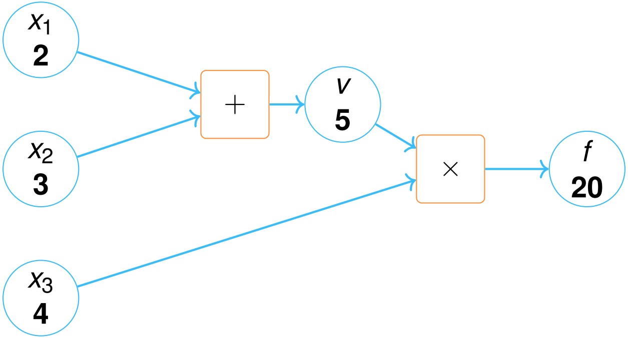

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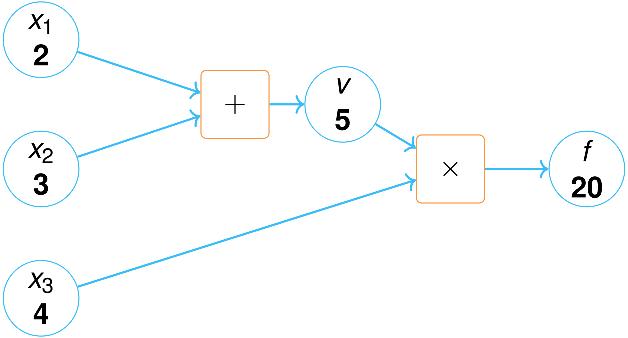

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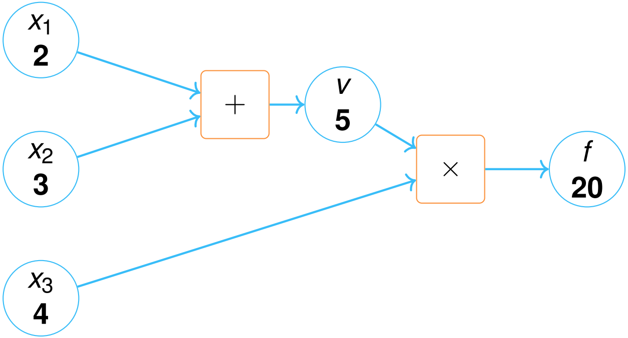

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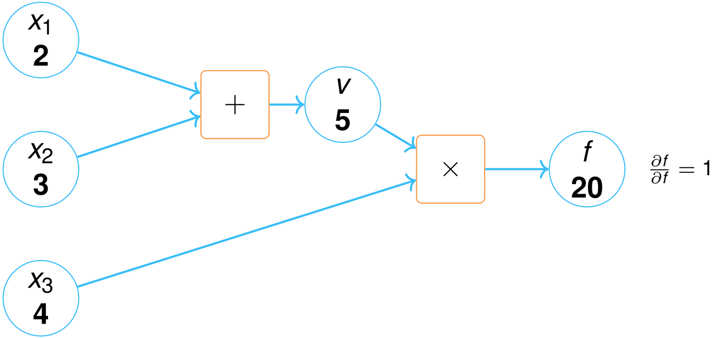

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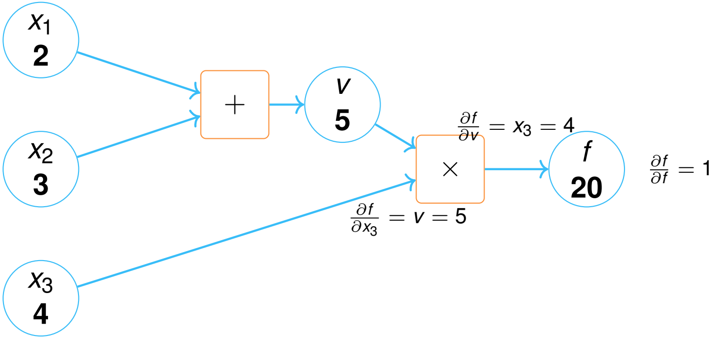

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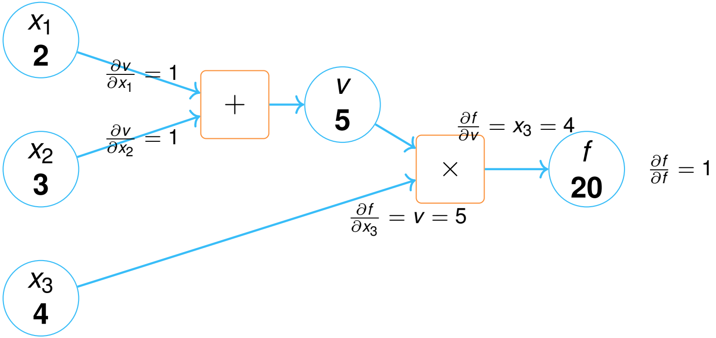

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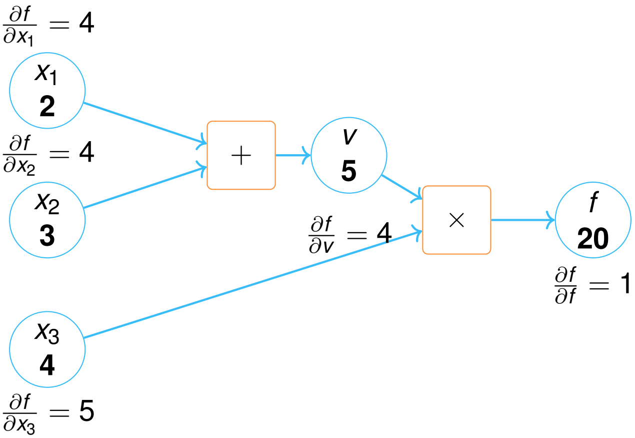

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial v} \cdot \frac{\partial v}{\partial x_1} = 4 \qquad \frac{\partial f}{\partial x_2} = \frac{\partial f}{\partial v} \cdot \frac{\partial v}{\partial x_2} = 4 \qquad \frac{\partial f}{\partial x_3} = 5$$

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To compute the gradient of any composite function, PyTorch just **chains** these local rules. That is all autograd does.

How PyTorch Builds the Graph

Every tensor remembers **how it was created**:

```
import torch

x = torch.tensor(3.0, requires_grad=True)

v = x ** 2           # v = 9.0
print(v.grad_fn)     # <PowBackward0>  -- "I was made by **2"

w = v + 1             # w = 10.0
print(w.grad_fn)     # <AddBackward0>  -- "I was made by +"

f = torch.log(w)      # f = log(10)
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What `f.backward()` does

Starting from f, it follows the chain of `.grad_fn` pointers backwards, applying each operation's local derivative rule, multiplying via the chain rule, and storing the final result in `x.grad`.

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class MyCube(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        ctx.save_for_backward(x)    # stash x for the backward pass
        return x ** 3               # forward: f(x) = x^3

    @staticmethod
    def backward(ctx, grad_output):
        x, = ctx.saved_tensors
        return grad_output * 3 * x**2    # f/x = f/MyCube · MyCube/x =
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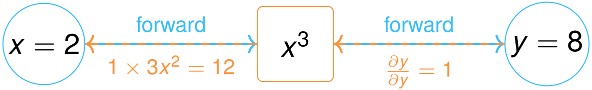
x = torch.tensor(2.0, requires_grad=True)
y = MyCube.apply(x)   # y = 8.0
y.backward()
print(x.grad)          # tensor(12.)  = 3 * 4
```

Adding a New Op: What Just Happened



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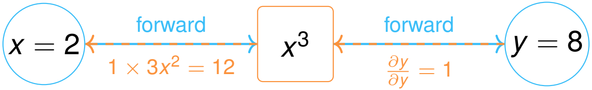

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Forward: you tell PyTorch what $f(x)$ returns.
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PyTorch handles the rest: chaining, accumulation, storage.

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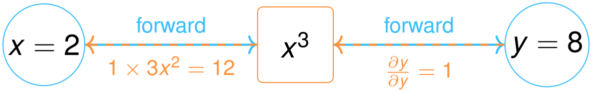

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In practice, you rarely need custom ops: PyTorch already knows hundreds of operations. But it's good to know the mechanism.

Warning: Gradients Accumulate by Default

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f1 = x**2
f1.backward()
print(x.grad)    # ?
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So `x.grad = 4`.

Warning: Second Backward Without Zeroing

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# Second backward pass (without zeroing!)
f2 = x**2
f2.backward()
print(x.grad)    # ?
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Expected gradient at $x = 2$:

$$2x = 4$$

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_().

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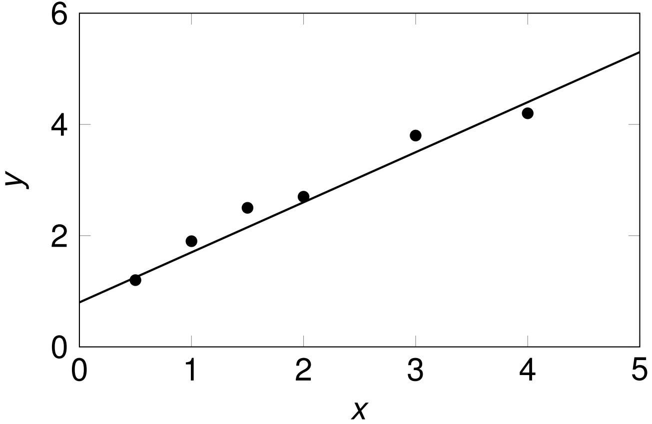
We cannot usually fit all points exactly.
So we minimize squared residuals:

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

Recall: Least Squares Fit



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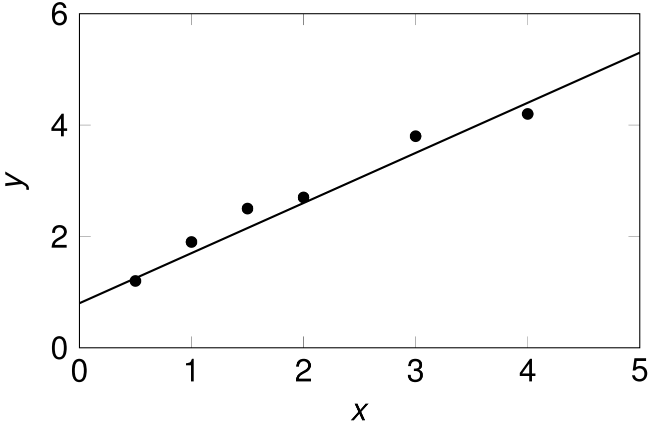

Minimize $\sum_i (\text{vertical errors})^2$.

Recall: Matrix Form and Gradient

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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Gradient (from last lecture):

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Last time

We implemented GD for this problem using NumPy, computing ∇f by hand. **Now:** let PyTorch compute the gradient automatically.

Vanilla Autograd: Write the Update Yourself

```
import torch

x = torch.zeros(n, requires_grad=True)
alpha = 1e-3    # step size

for k in range(1000):
    if x.grad is not None:
        x.grad.zero_()          # clear old gradients

    loss = (A @ x - b) @ (A @ x - b)
    loss.backward()             # compute gradient

    # gradient descent update
    x.data -= alpha * x.grad
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What's happening

`loss.backward()` computes ∇_x`loss` and stores it in `x.grad`.
`x.data -= alpha * x.grad` performs the update manually.

torch.optim: Don't Write the Loop Yourself

PyTorch packages the update step into **optimizers**:

```
import torch
import torch.optim as optim

x = torch.zeros(n, requires_grad=True)
optimizer = optim.SGD([x], lr=1e-3, momentum=0.0, weight_decay=0.0)    # basic gradient descent

for k in range(1000):
    optimizer.zero_grad()                  # zero gradients

    loss = (A @ x - b) @ (A @ x - b)
    loss.backward()                        # compute gradients
    optimizer.step()                       # x -= lr * x.grad  (handled for you)
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What changed

`optimizer.zero_grad()` replaces `x.grad.zero_()`.

`optimizer.step()` replaces the manual `x -= alpha * x.grad`.

Same math. Cleaner code. And you can swap in fancier optimizers (`Adam`, `RMSProp`, `LBFGS`) by changing one line.

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Let's start with the simplest case: **one variable.**

$$\min_\beta \sum_i (y_i - \beta x_i)^2 \quad \Rightarrow \quad \hat{\beta} = \frac{\sum_i x_i y_i}{\sum_i x_i^2}.$$

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What if $\sum x_i^2$ is very small (features close to zero)?

$$\hat{\beta} = \frac{\text{something}}{\text{tiny number}} = \textbf{huge.}$$

A tiny change in y gets amplified into a massive change in $\hat{\beta}$.

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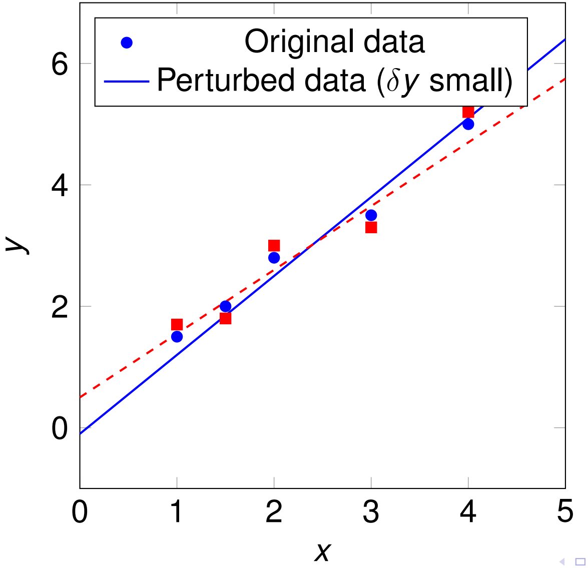
If the smallest eigenvalue $\sigma_n^2 \approx 0$ (columns of A nearly collinear):

$$\hat{\beta} \text{ blows up in the direction of that eigenvector.}$$

The Same Problem in Higher Dimensions



The Fix: Stop Dividing by Tiny Numbers

1D intuition:

$$\hat{\beta} = \frac{\sum x_i y_i}{\sum x_i^2} \quad \longrightarrow \quad \hat{\beta}_{\text{ridge}} = \frac{\sum x_i y_i}{\sum x_i^2 + \lambda}.$$

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Key insight

λ puts a **floor** under every eigenvalue. We never divide by anything smaller than λ. No blow-up. Stable $\hat{\beta}$.

Ridge Regression: Gradient and GD Step

Penalize values of x that "blow up" or are large.

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But with PyTorch, we don't need this formula at all.

Ridge Regression in PyTorch

```
import torch
import torch.optim as optim

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)
optimizer = optim.SGD([x], lr=1e-3)

for k in range(1000):
    optimizer.zero_grad()
    loss = (A @ x - b) @ (A @ x - b) + lam * (x @ x)   # ridge loss
    loss.backward()
    optimizer.step()

print(f"Final loss: {loss.item():.4f}")
```

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Observation

Compared to least squares, we added **ten characters**: `+lam*(x@x)`.

Effect of λ

$\lambda = 0$

Ordinary least squares.
No regularization.

Can be unstable when $A^\top A$ is ill-conditioned.

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Bigger picture

This idea: **penalizing complexity to get a better solution** is one of the most important ideas in machine learning. It will return when we train neural networks in a few weeks.

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So far today, we solved:

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No constraints. The gradient descent step is always valid.

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Example

Part I was *entirely* about constrained optimization (LP, IP).
We now have gradient tools (gradient descent, PyTorch). How do we put them together?

Approach 1: Projected Gradient Descent

Idea: take a gradient step, then **project** back onto the feasible set C.

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

where $\Pi_C(z) = \arg\min_{x \in C} \|x - z\|$ is the **Euclidean projection** onto C.

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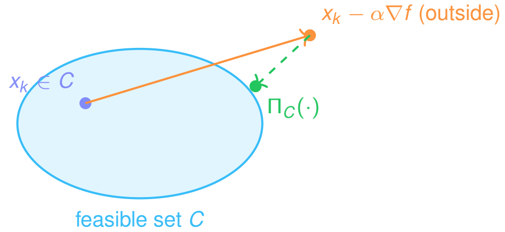

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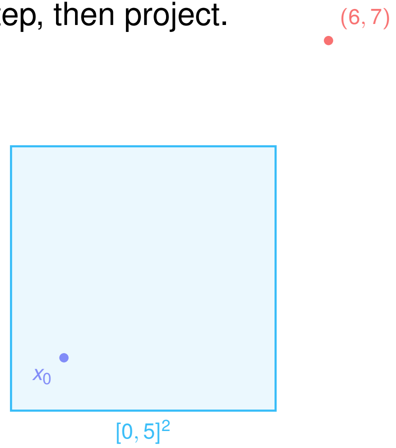

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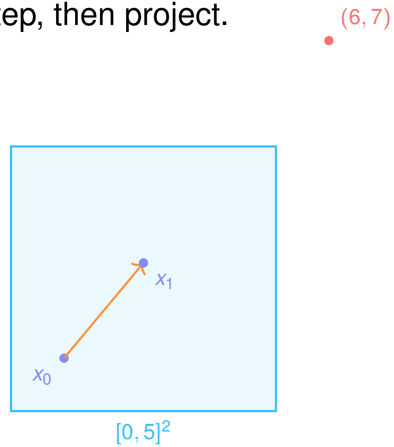

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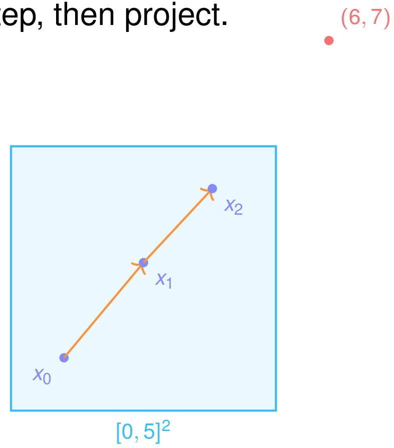

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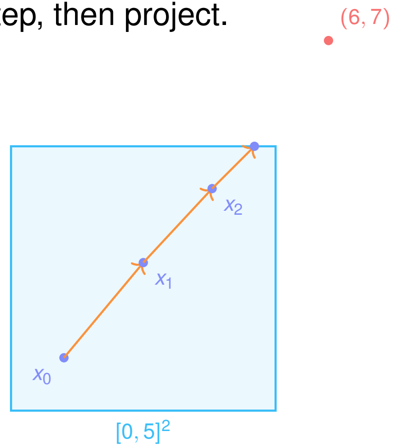

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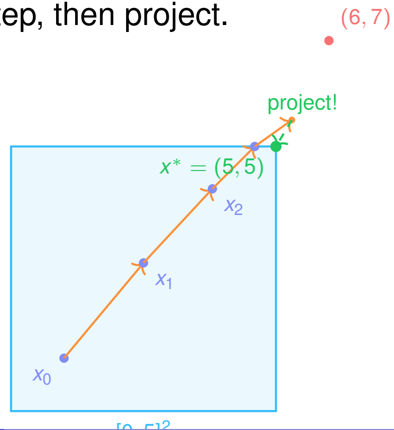

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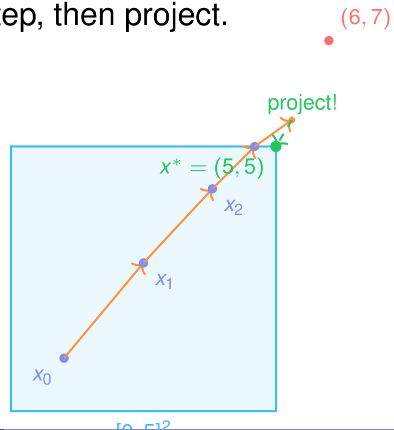

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Cost: $O(n)$
PyTorch: `x.clamp(min=l, max=u)`

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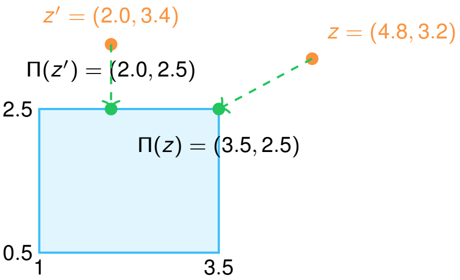

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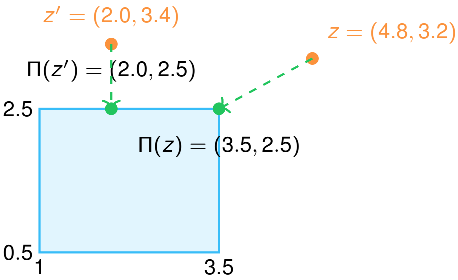

$$\Pi(4.8, 3.2) = (3.5, 2.5), \qquad \Pi(2.0, 3.4) = (2.0, 2.5)$$

Example: Box Projection in PyTorch

```
import torch

x = torch.tensor([1.0, 1.0], requires_grad=True)
alpha = 0.1

for k in range(100):
    loss = (x[0] - 6)**2 + (x[1] - 7)**2

    loss.backward()

    with torch.no_grad():
        x -= alpha * x.grad          # gradient step
        x.clamp_(min=0.0, max=5.0)   # project onto [0, 5]^2
        x.grad.zero_()

print(x)   # tensor([5., 5.])
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Observation

One extra line: `x.clamp_(min=0.0, max=5.0)`. That's the entire projection step.

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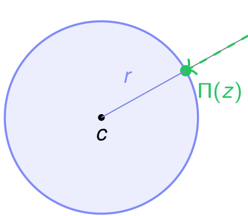

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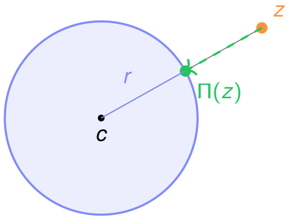

Cost: $O(n)$. Compute $\|z - c\|$, rescale if needed.

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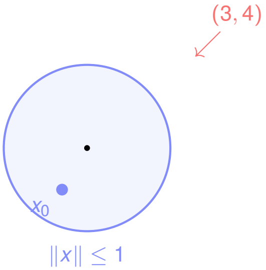

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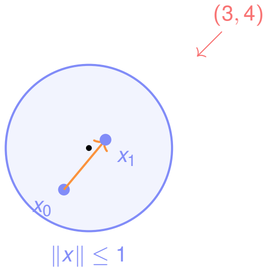

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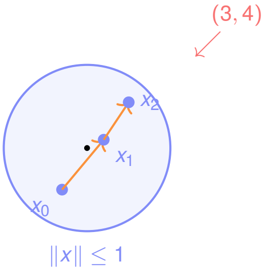

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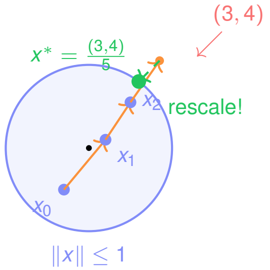

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import torch

x = torch.tensor([-0.3, -0.5], requires_grad=True)
r = 1.0
alpha = 0.1

for k in range(100):
    loss = (x[0] - 3)**2 + (x[1] - 4)**2

    loss.backward()

    with torch.no_grad():
        x -= alpha * x.grad                          # gradient step
        norm = torch.norm(x)
        if norm > r:
            x *= r / norm                            # project onto ball
        x.grad.zero_()

print(x)   # tensor([0.6000, 0.8000])
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```
import torch

x = torch.tensor([-0.3, -0.5], requires_grad=True)
r = 1.0
alpha = 0.1

for k in range(100):
    loss = (x[0] - 3)**2 + (x[1] - 4)**2

    loss.backward()

    with torch.no_grad():
        x -= alpha * x.grad                          # gradient step
        norm = torch.norm(x)
        if norm > r:
            x *= r / norm                             # project onto ball
        x.grad.zero_()

print(x)   # tensor([0.6000, 0.8000])
```

Same pattern: gradient step, then project. Two extra lines.

When Projection is Hard

Box and ball projections are cheap and have closed forms.

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The problem

When the feasible set is complex, projection is too expensive to call at every iteration.
We need a fundamentally different approach to handle constraints.

Approach 2: Penalty Methods

Idea: remove the constraints, but **punish violations** in the objective.

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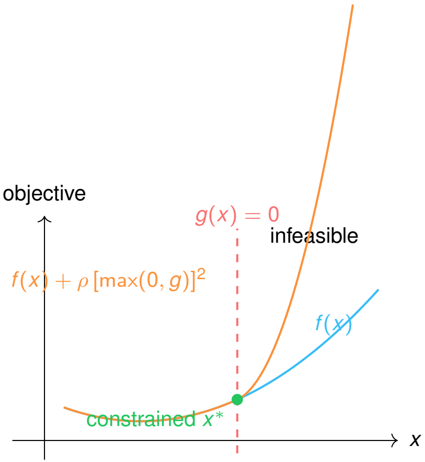
Penalty reformulation:

$$\min_x f(x) + \rho \cdot \left[\max(0,\; g(x))\right]^2, \qquad \rho > 0.$$

Approach 2: Penalty Methods



Penalty Methods: The Tradeoff

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Can we do better?

Is there a principled way to handle constraints that doesn't require $\rho \to \infty$?

Teaser: Lagrangian Duality

Instead of a brute-force penalty, introduce a **Lagrange multiplier** $\mu \geq 0$:

$$\mathcal{L}(x, \mu) = f(x) + \mu\, g(x).$$

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Next lecture

- Lagrangian duality and KKT conditions.
- Connects Part I (LP duality) with Part II (gradient methods).
- A principled framework for constrained nonlinear optimization.