CS498: Algorithmic Engineering

Lecture 12: Penalty Methods, Lagrangian Duality & Constrained Optimization

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Week 06 – 02/26/2026

Outline

Where We Left Off

Last lecture: **projected gradient descent** for constrained optimization.

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We worked through **box projections**:

- Constraint: $x \in [\mathbf{l}, \mathbf{u}]$.
- Projection: coordinate-wise clamp $\Pi(z)_i = \min(u_i, \max(l_i, z_i))$.
- Cost: $O(n)$. In PyTorch: `x.clamp_(min=l, max=u)`.

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Let's do one more easy projection, then see what happens when things get hard.

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$$\Pi(z) = \begin{cases} z & \text{if } \|z - c\| \leq r, \\ c + r \cdot \dfrac{z - c}{\|z - c\|} & \text{if } \|z - c\| > r. \end{cases}$$

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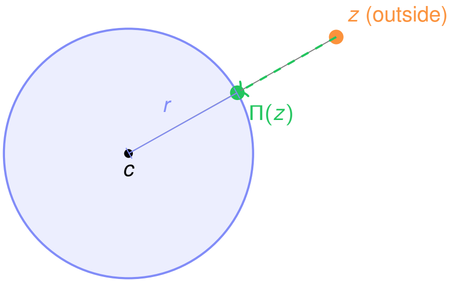
Intuition: walk from the center toward z, stop at the surface. Cost: $O(n)$.

Ball Projection: Picture



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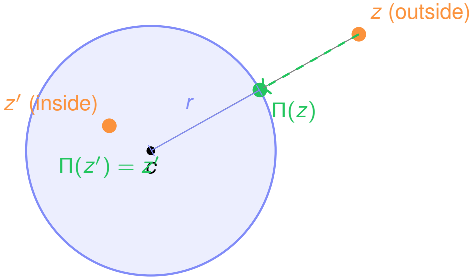

Example: Minimizing over a Ball

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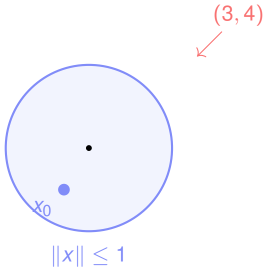

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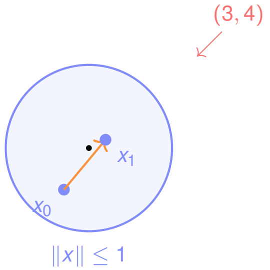

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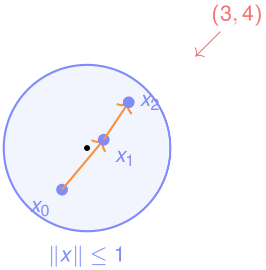

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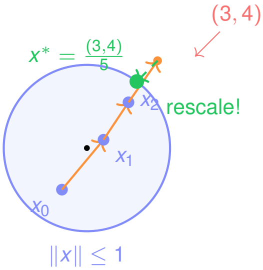

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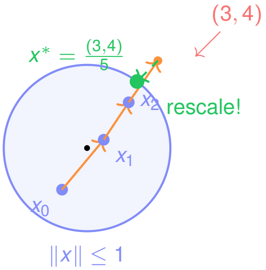

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Ball Projection in PyTorch (and with torch.no_grad())

```
import torch

x = torch.tensor([0.1, 0.2], requires_grad=True)
r = 1.0
alpha = 0.1

for k in range(100):
    loss = (x[0] - 3)**2 + (x[1] - 4)**2
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    #x.data -= alpha * x.grad
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    #x.data -= alpha * x.grad
    with torch.no_grad():
        x -= alpha * x.grad           # gradient step
        norm = torch.norm(x)
        if norm > r:
            x *= r / norm              # project: rescale to boundary
        x.grad.zero_()

print(x)   # tensor([0.6000, 0.8000], requires_grad=True)
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Same pattern as boxes: gradient step, then project. Two extra lines for the projection.

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Bottom line

Projected GD is beautiful when projection is "cheap". But for complex feasible sets, we need something else entirely.

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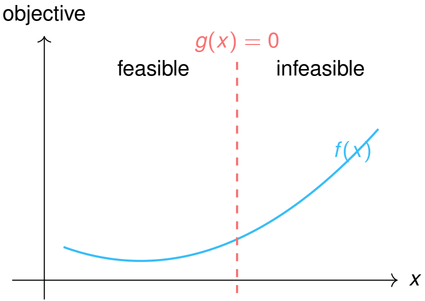
- If $g(x) \leq 0$ (feasible): penalty term $= 0$. No effect.
- If $g(x) > 0$ (violated): $f(x) + \rho g(x)^2$. GD pushes you back.

Penalty Methods: The Picture



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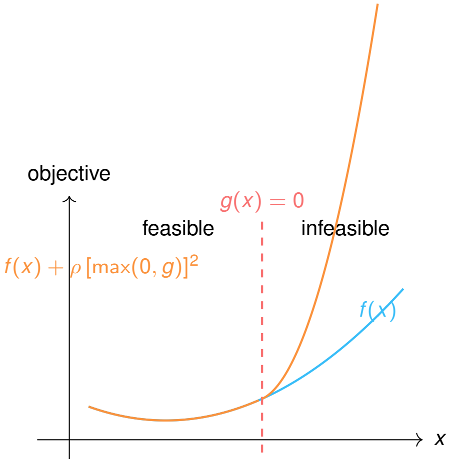

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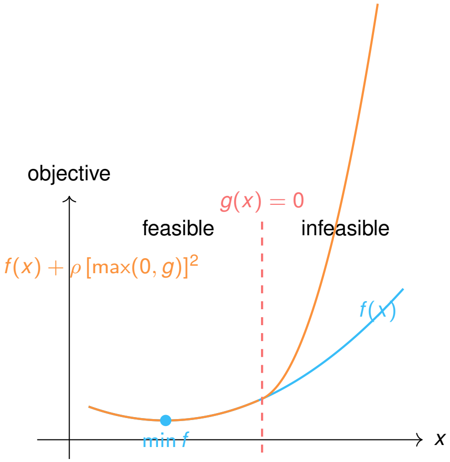

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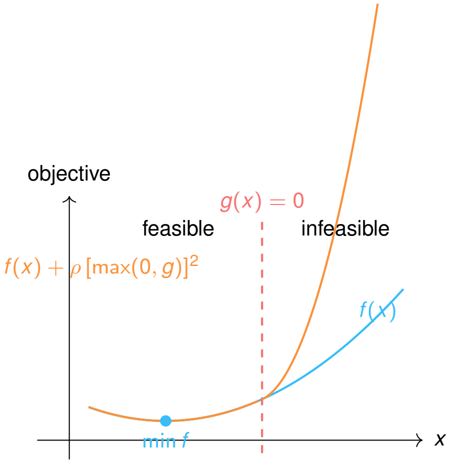

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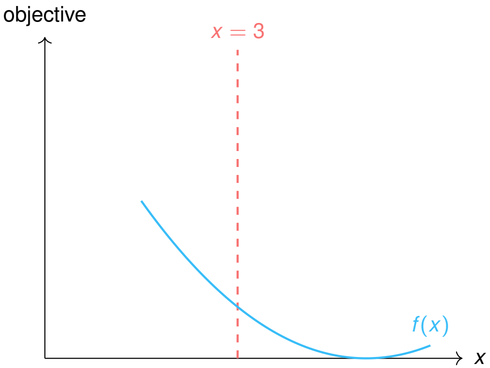
A Concrete Example

$$\min_x \, (x-5)^2 \quad \text{subject to} \quad x \le 3.$$

Penalty version with $g(x) = x - 3$:

$$\min_x \, (x-5)^2 + \rho\,[\max(0,\ x-3)]^2.$$

Penalty Methods: Visualizing ρ



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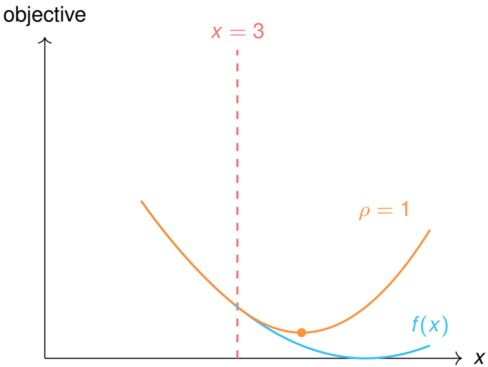

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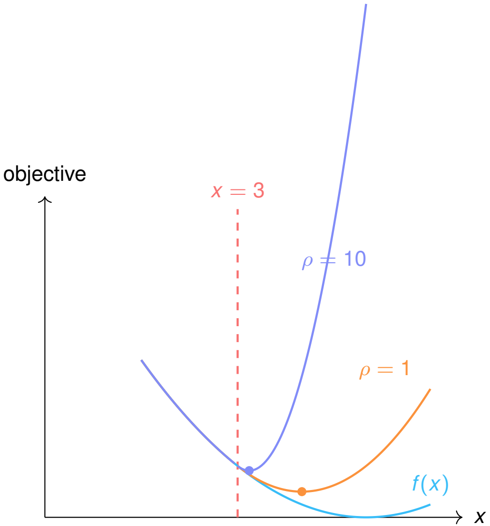

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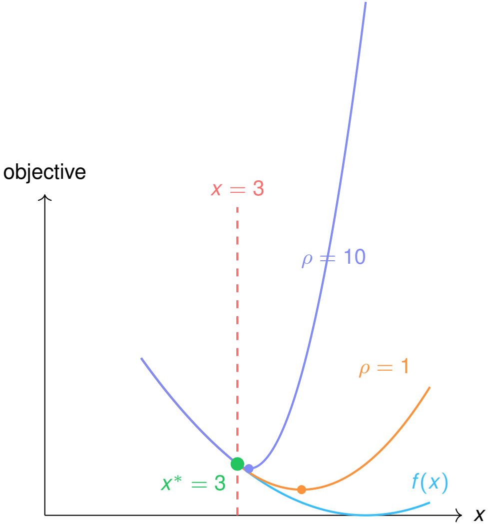

Penalty Method in PyTorch

```
x = torch.tensor([0.0, 0.0], requires_grad=True)
rho = 500.0
alpha = 0.005

for k in range(2000):
    obj = (x[0]-5)**2 + (x[1]-5)**2

    # single constraint: x1 + x2 <= 6  (i.e., g(x) = x1+x2-6 <= 0)
    # g(x) = x1 + x2 - 6 <= 0
    g = x[0] + x[1] - 6
    penalty = torch.maximum(torch.tensor(0.0), g)**2

    loss = obj + rho * penalty
    loss.backward()

    with torch.no_grad():
        x -= alpha * x.grad
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print(f"x = [{x[0].item():.3f}, {x[1].item():.3f}]")  # [3.002, 3.002]
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Notice: **no projection step at all**. The penalty does all the work. But we get 3.002, not 3.0. We'd need $\rho \to \infty$ for exactness.

Multiple Constraints? Just Add More Penalties

$$\min_x \, (x_1 - 5)^2 + (x_2 - 5)^2 \quad \text{s.t.} \quad x_1 + x_2 \leq 6, \quad x_1 \geq 0, \quad x_2 \geq 0.$$

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The question

Is there a smarter version of “penalize violations” that doesn’t require $\rho \to \infty$?

From Penalty to Lagrangian: The Key Insight

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

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- λ is not chosen by us: it's a **variable** that we optimize.
- We **minimize** over x (make the objective small).
- We **maximize** over λ (make constraint violations expensive).

What's the trick?

Consider what happens when we maximize over $\lambda \geq 0$:

$$\max_{\lambda \geq 0} \mathcal{L}(x, \lambda) = \max_{\lambda \geq 0} \left(f(x) + \lambda\, g(x)\right).$$

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Therefore:

$$\max_{\lambda \geq 0} \mathcal{L}(x, \lambda) = \begin{cases} f(x) & \text{if } x \text{ is feasible} \\ +\infty & \text{if } x \text{ is infeasible} \end{cases}$$

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$$\max_{\lambda \geq 0} \mathcal{L}(x, \lambda) = \max_{\lambda \geq 0} (f(x) + \lambda\, g(x)).$$

If $g(x) \leq 0$ (feasible): best $\lambda = 0$, so max $= f(x)$.
If $g(x) > 0$ (infeasible): can send $\lambda \to \infty$, so max $= +\infty$.

Therefore:

$$\max_{\lambda \geq 0} \mathcal{L}(x, \lambda) = \begin{cases} f(x) & \text{if } x \text{ is feasible} \\ +\infty & \text{if } x \text{ is infeasible} \end{cases}$$

So:

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The Lagrangian min-max is **exactly** the original constrained problem!

Primal-Dual Gradient Descent

We want to solve:

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Step 1 — Primal update (gradient *descent* in x):

$$x_{k+1} = x_k - \alpha\, \nabla_x \mathcal{L}(x_k, \lambda_k) = x_k - \alpha\left(\nabla f(x_k) + \lambda_k \nabla g(x_k)\right).$$

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But project on $\lambda \geq 0$ (clamp!):

$$\lambda_{k+1} = \max\big(0, \lambda_k + \alpha\, g(x_k)\big)$$

Primal–Dual Gradient Method: Update Rules Summary

We solve

$$\min_{x} \max_{\lambda \geq 0} \mathcal{L}(x, \lambda) = f(x) + \lambda g(x).$$

Initialize x_0, λ_0.

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Dual step (ascent in λ):

$$\lambda_{k+1} = \max\big(0, \lambda_k + \alpha\, g(x_k)\big)$$

Interpretation

- $g(x_k) > 0$ (constraint violated) $\Rightarrow \lambda$ increases.
- $g(x_k) < 0$ (constraint slack) $\Rightarrow \lambda$ decreases toward 0.

Concrete Example: Setup

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$$\frac{\partial \mathcal{L}}{\partial x} = 2(x-5) + \lambda$$

Updates:

$$x_{k+1} = x_k - \alpha\,[2(x_k - 5) + \lambda_k] \qquad \lambda_{k+1} = \max(0,\ \lambda_k + \alpha\,(x_k - 3))$$

Lagrangian Gradient Descent in PyTorch

```
import torch

x = torch.tensor(0.0, requires_grad=True)
lam = torch.tensor(0.0)
alpha = 0.05

for k in range(500):
    L = (x - 5)**2 + lam * (x-3)             # Lagrangian
    L.backward()                            # computes dL/dx automatically

    with torch.no_grad():
        x_old = x.clone()
        x -= alpha * x.grad                 # primal step: descend in x
        lam = torch.clamp(lam + alpha * (x_old-3), min=0)  # dual step: ascend in lambda
        x.grad.zero_()

print(f"x = {x.item():.4f}, lambda = {lam.item():.4f}")
# x ~ 3.0, lambda ~ 4.0
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# x ~ 3.0, lambda ~ 4.0
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No $\rho \to \infty$ needed. The multiplier λ **finds the right price** by itself.

The Lagrangian: General Form

Problem:

$$\min_x \; f(x) \quad \text{s.t. } g_i(x) \le 0 \; (i = 1, \ldots, m), \quad h_j(x) = 0 \; (j = 1, \ldots, p).$$

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$$\boxed{\mathcal{L}(x, \lambda, \nu) = f(x) + \sum_{i=1}^{m} \lambda_i \, g_i(x) + \sum_{j=1}^{p} \nu_j \, h_j(x)}$$

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- $\lambda_i \ge 0$: multiplier ("price") for inequality $g_i(x) \le 0$.
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Optimization:

$$\min_{x} \max_{\lambda \geq \mathbf{0},\, \nu} \mathcal{L}(x, \lambda, \nu) = f^*.$$

Primal–Dual Updates: General Case

We solve

$$\min_{x} \max_{\lambda \geq 0,\, \nu} \left(f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) + \sum_{j=1}^{p} \nu_j h_j(x) \right).$$

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$$x^{(k+1)} = x^{(k)} - \alpha\Big(\nabla f(x^{(k)}) + \sum_{i=1}^{m} \lambda_i^{(k)} \nabla g_i(x^{(k)}) + \sum_{j=1}^{p} \nu_j^{(k)} \nabla h_j(x^{(k)})\Big)$$

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$$\min_{x}\ \max_{\lambda\geq 0,\ \nu}\left(f(x)+\sum_{i=1}^{m}\lambda_i g_i(x)+\sum_{j=1}^{p}\nu_j h_j(x)\right).$$

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Convex Example: 2 Inequalities + 1 Equality

$$\min_{x} \, (x_1 - 5)^2 + (x_2 - 5)^2$$

$$\text{s.t.} \quad \underbrace{x_1 + x_2 \le 6}_{g_1(x) \le 0}, \qquad \underbrace{x_1^2 + x_2^2 \le 25}_{g_2(x) \le 0}, \qquad \underbrace{x_1 - x_2 = 0}_{h(x)=0}.$$

Primal–Dual Gradient Method

```
x = torch.tensor([0.0, 0.0], requires_grad=True)
lam = torch.tensor([0.0, 0.0])  # inequality multipliers (>=0)
nu = torch.tensor(0.0)   # equality multiplier
alpha = 0.02

for _ in range(2000):
    L = (x[0]-5)**2 + (x[1]-5)**2 \
            + lam[0]*(x[0]+x[1]-6)  \
            + lam[1]*(x[0]**2 + x[1]**2 - 25) \
            + nu * (x[0] - x[1])
    L.backward()
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        nu += alpha *(x_old[0] - x_old[1])   # ascent (no need to project)
        x.grad.zero_()
print(x) #tensor([3.0000, 3.0000], requires_grad=True)
print(lam) #tensor([4.0000, 0.0000])
print(nu) # tensor(0.)
```

KKT: When Are We at the Optimum?

We've been running gradient descent to *find* the solution. The **KKT conditions** tell us how to *check* it.

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KKT Check: Our Running Example

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3. **Dual feasibility:** $\lambda^* = 4 \geq 0$. $\checkmark$

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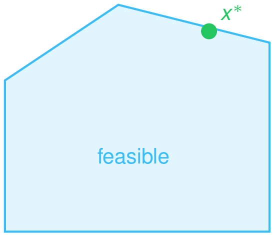
All four conditions hold $\Rightarrow$ $(3, 4)$ is **certifiably optimal**.

KKT: Geometric Picture



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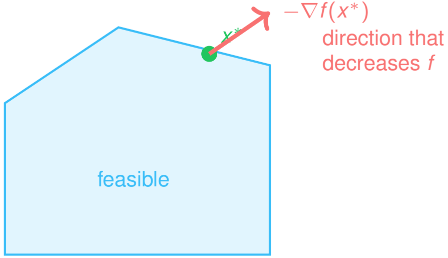

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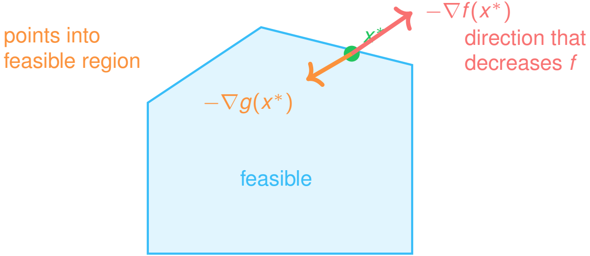
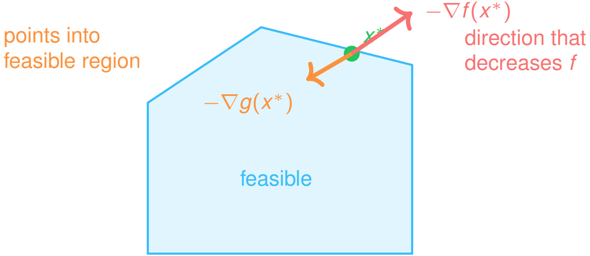


KKT: Geometric Picture



Stationarity: $\nabla f + \lambda^* \nabla g = 0$

Every improving direction violates a constraint. Stuck.

Looking Ahead: Semidefinite Programming

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To solve SDPs in practice, we use **CVXPY**: a Python library for convex optimization. Let me show you the bare minimum you'll need.

CVXPY for SDPs

An SDP optimizes over **positive semidefinite matrices**:

$$\min \langle C, X \rangle \quad \text{s.t.} \quad \langle A_i, X \rangle = b_i, \quad X \succeq 0.$$

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```
import cvxpy as cp
import numpy as np
np.random.seed(0)
n = 5
C = np.random.randn(n, n)
C = (C + C.T) / 2
A1, A2 = np.eye(n), np.ones((n, n))
b1, b2 = 1.0, 0.0

X = cp.Variable((n, n), symmetric=True)
constraints = [
    X >> 0, #positive semidefinite constraint
    cp.trace(A1 @ X) == b1, #Trace(A1 @ X) = <A1, X>
    cp.trace(A2 @ X) == b2 #Trace(A2 @ X) = <A2, X>
]
objective = cp.Minimize(cp.trace(C @ X))  #Trace(C @ X) = <C, X>
prob = cp.Problem(objective, constraints)
prob.solve(solver=cp.SCS, eps=1e-4, max_iters=300000)
```