# A Roadmap for Enforcing Hard Constraints in AI Models

## A Tutorial on Lagrangian and Repair Methods

# The Critical Need for Hard Constraints

Standard AI/ML models are trained to minimize a loss function, but they offer no guarantees that their outputs will satisfy critical operational constraints. This is a major barrier to deployment in high-stakes domains:

- **Robotics**: A robot arm's trajectory must remain within its joint limits and avoid collisions.
- **Power Grids**: Power generation schedules must exactly match demand to prevent blackouts.
- **Logistics**: A delivery route must respect vehicle capacity and driver work-hour limits.

In these applications, constraint violations are not just suboptimal; they are failures. Our goal is to bridge the gap between AI-driven decisions and the strict requirements of the physical world.

# Two Paths to Guaranteed Constraints

We can frame the problem of enforcing constraints as a choice between two fundamental strategies. Both leverage classical optimization theory as a foundation.

AI Model Output

## Path 1: Pricing Constraints (Lagrangian Methods)

**The Idea:** Relax hard constraints and incorporate them as tunable penalties in the training objective. We find the right "price" for each constraint violation.

**The Story:** An economic interpretation of constraints.

## Path 2: Projecting Solutions (Repair Methods)

**The Idea:** Allow a model to produce an unconstrained output, then use an explicit "repair" step to project it onto the feasible set.

**The Story:** A geometric interpretation of feasibility.

# The Toolkit: A Refresher on Lagrangian Duality

Let's revisit the standard constrained optimization problem:

The Primal Problem

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \end{aligned}$$

The Lagrangian Relaxation
We relax the hard constraints into a 'soft' penalty in the objective using non-negative Lagrange multipliers $\lambda_i \geq 0$:

$$\mathcal{L}(x, \lambda) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x)$$

Key Property: For any feasible point $x^*$ (a point satisfying all constraints) and any $\lambda \geq 0$, the Lagrangian provides a lower bound on the optimal value $f(x^*)$:

$$\min_x \mathcal{L}(x, \lambda) \leq \mathcal{L}(x^*, \lambda) = f(x^*) + \sum \lambda_i g_i(x^*) \leq f(x^*)$$

This holds because $g_i(x^*) \leq 0$ and $\lambda_i \geq 0$, making the sum non-positive.

# Finding the Best Lower Bound: The Dual Problem

## The Lagrange Dual Function

The dual function $q(\lambda)$ is the minimum value of the Lagrangian over the primal variable $x$. It is a function of the multipliers $\lambda$.

$$q(\lambda) = \inf_x \mathcal{L}(x, \lambda) = \inf_x \left( f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) \right)$$

## The Dual Problem

The dual problem is to find the multipliers $\lambda$ that provide the tightest possible lower bound on the primal problem. This is always a convex optimization problem.

$$\begin{aligned} \underset{\lambda}{\text{maximize}} \quad & q(\lambda) \\ \text{subject to} \quad & \lambda \geq 0 \end{aligned}$$

## Solving the Dual: Subgradient Ascent

We can solve the dual problem iteratively. If $x_k$ minimizes $\mathcal{L}(x, \lambda_k)$, then the constraint violations $g_i(x_k)$ form a subgradient of $q(\lambda)$ at $\lambda_k$. We can ascend in the direction of violation:

$$\lambda_{k+1} = [\lambda_k + s_k \nabla_\lambda \mathcal{L}(x_k, \lambda_k)]^+ = [\lambda_k + s_k \, g(x_k)]^+$$

where $s_k$ is a step size and $[\cdot]^+$ denotes projection onto the non-negative orthant.

# The Standard Form and Our Foundation

We consider a general optimization problem where the decision variable $x$ is the output of an AI model, $x = M_\theta(\text{input})$:

$$\begin{aligned} \underset{x \in \mathbb{R}^n}{\text{minimize}} \quad & f_0(x) \\ \text{subject to} \quad & f_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{aligned}$$

- $f_0(x)$ is the objective function we wish to minimize (e.g., tracking error, cost).
- $f_i(x)$ are the inequality constraints.
- $h_i(x)$ are the equality constraints.

The feasible set is $C = \{x \mid f_i(x) \leq 0, h_i(x) = 0\}$. Throughout this tutorial, we will use the notation and concepts from Boyd & Vandenberghe's Convex Optimization, which we assume as a shared foundation.

# Path 1: The Lagrangian "Pricing" Strategy

The core idea of Lagrangian relaxation is to transform a constrained problem into an unconstrained one by associating a "price" or penalty with each constraint. Let's revisit the Lagrangian from B&V, Chapter 5:

$$L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

- $\lambda_i \geq 0$ and $\nu_i$ are the Lagrange multipliers or dual variables.
- We can interpret $\lambda_i$ as the price per unit violation of the constraint $f_i(x) \leq 0$.
- The goal is to find prices $(\lambda^*, \nu^*)$ so that the minimizer of $L(x, \lambda^*, \nu^*)$ is also the solution to our original constrained problem.

The Lagrange dual function gives the optimal value of this "priced" problem for a fixed set of prices:

$$g(\lambda, \nu) = \inf_x L(x, \lambda, \nu)$$

For any $\lambda \geq 0$, $g(\lambda, \nu)$ provides a lower bound on the optimal value $p^*$ of the original problem (Weak Duality).

# Application: Integrating the Lagrangian into the Learning Objective

To apply this to an AI model $M_\theta$ that outputs $x$, we can define the training loss using the Lagrangian. The key question is how to handle the dual variables $(\lambda, \nu)$.

## Strategy 1: Fixed Hyperparameter Prices

The simplest approach is to treat $\lambda$ and $\nu$ as fixed, user-defined hyperparameters.

$$\mathcal{L}(\theta) = f_0(M_\theta(z)) + \lambda^T f(M_\theta(z)) + \nu^T h(M_\theta(z))$$

- **Pros:** Easy to implement.
- **Cons:** Extremely difficult to tune the prices $\lambda, \nu$ to achieve feasibility. No guarantee of satisfaction.

## Strategy 2: Learning the Prices via Dual Ascent (Fioretto et al.)

A more powerful approach is to learn the prices simultaneously with the model parameters. This mimics the saddle-point formulation of the dual problem. The training process becomes a two-player game:

1. **Primal Step:** Update model parameters $\theta$ to minimize $\mathcal{L}$ for fixed $(\lambda, \nu)$:
$$\theta \leftarrow \theta - \alpha \nabla_\theta \mathcal{L}(M_\theta(z), \lambda, \nu)$$
2. **Dual Step:** Update dual variables $\lambda$, $\nu$ to maximize $\mathcal{L}$ (i.e., raise the price on violated constraints):
$$\lambda_i \leftarrow [\lambda_i + \beta f_i(M_\theta(z))]_+$$
$$\nu_i \leftarrow \nu_i + \beta h_i(M_\theta(z))$$

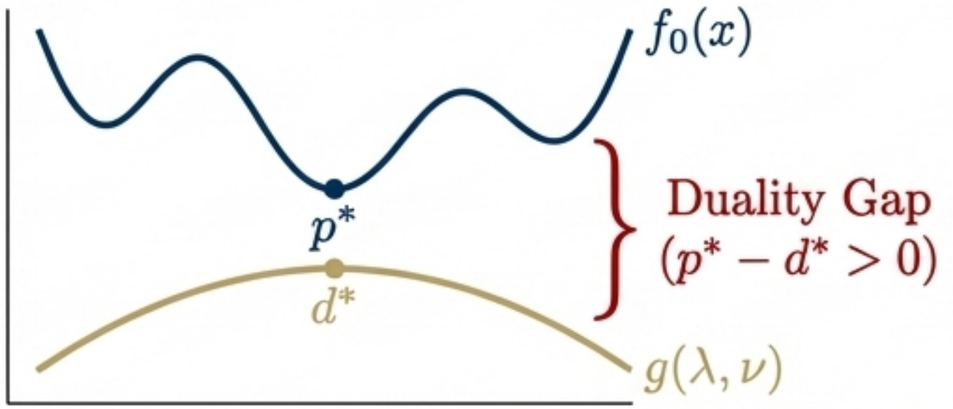
# Lagrangian Methods: Success and Failure

## When it Succeeds

- **Convex Problems with Strong Duality**: If the original problem is convex and satisfies a constraint qualification (e.g., Slater's condition), then strong duality holds ($p^* = d^*$). In this case, finding the optimal dual variables $(\lambda^*, \nu^*)$ and then minimizing $L(x, \lambda^*, \nu^*)$ solves the primal problem. The method is powerful as $\inf_x L(x, \dots)$ may be an easy unconstrained problem.
- **Provides a Bound**: Weak duality always holds, meaning $g(\lambda, \nu)$ is always a valid lower bound on the true optimal value $p^*$.

## When it Fails (Guarantees are Lost)

- **Non-Convexity and the Duality Gap**: For non-convex problems, such as training a deep neural network, a non-zero duality gap ($p^* > d^*$) is common. This means that even for the optimal dual variables $(\lambda^*, \nu^*)$, the minimizer of the Lagrangian, $x_L = \text{argmin}_x L(x, \lambda^*, \nu^*)$, is **not guaranteed to be feasible** for the original problem.
- **Result**: The method devolves into a sophisticated penalty method. It will push solutions *towards* feasibility, but it does not provide a **hard guarantee**. Violations, though often small, can persist.



# Path 2: The Repair ‘Projection’ Strategy

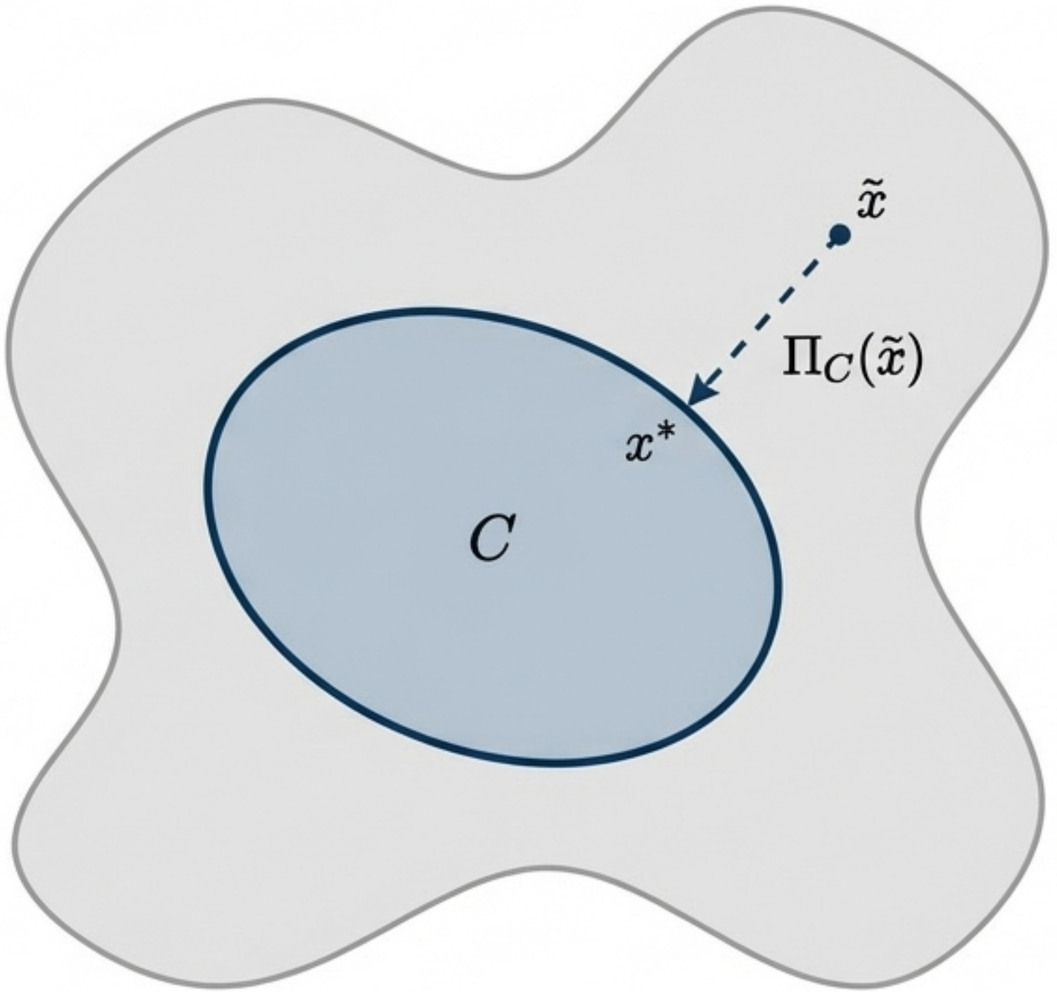
The repair method takes a different philosophical approach:

1. Train a model $M_\theta$ to produce a ‘best guess’ solution $\tilde{x} = M_\theta(z)$, ignoring the constraints.
2. In a separate, deterministic step, ‘repair’ $\tilde{x}$ by finding the closest point to it that lies within the feasible set $C$.

This repair step is a **projection**. The final, guaranteed-feasible output $x^*$ is:

$$x^* = \Pi_C(\tilde{x}) = \underset{x \in C}{\operatorname{argmin}} \|x - \tilde{x}\|_2.$$

- $C = \{x \mid f_i(x) \leq 0, h_i(x) = 0\}$ is the feasible set.
- This approach guarantees feasibility by construction.
- The key challenge is how to train the model $M_\theta$ end-to-end *through* this projection operator.



# Application: The Differentiable Repair Layer

To enable end-to-end training, the projection operator $\Pi_C(\cdot)$ must be differentiable. The model's loss depends on the final, projected output:

$$\mathcal{L}(\theta) = f_0(x^*) = f_0(\Pi_C(M_\theta(z)))$$

To compute the gradient $\partial\mathcal{L}/\partial\theta$, the chain rule requires the Jacobian of the projection, $\partial\Pi_C(\tilde{x})/\partial\tilde{x}$.

**How can we differentiate through `argmin`?**

- The projection $x^* = \Pi_C(\tilde{x})$ is the solution to a convex optimization problem.
- We can use the KKT conditions that define $x^*$. For a convex set $C$, these conditions implicitly define $x^*$ as a function of $\tilde{x}$.
- Using the **Implicit Function Theorem** on the KKT conditions, we can compute the Jacobian $\partial x^*/\partial\tilde{x}$. This is particularly straightforward when the projection is a Quadratic Program (QP).

This technique allows gradients to flow back from the final objective $f_0(x^*)$ through the repair layer to the underlying model $M_\theta$, as demonstrated in frameworks like HardNet.

# Repair Methods: Success and Failure

## When it Succeeds

- **Hard Feasibility Guarantee:** This is the primary advantage. The output is *always* feasible by construction, which is non-negotiable for high-stakes applications.
- **Efficient for Simple Sets:** If the feasible set $C$ allows for an efficient projection (e.g., affine sets, boxes, balls, probability simplex), the repair step is fast and its derivative is easy to compute.

## When it Fails (or is Impractical)

- **Computational Cost:** If $C$ is defined by complex constraints, solving the projection problem at every forward pass of the network can be prohibitively expensive.
- **Information Loss:** The projection can be a "violent" operation. It might move $\tilde{x}$ a large distance, potentially discarding useful information learned by the model and hurting the primary objective $f_0$. The model might learn to rely on the projection as a crutch.
- **Requires Convexity:** The projection $\Pi_C(\tilde{x})$ is a well-defined and tractable convex optimization problem only if the feasible set $C$ is itself convex. This limits applicability for problems with non-convex constraints.

# Example Showdown: Projection onto the Probability Simplex

**Problem:** An AI model outputs a logit vector $\tilde{\boldsymbol{x}} \in \mathbb{R}^n$. We want to produce a probability distribution $\boldsymbol{x}$ that minimizes $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2^2$ subject to the simplex constraints $C = \{\boldsymbol{x} \mid \boldsymbol{x} \geq 0, 1^T\boldsymbol{x} = 1\}$.

## Path 1: Lagrangian Approach

1. Form the Lagrangian:

$$L(\boldsymbol{x}, \lambda, \nu) = \|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2^2 - \lambda^T\boldsymbol{x} + \nu(1^T\boldsymbol{x} - 1).$$

2. Minimize $L$ with respect to $\boldsymbol{x}$ by setting $\nabla_x L = 0$:

$$2(\boldsymbol{x} - \tilde{\boldsymbol{x}}) - \lambda + \nu 1 = 0 \;\Rightarrow\; \boldsymbol{x}_i = \tilde{\boldsymbol{x}}_i + \frac{\lambda_i - \nu}{2}.$$

3. The training process must then learn $\lambda \geq 0$ and $\nu$ that satisfy the KKT conditions (stationarity, primal/dual feasibility, complementarity). The final $\boldsymbol{x}$ is not guaranteed to be exactly on the simplex.

## Path 2: Repair Approach

1. The model produces $\tilde{\boldsymbol{x}}$.
2. The repair layer solves the projection problem:

$$\boldsymbol{x}^* = \text{argmin}_{x \in C} \|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2^2.$$

3. This is a standard Quadratic Program (QP) with a known, efficient solution algorithm.
4. The final output $\boldsymbol{x}^*$ is guaranteed to be a valid probability distribution. Gradients are computed by differentiating through the KKT solution of the QP.

# A Traveler's Guide: Choosing Your Path

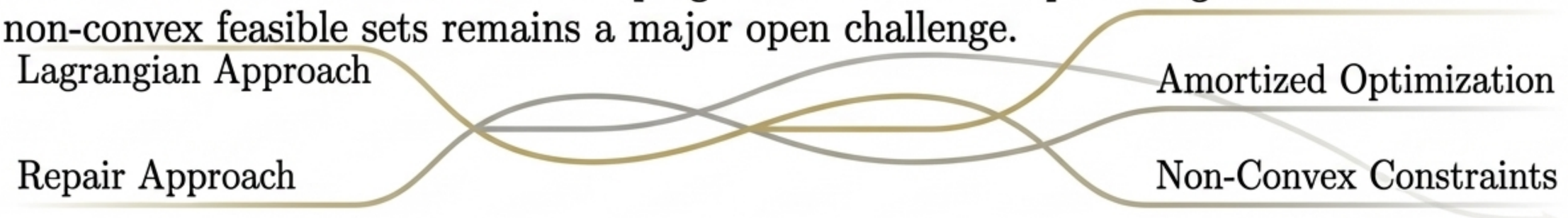
The choice between Lagrangian and Repair methods depends on the specific problem's requirements.

| Feature | Lagrangian Methods | Repair Methods |
|---|---|---|
| **Feasibility Guarantee** | **Soft**. Prone to small violations in non-convex cases. | **Hard**. Guaranteed by construction. |
| **Core Idea** | Economic: 'Pricing' constraints via dual variables. | Geometric: 'Projecting' solutions onto the feasible set. |
| **Computational Cost** | Solving $\inf_x L(x, \lambda, \nu)$ + dual updates during training. | Solving the projection problem $\Pi_C(\cdot))$ in every forward and backward pass. |
| **Primary Requirement** | Differentiable objective $f_0$ and Lagrangian. | A convex feasible set $C$ with a tractable and differentiable projection. |
| **Best Suited For...** | Problems where small violations are tolerable and constraints might be non-differentiable. | High-stakes problems requiring strict feasibility where $C$ is a convex set amenable to fast projection. |
| **B&V Foundation** | Chapter 5: Duality | Chapter 8: Projection on a Set |

# The Frontier: A Synthesis of Learning and Optimization

Enforcing hard constraints is not just about retrofitting classical optimization onto modern AI. It is about creating a true synthesis. The frontier of this field lies in pushing beyond these two fundamental paths:

- **Hybrid Methods:** Can we use a Lagrangian penalty to guide a model's output $\tilde{x}$ to be closer to the feasible set, thereby making the final repair projection less "violent" and more efficient?
- **Amortized Optimization:** Instead of solving a projection problem from scratch every time, can we train a separate neural network to *approximate* the projection operator $\Pi_C(\cdot)$ for faster inference?
- **Non-Convex Constraints:** Developing methods that can provide guarantees for structured non-convex feasible sets remains a major open challenge.




The principles laid out in texts like Boyd & Vandenberghe are not relics; they are the essential grammar for building the next generation of robust, reliable, and deployable AI systems.

# Key References


**Foundation**

Boyd, S., & Vandenberghe, L. (2004). *Convex Optimization*. Cambridge University Press.

**Roadmap**

Van Hentenryck, P. (2020). AI and optimization: A roadmap for constraint satisfaction. *AI Magazine*.

**Methodology Examples**

- **Lagrangian Methods**: Fioretto, F., et al. (2020). Lagrangian Duality for Constrained Deep Learning. *AAAI Conference on Artificial Intelligence*.
- **Repair Methods**: Vlastelica, M., et al. (2019). Differentiation of Blackbox Combinatorial Solvers. *International Conference on Learning Representations* (Introduced concepts for differentiating through solvers, relevant to HardNet).


Note: Full citations for Fioretto and HardNet papers are representative examples. Replace with the exact papers if they differ.