Numerical Optimization 18: Symbolic Regression

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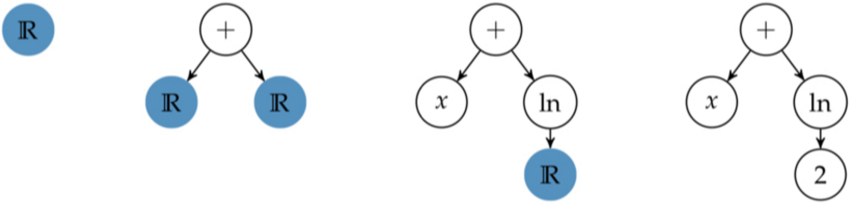
Overview

Grammars

An expression can be represented by a tree of symbols. For example, the mathematical expression $x + \ln 2$ can be represented using the tree consisting of the symbols $+, x, \ln$, and 2. Grammars specify constraints on the space of possible expressions.



Constraints

Constraints are not typically specified directly through a known feasible set X . Instead, the feasible set is typically formed from two types of constraints:

- equality constraints, $h(x) = 0$
- inequality constraints, $g(x) \leq 0$

Any optimization problem can be rewritten using these constraints

$$\begin{aligned} & \min_{\boldsymbol{x}} \; f(\boldsymbol{x}) \\ s.t. \quad & h_i(x) = 0 \\ & g_j(x) = 0 \end{aligned}$$

Genetic Programming

Genetic programming represents individuals using trees instead, which are better at representing mathematical functions, programs, decision trees, and other hierarchical structures.

$$x = \frac{b+a}{2} + \frac{b-a}{2}\left(\frac{2\hat{x}}{1+\hat{x}^2}\right)$$

Lagrange Multipliers

The method of Lagrange multipliers is used to optimize a function subject to equality constraints.

$$\min_{\boldsymbol{x}} \ f(\boldsymbol{x})$$
$$s.t. \quad h_i(x) = 0$$

where f and h have continuous partial derivatives.
We can formulate the Lagrangian, which is a function of the design variables,

$$\mathcal{L}(x, \lambda) = f(x) - \lambda h(x)$$

Solving $\nabla \mathcal{L}(x, \lambda) = 0$. Specifically, $\nabla_x \mathcal{L} = 0$ gives us the condition $\nabla f = \lambda \nabla h$, and $\nabla \lambda \mathcal{L} = 0$ gives us $h(x) = 0$. Any solution is considered a critical point.

Lagrange Multipliers to a single equality condition

The method of Lagrange multipliers is used to optimize a function subject to equality constraints.

$$\min_{\boldsymbol{x}} \; -\exp[-(x_1x_2 - 3/2)^2 - (x_2 - 3/2)^2]$$
$$s.t. \quad x_1 - x_2^2 = 0$$

We can formulate the Lagrangian,

$$\mathcal{L}(x,\lambda) = -\exp[-(x_1x_2 - 3/2)^2 - (x_2 - 3/2)^2] + \lambda(x_1 - x_2^2)$$

We compute

- $\frac{\partial \mathcal{L}}{\partial x_1}$
- $\frac{\partial \mathcal{L}}{\partial x_2}$
- $\frac{\partial \mathcal{L}}{\partial \lambda}$

Lagrange Multipliers to multiple equality conditions

The method of Lagrange multipliers is used to optimize a function subject to equality constraints.

$$\min_{\boldsymbol{x}} \; -\exp[-(x_1x_2 - 3/2)^2 - (x_2 - 3/2)^2]$$
$$s.t. \quad x_1 - x_2^2 = 0$$

We can formulate the Lagrangian,

$$\mathcal{L}(x, \lambda) = -\exp[-(x_1x_2 - 3/2)^2 - (x_2 - 3/2)^2] + \lambda(x_1 - x_2^2)$$

We compute

- $\frac{\partial \mathcal{L}}{\partial x_1}$
- $\frac{\partial \mathcal{L}}{\partial x_2}$
- $\frac{\partial \mathcal{L}}{\partial \lambda}$

Summary

- Constraints are requirements on the design points that a solution must satisfy.
- Some constraints can be transformed or substituted into the problem to result in an unconstrained optimization problem.
- Analytical methods using Lagrange multipliers yield the generalized Lagrangian and the necessary conditions for optimality under constraints.
- A constrained optimization problem has a dual problem formulation that is easier to solve and whose solution is a lower bound of the solution to the original problem.