Outline

In this lecture, we cover several black-box optimization frameworks that are often very useful for practical problems. Many decision-making problems that arise in practice often incorporate uncertain problem parameters, which is not accessible until we decide on an action. We introduce a global search-based algorithms and regression-based methods.

1 (Non-Convex) Black-Box Optimization

Many problems in practice involve non-convex loss functions. Loss functions that arise in real-world applications can be as complex as the example in Figure 11.1. In fact, there are various

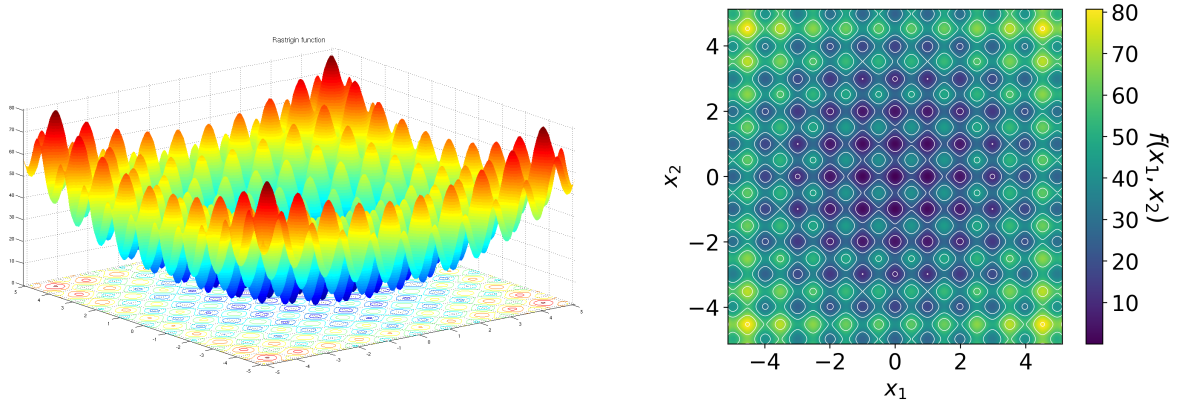

Figure 11.1: Rastrigin Function in 2D

algorithms for non-convex optimization, including gradient descent with Hessian steps, the cubic regularization method, and perturbed gradient descent. Recall that these algorithms are designed to find second-order stationary points or local minima under appropriate assumptions on the loss function.

Although the aforementioned algorithms for non-convex optimization are commonly used in practice, they require knowledge of the loss function's gradient and possibly Hessian. There indeed exist many applications where it is difficult to analyze the gradient and Hessian of the underlying loss function. The following provides a list of such applications.

- Engineering Design: Optimizing the design of complex systems and structures (e.g., aerodynamics of aircraft, structural design of bridges) where simulations are used to evaluate performance.
- Machine Learning and Hyperparameter Tuning: Tuning hyperparameters of machine learning models, such as neural networks, support vector machines, and random forests, to achieve better performance on training and validation data.

- Robotics: Optimizing control parameters and policies for robotic systems where the dynamics are complex and non-linear.
- Gaming and AI: Developing and tuning artificial intelligence for games, including the optimization of strategies and behaviors in complex environments.
- Finance and Trading: Developing and optimizing trading algorithms and strategies, as well as portfolio optimization, where the financial models are often noisy and non-differentiable.
- Energy Systems: Optimizing the operation and design of energy systems, such as power grids, renewable energy installations, and energy storage systems, to improve efficiency and stability.
- Material Science: Discovering new materials with desirable properties (e.g., strength, conductivity) by optimizing the composition and processing parameters.
- Healthcare and Medicine: Personalizing treatment plans and drug formulations by optimizing the dosage and combination of therapies for individual patients.
- Chemistry and Biochemistry: Optimizing chemical reactions and biological processes for higher yield, efficiency, and reduced side products in chemical engineering and biotechnology.

In these application settings, the associated loss function is ofen complex, non-differentiable, noisy, or not explicitly known. As a result, we cannot hope for computing the gradient nor the Hessian of the underlying loss function. This problem is often referred to as **black-box optimization**.

2 Discretization-Based Search

Let us consider

$$\min_{x \in C} \quad f(x)$$

where C is the domain and f is the loss function. For black-box optimization, we make minimal assumptions on the loss function f. That said, we consider the general setting where the loss function can be non-convex and non-differentiable. On the other hand, in some applications, the underlying loss function is continuous. The example in Figure 11.1 is indeed continuous, even though its structure is highly complex. Motivated by this, we consider the setting where the loss function is **Lipschitz continuous**. Throughout this section, we assume that f is L-Lipschitz continuous in a norm $\|\cdot\|$, i.e.,

$$|f(x) - f(y)| \leq L\|x - y\|.$$

The goal is to find a near-optimal solution x_ϵ for a given $\epsilon > 0$ such that

$$f(x_\epsilon) \leq \min_{x \in C} f(x) + \epsilon.$$

As the loss function f is Lipschitz continuous, our approach is to find a point that is close to an optimal solution. Then, how do we find such a point? The most naïve way is to discretize the solution space and search over the discrete set of points. To be more precise, we consider the following two steps.

1. First, discretize the domain C to obtain a finite subset $C_\epsilon \subseteq C$ containing an ϵ-optimal solution.
2. Next, enumerate all points in C_ϵ.

Hence, as long as the discretization C_ϵ contains an ϵ-optimal solution x_ϵ, the search procedure will find one. The iteration complexity of this algorithm is the number of points in C_ϵ. Therefore, the part of constructing a discretization C_ϵ is crucial.

To simplify our presentation, we assume that

- the domain is given by $C = [0,1]^d$,
- we use the ℓ_∞-norm, i.e., $\|\cdot\| = \|\cdot\|_\infty$, and
- $1/L\epsilon$ is an integer.

Based on these assumptions, we partition the domain $C = [0,1]^d$ into $(1/L\epsilon)^d$ boxes by decomposing each coordinate interval $[0,1]$ into

$$[0, \epsilon/L], \quad [\epsilon/L, 2\epsilon/L], \quad \ldots, \quad [1-\epsilon/L, 1].$$

Then a box has the form

$$\begin{aligned}&\left[\frac{(i_1-1)\epsilon}{L}, \frac{i_1\epsilon}{L}\right] \times \left[\frac{(i_2-1)\epsilon}{L}, \frac{i_2\epsilon}{L}\right] \times \cdots \times \left[\frac{(i_d-1)\epsilon}{L}, \frac{i_d\epsilon}{L}\right] \\ &= \left\{x \in \mathbb{R}^d : \ \frac{(i_j-1)\epsilon}{L} \le x_j \le \frac{i_j\epsilon}{L} \quad \forall j \in [d]\right\}.\end{aligned}$$

For a given box, we take the center point given by

$$\left(\frac{\left(i_1 - \frac{1}{2}\right)\epsilon}{L}, \quad \frac{\left(i_2 - \frac{1}{2}\right)\epsilon}{L}, \quad \ldots, \frac{\left(i_d - \frac{1}{2}\right)\epsilon}{L}\right).$$

Note that there are $(1/L\epsilon)^d$ center points from the $(1/L\epsilon)^d$ boxes. Basically, the set of center points gives rise to a desired discretization C_ϵ. The algorithm is to enumerate all center points and return the one achieving the minimum loss value.

How do we establish the correctness of this approach? Note that any two points x, y in a piece satisfies

$$\|x - y\|_\infty \le \epsilon/L,$$

which implies that

$$|f(x) - f(y)| \le L\|x - y\|_\infty \le \epsilon.$$

Let c^* be the center point of the box containing an optimal solution. Then it follows that

$$f(c^*) \le \min_{x \in C} f(x) + \epsilon.$$

Let $\bar{c}$ be the center point returned by the algorithm. By the choice of $\bar{c}$, we have that

$$f(\bar{c}) \le f(c^*) \le \min_{x \in C} f(x) + \epsilon,$$

as required.

3 Optimistic Optimization

The algorithm from the previous section is based on a fixed discretization. As a result, the algorithm always takes $(1/L\epsilon)^d$ steps to finish search over all points in the discretization. Another issue is that we require knowledge of the Lipschitz constant L. Furthermore, the most critical issue with the method is that we need the assumption that the loss function is Lipschitz continuous over the entire domain.

In this section, we cover a framework of Munos [Mun11], referred to as **simultaneous optimistic optimization (SOO)**. The SOO framework works under the following weaker assumption than the global Lipschitz continuity assumption.

Assumption 11.1. There exists some $L > 0$ such that for any $x \in C$,

$$f(x) - f(x^*) \leq L\|x - x^*\|$$

where x^* is an optimal solution to $\min_{x \in C} f(x)$.

Hence, we assume Lipschitz continuity around an optimal solution, which is essentially a local Lipschitz continuity assumption.

Another favorable aspect of SOO is that it does not need to know the Lipschitz constant L. How is this possible? Recall that the previous approach needs to know L because it prepares a fixed discretization based on the parameter L. In contrast, instead of one fixed discretization, the SOO framework starts with a rough partition of the domain, and it gradually refines it.

To be more specific, SOO works with the idea of **hierarchical partitioning**. First, the domain C is partitioned into K subsets. Here, one may represent the K subsets as K children of paraent C. Then, we may choose one of the K subsets and partition it into K subsets, as in Figure 11.2.

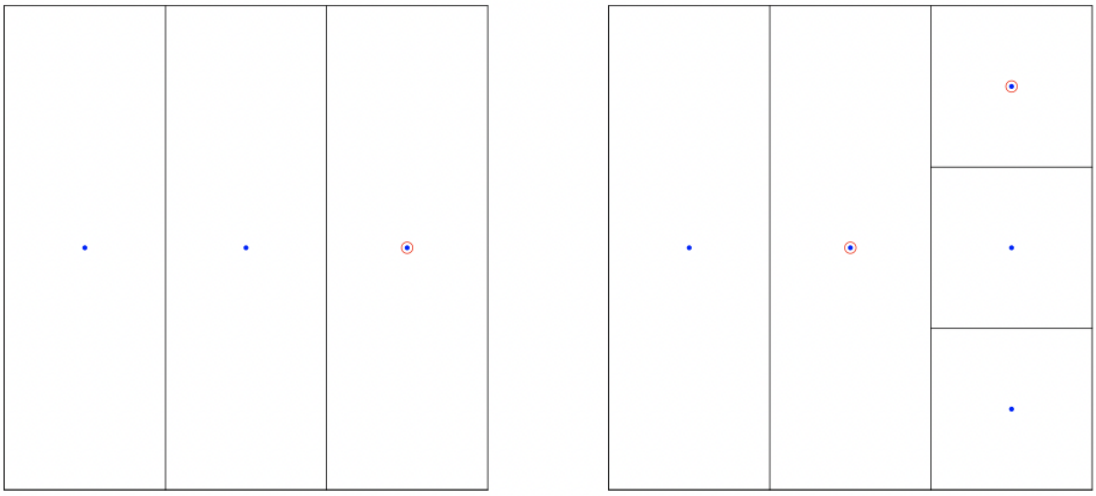

Figure 11.2: Partitioning of the domain

We may continue partitioning pieces. From the second partition of Figure 11.2, we can choose one of the two large subsets or one of the three smaller subsets. Figure 11.3 shows a sequence of more refined partitions of the domain C.

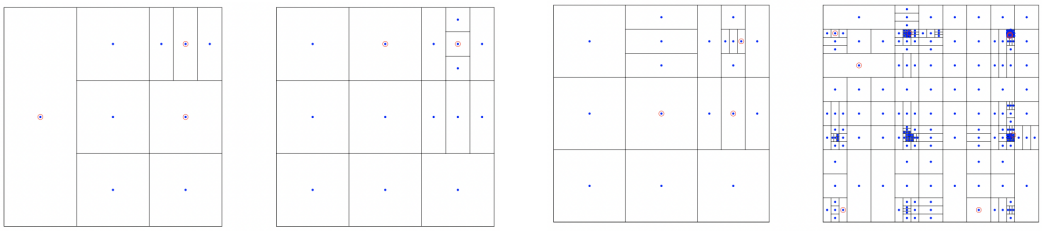

Figure 11.3: Refined partitions

The hierarchical partitioning structure naturally gives rise to a tree representation as in Figure 11.4.

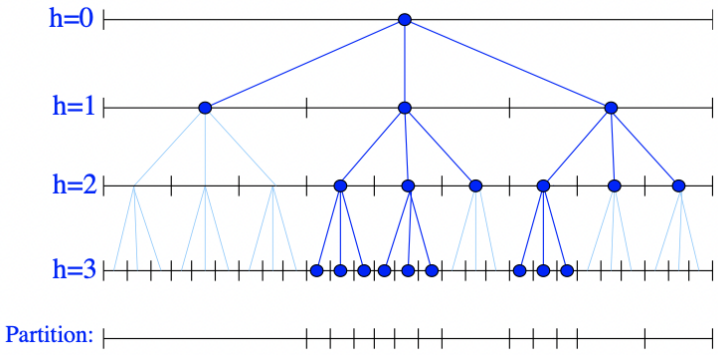

Figure 11.4: Tree representation of a partition

Note that hierarchical partitioning can be done without knowledge of the Lipschitz constant L. The main idea behind the SOO framework is to choose subsets that are expected to contain an optimal solution and refine them gradually. As the algorithm from the previous section, SOO takes a center point of each subset. Then the quality of the subset is measured by the loss value of its center point.

Another important component of SOO is the idea of **optimistic search**. At each iteration, we need to choose which subset to be partitioned. The choice is made based on two criteria. On one hand, it makes sense to focus on subsets whose center points have low loss values. On the other hand, a large subset is not explored enough yet, so its unexplored region may contain a good solution. This is similar in spirit to **the exploration-exploitation tradeoff**.

To be more specific, we use notation (h, j) to denote the jth subset at depth h. Here, $(0, 0)$ refers to the original domain C. Then we denote by $x_{h,j}$ the center point of (h, j). Then the quality of subset (h, j) is measured by $f(x_{h,j})$. Then, the next question is about how to choose a subset that is unexplored? We may select a subset at a high hierarchy in the tree representation. The SOO algorithm is given as follows.

Algorithm 1 Simultaneous Optimistic Optimization

Input: the maximum depth function $h_{\max} : \mathbb{Z} \to \mathbb{Z}$.
Initialize $\mathcal{T}_1 = \{(0, 0)\}$ and $t = 1$.
while True **do**
  Set $v_{\min} = \infty$.
  for $h = 0$ to $\min\{\text{depth}(\mathcal{T}_t), h_{\max}(t)\}$ **do**
    Among all leaves $(h, j) \in \mathcal{L}_t$ of depth h, select

$$(h, i) \in \text{argmin}_{(h,j)\in\mathcal{L}_t} f(x_{h,j})$$

    if $f(x_{h,i}) \leq v_{\min}$ **then**
      Partition the subset (h, i) into K subsets $(h + 1, i_1), \ldots, (h + 1, i_K)$.
      Add them to $\mathcal{T}_t$.
      Evaluate $f(x_{h+1,i_1}), \ldots, f(x_{h+1,i_K})$.
      Set $v_{\min} = f(x_{h,i})$.
      if $t = T$ **then**
        Return

$$\text{argmax}_{(h,i)\in\mathcal{T}_T} f(x_{h,i})$$

      end if
    end if
  end for
end while

4 Black-Box Optimization by Supervised Learning

In the previous section, we introduced the black-box optimization framework which applies to settings where the objective function is not known to the decision-maker. We consider

$$\min_{x\in C} \quad f(x)$$

where the decision-maker has access to none of the gradient $\nabla f(x)$ and the Hessian $\nabla^2 f(x)$. We find a solution based on bandit feedback which exhibits the value $f(x)$ of a chosen solution x. We learned optimistic optimization methods, which explore the solution space based on continuity of the objective function. The main idea behind the optimistic optimization methods is that we provide a hierarchical partitioning of the search space based on which we can optimistically explore subsets of the search space.

The optimistic optimization algorithms are widely used in practice because they rely on minimal structural assumptions on the objective function. On the other hand, as they do not exploit any underlying structures of the objective function, they often fall into inferior performance than instance-specific methods that are implemented with some knowledge of the problem environment. This motivates the question of how to explore and exploit the underlying structure of the function.

In this lecture, we discuss some supervised learning methods to learn and approximate the unknown objective function. More importantly, based on the learned model and function, we are interested in finding a good solution that guarantees a small loss value. Basically, we are given n data points $(x_1, f(x_1)), \ldots, (x_n, f(x_n))$, from which we infer the underlying function f.

One of the most practical supervised learning is to use a neural network to learn the underlying model. Based on a data set of n points $(x_1, y_1), \ldots, (x_n, y_n)$ with $y_i = f(x_i)$ for $i \in [n]$, one may

train a neural network by considering

$$\min_{\theta} \quad \sum_{i=1}^{n} \ell(f_\theta(x_i), y_i).$$

Here, the trained neural network f_θ provides an approximation of the objective function f. Then, we may find a solution that achieves a small f value by considering

$$\min_{x \in C} \quad f_\theta(x).$$

Feed-forward neural networks with ReLU activations functions are commonly used for approximating the unknown objective function in practice [PTA+22]. Throughout this section, we discuss how to find an input solution that optimizes the output value of a trained feed-forward neural network with ReLU activation. In particular, we explain the basic formulation due to Fischetti and Jo [FJ18] and Serra et al. [STR18].

Let us discuss the case of a neural network with a single hidden layer. Let $x \in \mathbb{R}^d$ be the input, prepared by d input neurons. There are m neurons in the single hidden layer. Let the input of the ith neuron in the hidden layer be given by $w_i^\top x + b_i$. Then the output of the neuron is

$$\mathrm{ReLU}(w_i^\top x + b_i).$$

Let a_i denote the weight between the ith neuron in the hidden layer and the output node. Then the output of the neural network is given by

$$f_\theta(x) = \sum_{i=1}^{n} a_i \cdot \mathrm{ReLU}(w_i^\top x + b_i).$$

Then the problem boils down to solving

$$\begin{aligned} \min_{x \in C} \quad & \sum_{i=1}^{n} a_i t_i \\ \text{s.t.} \quad & t_i = \mathrm{ReLU}(w_i^\top x + b_i), \quad i \in [n]. \end{aligned} \tag{11.1}$$

Recall that

$$\mathrm{ReLU}(x) = \begin{cases} x, & \text{if } x > 0, \\ 0, & \text{otherwise.} \end{cases}$$

Let ℓ_i and u_i denote the lower and upper bounds of $w_i^\top x + b_i$ over C given by

$$\ell_i = \inf_{x \in C} \left\{ w_i^\top x + b_i \right\}, \quad u_i = \sup_{x \in C} \left\{ w_i^\top x + b_i \right\}.$$

Then, we can argue that $t_i = \mathrm{ReLU}(w_i^\top x + b_i)$ holds if and only if t_i satisfies

$$\begin{aligned} & t_i \geq 0, \\ & t_i \geq w_i^\top x + b_i, \\ & t_i \leq u_i^\top z_i, \\ & t_i \leq w_i^\top x + b_i - \ell_i(1 - z_i), \end{aligned}$$

for some $z_i \in \{0,1\}$. Therefore, (11.1) can be formulated as

$$\begin{aligned} \min_{x \in C} \quad & \sum_{i=1}^{n} a_i t_i \\ \text{s.t.} \quad & t_i \geq 0, \quad i \in [n] \\ & t_i \geq w_i^\top x + b_i, \quad i \in [n] \\ & t_i \leq u_i^\top z_i, \quad i \in [n] \\ & t_i \leq w_i^\top x + b_i - \ell_i(1 - z_i), \quad i \in [n] \\ & z_i \in \{0,1\}, \quad i \in [n]. \end{aligned} \tag{11.2}$$

The formulation simply extends to the case of multiple hidden layers.

More recently, Anderson et al. [AHM+20] and Tsay et al. [TKTM21] developed computationally improved formulations for optimizing a trained feed-forward neural network with ReLU activation.

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