Optimization, Convexity, and Hyperplanes

We formulated the least squares method and linear regression as optimization problems. Our goal was to minimize the sum of the squared errors by choosing parameters for the linear model. Optimization problems have enormous utility in data science, and most model fitting techniques are cast as optimizations. In this chapter, we will develop a general framework for describing and solving several classes of optimization problems. We begin by reviewing the fundamentals of optimization. Next, we discuss convexity, a property that greatly simplifies the search for optimal solutions. Finally, we derive vector expressions for common geometric constructs and show how linear systems give rise to convex problems.

Optimization

Optimization is the process of minimizing or maximizing a function by selecting values for a set of variables or parameters (called decision variables). If we are free to choose any values for the decision variables, the optimization problem is unconstrained. If our solutions must obey a set of constraints, the problem is a constrained optimization. In constrained optimization, any set of values for the decision variables that satisfies the constraints is called a feasible solution. The goal of constrained optimization is to select the “best” feasible solution.

Optimization problems are formulated as either minimizations or maximizations. We don’t need to discuss minimization and maximization separately, since minimizing $f(x)$ is equivalent to maximizing $-f(x)$. Any algorithm for minimizing can be used for maximizing by multiplying the objective by $-1$, and vice versa. For the rest of this chapter, we’ll talk about minimizing functions. Keep in mind that everything we discuss can be applied to maximization problems by switching the sign of the objective.

During optimization we search for minima. A minimum can either be locally or globally minimal. A global minimum is has the
smallest objective value of any feasible solution. A local minimum has the smallest objective value for any of the feasible solutions in the surrounding area. The input to a function that yields the minimum is called the \textit{argmin}, since it is the argument to the function that gives the minimum. Similarly, the \textit{argmax} of a function is the input that gives the function’s maximum. Consider the function \( f(x) = 3 + (x - 2)^2 \). This function has a single minimum, \( f(2) = 3 \). The minimum is 3, while the \textit{argmin} is \( x = 2 \), the value of the decision variable at which the minimum occurs. For optimization problems, the minimum (or maximum) is called the \textit{optimal objective value}. The \textit{argmin} (or \textit{argmax}) is called the \textit{optimal solution}.

\textit{Unconstrained Optimization}

You already know how to solve unconstrained optimization problems in a single variable: set the derivative to the function equal to zero and solve. This method of solution relies on the observation that both maxima and minima occur when the slope of a function is zero. However, it is important to remember that not all roots of the derivative are maxima or minima. Inflection points (where the derivative changes sign) also have derivatives equal to zero. You must always remember to test the root of the derivative to see if you’ve found a minimum, maximum, or inflection point. The easiest test involves the sign of the second derivative. If the second derivative at the point is positive, you’ve found a minimum. If it’s negative, you’ve found a maximum. If the second derivative is zero, you’ve found an inflection point.

A similar approach works for optimizing multivariate functions. In this case one solves for points where the gradient is equal to zero, checking that you’ve not found an inflection point (called “saddle points” in higher dimensions).

\textit{Constrained Optimization}

Constrained optimization problems cannot be solved by finding roots of the derivatives of the objective. Why? It is possible that the minima or maxima of the unconstrained problem lie outside the feasible region of the constrained problem. Consider our previous example of \( f(x) = 3 + (x - 2)^2 \), which we know has an \textit{argmin} at \( x = 2 \). Say we want to solve the constrained problem

\[ \min f(x) = 3 + (x - 2)^2 \quad \text{s.t.} \quad x \leq 1 \]

The root of the derivative of \( f \) is still at \( x = 2 \), but values of \( x \) greater than one are not feasible. From the graph we can see that the minimum feasible value occurs at \( x = 1 \). The value of the derivative at \( x = 1 \) is \(-2\), not zero.
In general, constrained optimization is a challenging field. Finding global optima for constrained problems is an unsolved area or research, one which is beyond the scope of this course. However, there are classes of problems that we can solve to optimality using the tools of linear algebra. These problems form the basis of many advanced techniques in data science.

**Convexity**

Many “solvable” optimization problems rely on a property called *convexity*. Both sets and functions can be convex.

**Convex sets**

A set of points is *convex* if given any two points in the set, the line segment connecting these points lies entirely in the set. You can move from any point in the set to any other point in the set without leaving the set. Circles, spheres, and regular polygons are examples of convex sets.

To formally define convexity, we construct the line segment between any two points in the set.

**Definition.** A set $S$ is convex if and only if given any $x \in S$ and $y \in S$ the points $\lambda x + (1 - \lambda)y$ are also in $S$ for all scalars $\lambda \in [0, 1]$.

The expression $\lambda x + (1 - \lambda)y$ is called a *convex combination* of $x$ and $y$. A convex combination of two points contains all points on the line segment between the two points. To see why, consider the 1-dimensional line segment between points 3 and 4.

$$\lambda(3) + (1 - \lambda)(4) = 4 - \lambda, \quad \lambda \in [0, 1]$$

When $\lambda = 0$, the value of the combination is 4. As $\lambda$ moves from 0 to 1, the value of the combination moves from 4 to 3, covering all values in between.

Convex combinations work in higher dimensions as well. The convex combination of the vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is

$$\lambda \begin{pmatrix} 1 \\ 0 \end{pmatrix} + (1 - \lambda) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \lambda \\ 1 - \lambda \end{pmatrix}$$

The combination goes from the first point $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ when $\lambda = 0$ to the second point $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ when $\lambda = 1$. Halfway in between, $\lambda = 1/2$ and...
the combination is \( \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \), which is midway along the line connecting \( \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} 0 \\ 1 \end{pmatrix} \). Sometimes it is helpful to think of a convex combination as a weighted sum of \( x \) and \( y \). The weighting (provided by \( \lambda \)) moves the combination linearly from \( y \) to \( x \) as \( \lambda \) goes from 0 to 1.

**Convex functions**

There is a related definition for **convex functions**. This definition formalizes our visual idea of convexity (lines that curve upward) and concavity (lines that curve downward).

**Definition 1.** A function \( f \) is convex if and only if

\[
f(\lambda x + (1 - \lambda) y) \leq \lambda f(x) + (1 - \lambda) f(y), \quad \lambda \in [0, 1]
\]

This definition looks complicated, but the intuition is simple. If we plot a convex (upward curving) function, any chord – a segment drawn between two points on the line – should lie above the line. We can define the chord between any two points on the line, say \( f(x) \) and \( f(y) \) as a convex combination of these points, i.e. \( \lambda f(x) + (1 - \lambda) f(y) \). This is the right hand side of the above definition. For convex functions, we expect this chord to be greater than or equal to the function itself over the same interval. The interval is the segment from \( x \) to \( y \), or the convex combination \( \lambda x + (1 - \lambda) y \). The values of the function over this interval are therefore \( f(\lambda x + (1 - \lambda) y) \), which is the left hand side of the definition.

**Convexity in Optimization**

Why do we care about convexity? In general, finding local optima during optimization is easy; just pick a feasible point and move downward (during minimization) until you arrive at a local minimum. The truly hard part of optimization is finding global optima. How can you be assured that your local optimum is a global optimum unless you try out all points in the feasible space?

Fortunately, convexity solves the local vs. global challenge for many important problems, as we see with the following theorem.

**Theorem.** When minimizing a convex function over a convex set, all local minima are global minima.

Convex functions defined over convex sets must have a special shape where no strictly local minima exist. There can be multiple local minima, but all of these local minima must have the same value (which is the global minimum).
Let’s prove that all local minima are global minima when minimizing a convex function over a convex set.

**Proof.** Suppose the convex function $f$ has a local minimum at $x'$ that is not the global minimum (which is at $x^*$). By the convexity of $f$, 

$$f(\lambda x' + (1 - \lambda)x^*) \leq \lambda f(x') + (1 - \lambda)f(x^*)$$

Since $x'$ is at a local, but not global, minimum, we know that $f(x') > f(x^*)$. If we replace $f(x^*)$ on the right hand side by the larger quantity $f(x')$, the inequality ($\leq$) becomes a strict inequality ($<$). (Even if both sides were equal, adding a small amount to the right hand side would still make it larger.) We now have 

$$f(\lambda x' + (1 - \lambda)x^*) < \lambda f(x') + (1 - \lambda)f(x^*)$$

which, by simplifying the right hand side, becomes 

$$f(\lambda x' + (1 - \lambda)x^*) < f(x')$$

This statement says that the value of the function $f$ on any point on the line segment from $x'$ to $x^*$ is less than the value of the function at $x'$. If this is true, we can find a point arbitrarily close to $x'$ that is below our supposed local minimum $f(x')$. Clearly, $f(x')$ cannot be a local minimum if we can find a lower point arbitrarily closer to it. Our conclusion contradicts our original supposition. No local minimum can exist that are not equal to the global minimum.

The previous proof seemed to rely only on the convexity of the objective function, not on the convexity of the solution set. The role of convexity of the set is hidden. When we make an argument about a line drawn from the local to the global minimum, we assume that all the points on the line are feasible. Otherwise, it does not matter if they have a lower objective than the local minimum, since they would not be allowed. By assuming the solution set is convex, we are assured that any point on this line is also feasible.