The following presentation uses materials from Numerical analysis (9th Edn.) by Burden & Faires, Brooks/Cole, 2011.

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Fixed point iteration

The idea of the fixed-point iteration method is to:

(1) Reformulate an equation to an equivalent fixed-point problem

$$f(x) = 0 \leftrightarrow x = g(x)$$

(2) Use iteration, with a chosen initial guess x_0, to compute a sequence

$$x_{n+1} = g(x_n)\big(= g^{n+1}(x_0)\big), \quad n = 0, 1, 2, \ldots$$

in hope that $x_n \to \alpha$ (the root of the non-linear equation).

There are numerous ways to introduce an equivalent fixed-point problem for a given equation. But convergence to α is not guaranteed, not to mention rapid convergence.

Lemma: Let $g(x)$ be a continuous function on the interval $[a, b]$, and suppose it satisfies the property

$$a \leq x \leq b \to a \leq g(x) \leq b$$

Then the equation $x = g(x)$ has at least on solution in the interval $[a, b]$.

Theorem: Assume $g(x)$ and $g'(x)$ exist and are continuous on the interval $[a, b]$; and further, assume

$$a \leq x \leq b \to a \leq g(x) \leq b$$

$$\lambda = \max_{a \leq x \leq b} |g'(x)| < 1$$

Then,

$\boldsymbol{Conclusion\ 1}$ (existence and uniqueness) The equation $x = g(x)$ has a unique solution α in $[a, b]$.

$\boldsymbol{Conclusion\ 2}$ (convergence) For any initial guess x_0 in $[a;\ b]$, in the iteration

$$x_{n+1} = g(x_n), n = 0, 1, 2, \ldots$$

Will converge to α.

$\boldsymbol{Conclusion\ 3}$ (error bound estimate)

$$|x_n - \alpha| \leq \frac{\lambda^n}{1 - \lambda} |x_1 - x_0|, \quad n > 0$$

$\boldsymbol{Conclusion\ 4}$

$$\lim_{n\to\infty} \frac{x_{n+1} - \alpha}{x_n - \alpha} = g'(\alpha)$$

Thus, for any x_n close to α, $x_{n+1} - \alpha \approx g'(\alpha)(x_n - \alpha)$

When converging near the root α, the errors will decrease by a constant factor of $g'(\alpha)$. If $g'(\alpha)$ is negative, then the errors will oscillate between positive and negative, and the iterates will be approaching from both sides. When $g'(\alpha)$ is positive, the iterates will approach α from only one side.

When $|g'(\alpha)| > 1$, the errors will increase as we approach the root rather than decrease in size.

Let's look at two examples:

Example 1

$x = \sin(0.9 - 0.7x) = g(x)$ which has a root of $\alpha = 0.514192160$

$g(\alpha) = \sin(0.9 - 0.7\alpha) = \alpha$ verified!

$g'(\alpha) = -0.7\cos(0.9 - 0.7\alpha) = -0.600372506$

$\therefore\ converge$ (absolute value less than 1)

Example 2

$x = \sin(2.5 + 1.3x) = g(x)$ which has a root of $\alpha = 0.277371219$

$g(\alpha) = \sin(2.5 + 1.3\alpha) = \alpha$ verified!

$g'(\alpha) = (1.3)\cos(2.5 + 1.3\alpha) = -1.24899179$

$\therefore\ diverge$ (absolute value greater than 1)

But the challenge remains that the interval $[a, b]$ may not be easily identified. This leads to the **localized fixed-point theorem** as follows:

Assume $x = g(x)$ has a solution α, both $g(x)$ and $g'(x)$ are continuous for all x In some interval about α, and $|g'(\alpha)| < 1$. Then for any sufficiently small number $\epsilon > 0$, the interval $[a, b] = [\alpha - \epsilon,\ \alpha + \epsilon]$ will satisfy the hypotheses of the fixed-point theorem. If we choose x_0 sufficiently close to α, then the fixed-point iteration $x_{n+1} = g(x),\ n = 0, 1, 2, \ldots$ will converge.

Example 3

The equation $f(x) = x^3 + 4x^2 - 10 = 0$ has a root of $\alpha = 1.36523001$.

Choices of $g(x)$ are:

$$g_1(x) = x - x^3 - 4x^2 + 10$$
$$g_2(x) = \frac{1}{2}\sqrt{10 - x^3}$$
$$g_3(x) = x - \frac{x^3 + 4x^2 - 10}{3x^2 + 8x}$$

Stopping/termination criterion is $|x_n - x_{n+1}| < 10^{-6}$. Use the fixed-point iteration method to find α.

- We should check which one has $g(\alpha) = \alpha$.

Solution

First off, $g_1(x)$ will not converge. So, use $g_2(x)$ and $g_3(x)$ only.

absolute error

$x_0 = 1;$

$g(x)$	# of iterations	x_n	$\lvert x_n - x_{n-1} \rvert$
$g_2(x)$	21	1.36523004	$6.57824 \cdot 10^{-7}$
$g_3(x)$	5	1.36523001	$2.12699 \cdot 10^{-11}$

$x_0 = 1.3;$

$g(x)$	# of iterations	x_n	$\lvert x_n - x_{n-1} \rvert$
$g_2(x)$	19	1.36523020	$5.52801 \cdot 10^{-7}$
$g_3(x)$	4	1.36523001	$2.70561 \cdot 10^{-12}$

It is seen that $g_3(x)$ outperforms $g_2(x)$.

It turns out that $g_3(x)$ represents the Newton's method or the Newton-Rhapson method, where $g(x)$ is

$$g(x) = x - \frac{f(x)}{f'(x)}$$

Newton's method has a quadratic convergence rate as long as x_0 is sufficiently close to α. The rate of convergence depends on the choice of x_0.

Another drawback is requiring $f'(x)$. The secant method uses finite difference to approximate the derivative. The rate of convergence of the secant method is, 1.618, as long as the initial points are sufficiently close to α.

The following presentation is based on https://neos-guide.org/, and "Numerical Methods for Engineers" (8th Edn.), Chapra and Canale, McGraw-Hill, 2021.

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Part 4: Optimization (I)

In mathematical terms, an ***optimization problem*** is the problem of finding the *best* solution from the set of all *feasible* solutions.

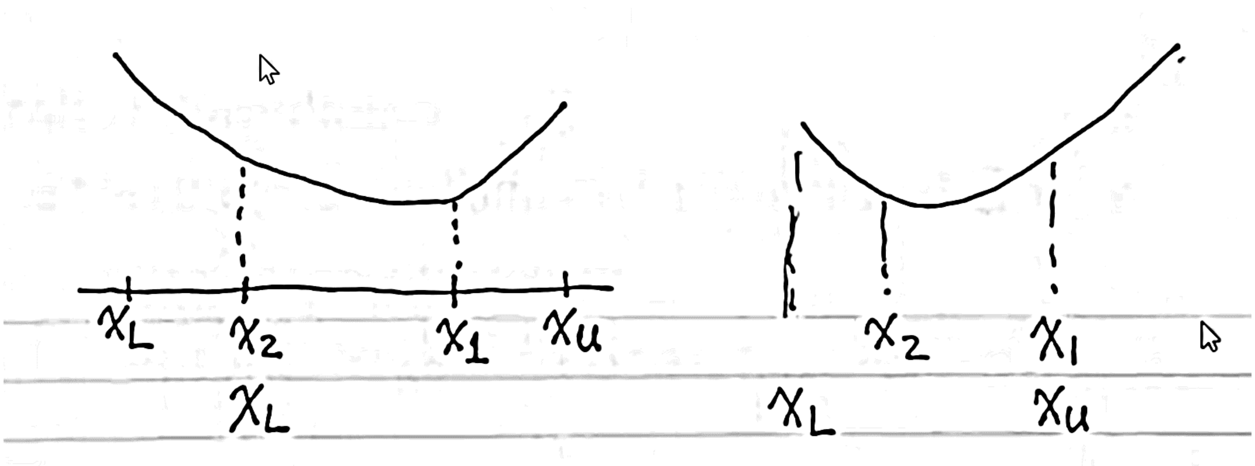
Formulating an optimization problem

The mathematical statement is as follows:

Let $f(\boldsymbol{x})$ be a continuous real-values function, the optimization problem is stated as:

$$\begin{aligned} &\min_{x} f(\boldsymbol{x}) && ; \quad for\ \boldsymbol{x} \in \boldsymbol{R^n} \\ &Subject\ to\ F_j(\boldsymbol{x}) = a_j && ; \quad j = 1, 2, \ldots, m_1 \\ &G_k(\boldsymbol{x}) \le b_k && ; \quad k = 1, 2, \ldots, m_2 \\ &and\ \boldsymbol{U_L} \le \boldsymbol{x} \le \boldsymbol{U_P} && \end{aligned}$$

which involves, the **objective** f($\boldsymbol{x}$), the **variables** $\boldsymbol{x}$, the **constraints** $F_j(\boldsymbol{x})$ and $G_k(\boldsymbol{x})$ of the problem, and the lower limit $\boldsymbol{U_L}$ and upper limit $\boldsymbol{U_p}$ on $\boldsymbol{x}$.



- An objective is a quantitative measure of the performance of the system that we want to minimize or maximize. For example, in manufacturing we may want to maximize the profits or minimize the cost of production; in fitting experimental data to the model, we may want to minimize the sum of squares of errors between the observed data and the predicted data.

- The *variables* or the *unknowns* are the components of the system for which we want to find values. For the manufacturing example, the variables may be the amount of each resource consumed or the time spent on each activity, whereas in data fitting, the variables may be the parameters of the model.

- The *constraints* are the functions that describe the relationships among the variables and that define the allowable values for the variables. For example, the manufacturing example, the amount of a resource consumed cannot exceed the available amount. Another example us, if a variable represents the number of people assigned to a specific task, the variable must be a positive integer.

Types of Optimization Problems

- ***Continuous Optimization*** versus ***Discrete Optimization***

Optimization problems with *discrete variables* are discrete optimization problems: on the other hand, problems with continuous variables are *continuous optimization* problems.

Continuous optimization problems tend to be easier to solve than discrete optimization problems.

However, recent improvements in algorithms coupled with advancements in computing technology have dramatically increased the size and complexity of discrete optimization problems that can be solved efficiently.

- ***Unconstrained Optimization*** versus ***Constrained Optimization***

Unconstrained optimization is one in which there are *no constraints* on the variables; optimization in which there are constraints on the variables is known as constrained optimization.

Both types arise directly from practical applications. Algorithm-wise, constrained optimization can be reformulated to become and unconstrained one.

The constraints on the variables can be from simple bounds, to systems of equalities and inequalities that model complex relationships of the variables.

- ***None, One or Many Objectives***

Most optimization problems have a single objective function. However, there are cases when optimization problems have no objective function or have multiple objective functions.

Feasibility problems are problems in which the goal is to find values for the variables that satisfy the constraints of a system with no objective to optimize.

Multi-objective optimization problems arise in many fields, such as engineering, economics, and logistics, when optimal decisions need to be taken I the presence of trade-offs between two or more conflicting objectives. For example, developing a new component might involve minimizing weight while maximizing strength.

In practice, problems with multiple objectives often are reformulated as single objective problems by either forming a weighted combination of the different objectives or by replacing some of the objectives by constraints.

- ***Deterministic Optimization*** versus ***Stochastic Optimization***

Deterministic optimization is optimization under certainty. It is assumed that the data for the given problem are known accurately.

Stochastic optimization is optimization under uncertainty.

- ***Local Optimization*** versus ***Global Optimization***

Local optimization seeks the optimal solution over a small neighborhood where the derivative of the objective is zero (or near zero).

Global optimization finds the smallest objective value over all feasible variables.

Note that each category of optimization problems has specifically developed algorithms so that the optimization can be done effectively.

Also note that the above classifications are not mutually exclusive. For example, a multi-objective optimization problem can be continuous and unconstrained.

Part 4: Optimization (II)

One-dimensional unconstrained optimization means, in mathematical terms,

$$\min_x f(x) \quad ; \quad for\ x \in (-\infty, \infty)$$

Where $f(x)$ is a continuous real-valued function.

Methods include:

- Golden-section search;
- Quadratic interpolation; and
- Newton's method.

One-dimensional unconstrained optimization is important in its own right, not to mention it is the foundation for multi-dimensional unconstrained optimization.

Golden-section Search

The method is similar to the bisection method in Part 3. It is simple to use.

Assume that there is a minimum in the interval $[x_L, x_U]$.

Step 1: Let $\ell_0 = x_U - x_L$.

Step 2: Two intermediate points are needed.

$$x_1 = x_L + d$$
$$x_2 = x_U - d$$
$$\text{with } d = (\sqrt{5} - 1)/2 \cdot \ell_0 = 0.618 \cdot \ell_0.$$

Step 3a: If $f(x_1) \geq f(x_2)$, $x_U \leftarrow x_1$, go back to Step 1 until $|x_2 - x_1|$ or $|f(x_2) - f(x_1)|$ is very small;

Step 3b: If $f(x_1) < f(x_2)$, $x_L \leftarrow x_2$, go back to Step 1 until $|x_2 - x_1|$ or $|f(x_2) - f(x_1)|$ is very small;

Quadratic Interpolation

Assume that there is a minimum in the interval $[x_L, x_U] = [x_0, x_2]$.

Step 1: One intermediate point is needed; $x_0 < x_1 < x_2$.

Step 2: A parabola is fitted onto the three points. Take the derivative of the parabolics function. The derivative is zero at x_3.

$$x_3 = \frac{1}{2} \frac{f_0(x_1^2 - x_2^2) + f_1(x_2^2 - x_0^2) + f_2(x_0^2 - x_1^2)}{f_0(x_1 - x_2) + f_1(x_2 - x_0) + f_2(x_0 - x_1)}$$

Where $f_i = f(x_i)$.

Step 3a: Drop x_0 is $f(x_0) \geq f(x_2)$, $x_0 \leftarrow x_1$ or x_3, $x_1 \leftarrow x_3$ or x_1, go back to Step 2 until $|x_3 - x_1|$ or $|f(x_3) - f(x_1)|$ is very small.

Step 3b: Drop x_2 is $f(x_0) < f(x_2)$, $x_2 \leftarrow x_1$ or x_3, $x_1 \leftarrow x_3$ or x_1, go back to Step 2 until $|x_3 - x_1|$ or $|f(x_3) - f(x_1)|$ is very small.