Hayato Fukuba (1856–1921) is one of the most important figures in the history of Shinjuku Gyoen. The father of modern horticulture in Japan, after studying agricultural chemistry, he entered the Ministry of the Interior in 1877.

In 1886 he traveled to France and Germany to study grape cultivation and brewing and brought back samples of grapes and other specimens. He was the first person in Japan to grow many fruits and vegetables not native to Japan in an unheated greenhouse. His extensive cross-breeding led to the creation of many new strains, such as the eponymous Fukuba Strawberry. In 1891 he was appointed as a technical expert to the Imperial Estates, from which time his connection with Shinjuku Gyoen began. He published an encyclopedia about vegetable cultivation in 1893.

In 1898 Fukuba was appointed to head what was then the Shinjuku Imperial Botanical Garden, and began work on implementing plans for a large-scale development of what is today's Shinjuku Gyoen.

In 1900 Fukuba traveled to Paris for the Exposition Universelle (World's Fair), where he displayed five large Japanese chrysanthemums to wide acclaim. In Paris he met with Professor Henri Martine, a noted professor from the Versailles horticultural school, and he asked Professor Martine to prepare designs for the Shinjuku Imperial Botanical Garden. After five years, the garden, now renamed the Shinjuku Gyoen National Garden, was completed in 1906 based on Martine's designs, and Emperor Meiji (1852–1912) attended the opening ceremony.

Professor Martine's original plans for the garden were destroyed, along with much of the garden itself, during the firebombing of 1945. The only remaining document of the original design is a "bird's-eye view" of the new garden, drawn by Professor Martine himself. After the war, Shinjuku Gyoen was rebuilt relying heavily on Martine's drawing, and the present Shinjuku Gyoen is a very close representation of that design.