Least-Squares Problems and Best-Fit Lines

Linear Algebra

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https://github.com/CU-Denver-MathStats-OER

Inconsistent Linear Systems

Consider solving $A\mathbf{x} = \mathbf{b}$.

- If the system is consistent, then $\mathbf{b}$ is in Col A.
- If the system is inconsistent, then $\mathbf{b}$ is not in Col A.

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As a consolation prize, let's find $\hat{\mathbf{x}}$ such that $A\hat{\mathbf{x}}$ is the closest vector in Col A to $\mathbf{b}$; that is,

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\| \text{ for all } \mathbf{x} \text{ in } \mathbb{R}^n.$$

Such a sol'n $\hat{\mathbf{x}}$ is called a least-squares solution since $\hat{\mathbf{x}}$ minimizes $\|\mathbf{b} - A\mathbf{x}\| = \|\mathbf{z}\| = \sqrt{\sum \mathbf{z}_i^2}$.

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Let $\hat{\mathbf{b}} = \text{proj}_{\text{Col } A}\mathbf{b}$. Then $\hat{\mathbf{b}}$ is the closest vector in Col A to $\mathbf{b}$, and $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$ is consistent.

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We know how to do each of these steps:

- Compute $\hat{\mathbf{b}} = \text{proj}_{\text{Col } A}\mathbf{b}$. (How?)
- Solve $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

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We know how to do each of these steps:

- Compute $\hat{\mathbf{b}} = \text{proj}_{\text{Col } A}\mathbf{b}$. (How?)
- Solve $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.

But there is a simpler way!

Least-Squares Solutions

We wish to find least-squares solutions $\hat{\mathbf{x}}$ to $A\mathbf{x} = \mathbf{b}$.

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By the Orthogonal Decomposition Theorem, $\mathbf{z} = \mathbf{b} - \hat{\mathbf{b}}$ is orthogonal to Col A.
Thus, $\mathbf{z} = \mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to each column $\mathbf{a}_j$ of the matrix A.

$$\mathbf{a}_j \cdot (\mathbf{b} - A\hat{\mathbf{x}}) = 0 \text{ for each } j.$$
$$\mathbf{a}_j^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \text{ for each } j.$$

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Rearranging, we have that $(A^T A)\hat{\mathbf{x}} = A^T\mathbf{b}$. These are called the normal equations.

Theorem

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ is given by the solutions of the normal equations.

Example

Find the least-squares solutions of $A\mathbf{x} = \mathbf{b}$, where $A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$.

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Notice that $\left[\begin{array}{cc|c} 4 & 0 & 2 \\ 0 & 2 & 0 \\ 1 & 1 & 11 \end{array}\right] \xrightarrow{\text{RREF}} \left[\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & {\color{red}1} \end{array}\right]$. Hence the system is inconsistent.

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We solve the normal equations:

$$A^T A\mathbf{x} = A^T\mathbf{b}.$$

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}\mathbf{x} = \begin{bmatrix} 19 \\ 11 \end{bmatrix} \qquad \text{one sol: } \hat{\mathbf{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

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Compare:

$$\text{G–S: } \left\{ \begin{bmatrix} 4 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -4/17 \\ 2 \\ 16/17 \end{bmatrix} \right\}, \qquad \hat{\mathbf{b}} = \text{proj}_{\text{Span}\{\mathbf{v}_1,\mathbf{v}_2\}}\mathbf{b} = \left(\frac{\mathbf{b}\cdot\mathbf{v}_1}{\mathbf{v}_1\cdot\mathbf{v}_1}\right)\mathbf{v}_1 + \left(\frac{\mathbf{b}\cdot\mathbf{v}_2}{\mathbf{v}_2\cdot\mathbf{v}_2}\right)\mathbf{v}_2 = \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix} = A\hat{\mathbf{x}}.$$

Unique solution to the Least-Squares Problem

Theorem

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Theorem

Let A be an $m \times n$ matrix. The following statements are logically equivalent:

(a) The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each $\mathbf{b}$ in $\mathbb{R}^m$.

(b) The columns of A are linearly independent.

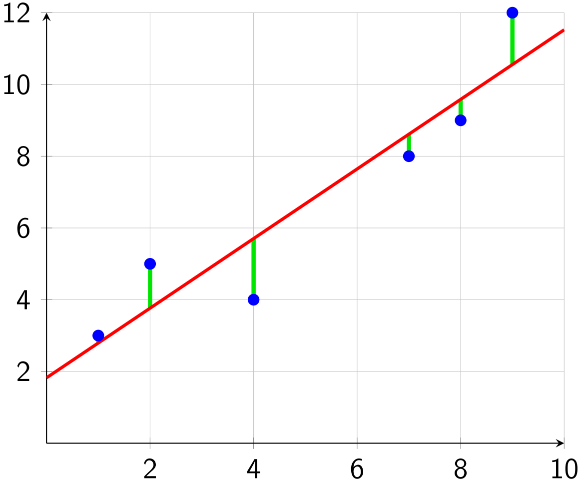
(c) The matrix $A^T A$ is invertible.

When these statements are satisfied, the least-squares solution $\hat{\mathbf{x}}$ is given by

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T\mathbf{b}.$$

Best-Fit Line

Suppose we have n data points $(x_1, y_1), \ldots, (x_n, y_n)$. What is the line that best fits this data?



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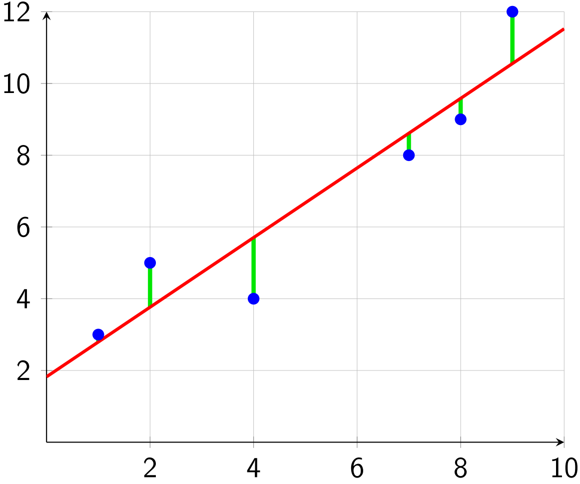

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Which line best fits the data?

We want to minimize the sum of squares

$$\sqrt{\sum_{i=1}^{n} \Big(y_i - (\beta_0 + \beta_1 x_i) \Big)^2}.$$

$y_i - (\beta_0 + \beta_1 x_i)$ is called the residual.

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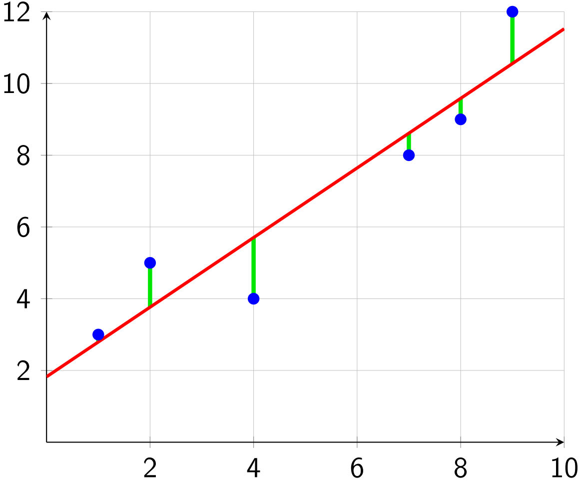

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Can we formulate as a least-squares problem?

Yes!

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We would like to solve:

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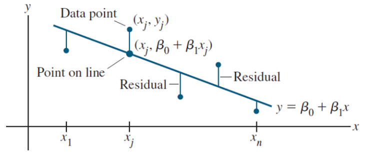

FIGURE 1 Fitting a line to experimental data.

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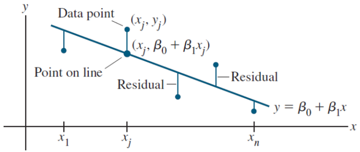
As a matrix equation:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

$$\mathbf{y} = A\boldsymbol{\beta}$$



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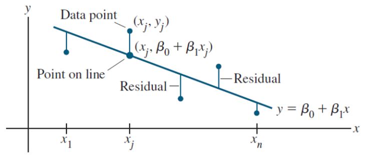


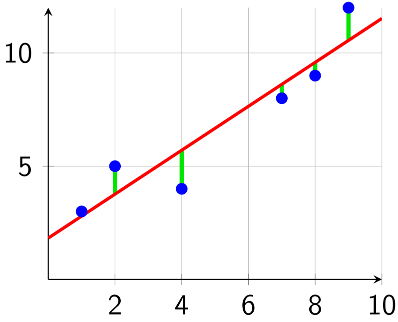
FIGURE 1 Fitting a line to experimental data.

- A is called the model matrix (or design matrix).
- $\mathbf{y}$ is the vector of observed responses.
- $\boldsymbol{\beta}$ is the vector of regression coefficients.

Computing the least-squares solution of $\mathbf{y} = A\boldsymbol{\beta}$ is equivalent to finding values for the regression coefficients β_0 and β_1 that minimize the sum of square residuals.

Example

Suppose we have data $(1,3),(2,5),(4,4),(7,8),(8,9),(9,12)$. What is the best-fit line?



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$$\begin{bmatrix} 3 \\ 5 \\ 4 \\ 8 \\ 9 \\ 12 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 7 \\ 1 & 8 \\ 1 & 9 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}.$$

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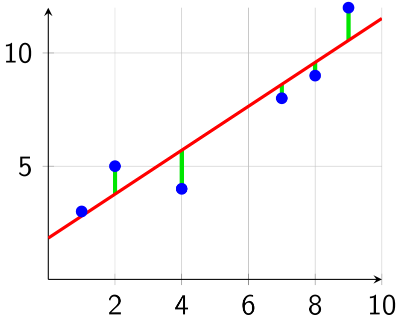

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We solve the normal equations by computing

$$\boldsymbol{\beta} = (A^T A)^{-1} A^T \mathbf{y} = \begin{bmatrix} 1.824 \\ 0.970 \end{bmatrix}.$$

So $y = 1.824 + 0.970x$ is the best-fit line.

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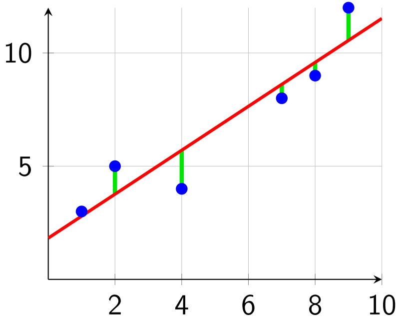

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We can quantify the error by $\mathbf{y} = A\boldsymbol{\beta} + \boldsymbol{\varepsilon} = \hat{\mathbf{y}} + \mathbf{z}$, $\|\mathbf{z}\| \approx 2.699$.

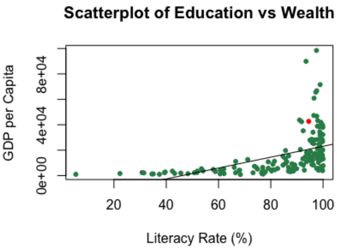
Predicting Wealth Based on Literacy Rate

Data scientists often begin with a simple model, and then determine whether predictions increase when new predictors are added. Let's first consider the following potential relationship:

- Let y denote the Gross Domestic Product (GDP) per capita of a country (in thousands of dollars).
- Let x_1 denote the literacy rate of the country's population (as a percentage).
- We collect a dataset that consists of n observations.
- Based on our data, what is the best model of the form $y = \beta_0 + \beta_1 x_1$?

$$
\begin{aligned}
2.079 &= \beta_0 + \beta_1(31.4) \\
13.440 &= \beta_0 + \beta_1(98.1) \\
11.324 &= \beta_0 + \beta_1(81.4) \\
&\vdots \\
3.537 &= \beta_0 + \beta_1(88.7)
\end{aligned}
$$

$$
\begin{bmatrix} 2.07 \\ 13.44 \\ 11.324 \\ \vdots \\ 3.537 \end{bmatrix} = \begin{bmatrix} 1 & 31.4 \\ 1 & 98.1 \\ 1 & 81.4 \\ \vdots & \vdots \\ 1 & 88.7 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}
$$



Interpreting the Results

Let's imagine that we randomly select four countries record the most recent data for each country's GDP per capita and literacy rate. $\widehat{\texttt{Wealth}} = -1.938 + 0.126(\texttt{Education})$

$$A = \begin{bmatrix} 1 & 31 \\ 1 & 98 \\ 1 & 81 \\ 1 & 89 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} 2 \\ 13 \\ 11 \\ 4 \end{bmatrix}$$

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For the least-squares solution to $A\boldsymbol{\beta} = \mathbf{y}$, we solve the normal equations $A^T A\boldsymbol{\beta} = A^T\mathbf{y}$:

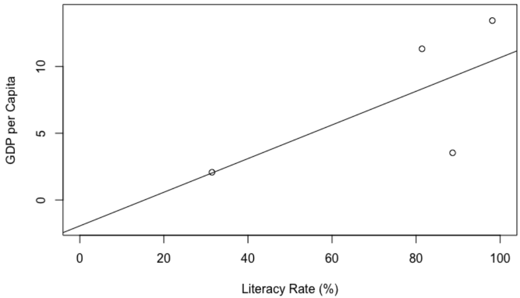
$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \left(\begin{bmatrix} 4 & 299 \\ 299 & 25{,}047 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 31 & 98 & 81 & 89 \end{bmatrix} \begin{bmatrix} 2 \\ 13 \\ 11 \\ 4 \end{bmatrix} \approx \begin{bmatrix} -1.938 \\ 0.126 \end{bmatrix}$$

Fitting a Model for Predicting Wealth of a Nation

Let's imagine that we randomly select four countries record the most recent data for each country's GDP per capita and literacy rate.

$\widehat{\texttt{Wealth}} = -1.938 + 0.126(\texttt{Education})$

1. The literacy rate in the United States in 2021 is approximately 80%. Based on our model predict the GDP per capita of the US? (Note the actual value is \$69,734.)
2. Interpret the practical meaning of the slope and vertical intercept of the linear model.



Multiple Regression

We can include other factors and also fit them.

Wealth	Literacy	Life Exp	Area
2	31	65	653
13	98	79	27
11	81	77	2381
4	89	61	387

$$A = \begin{bmatrix} 1 & 31 & 65 & 653 \\ 1 & 98 & 79 & 27 \\ 1 & 81 & 77 & 2381 \\ 1 & 89 & 61 & 387 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 2 \\ 13 \\ 11 \\ 4 \end{bmatrix}.$$

We wish to find the regression coefficients $\beta_0, \beta_1, \beta_2$, and β_3 that will give us the best fitting model of the form

$$\texttt{wealth} = \beta_0 + \beta_1(\texttt{Literacy}) + \beta_2(\texttt{LifeExp}) + \beta_3(\texttt{Area}) + \epsilon.$$

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Solving the normal equations, we obtain

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = (X^T X)^{-1} X^T \mathbf{y} \approx \begin{bmatrix} -30.458 \\ 0.067 \\ 0.467 \\ 0.00003 \end{bmatrix}$$

$$\widehat{\texttt{wealth}} = -30.458 + 0.067(\texttt{Literacy}) + 0.467(\texttt{LifeExp}) + 0.00003(\texttt{Area})$$

Fitting Other Models

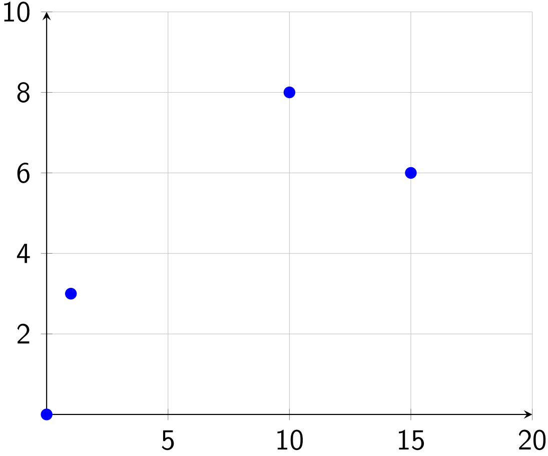
We call any model which is linear in the coefficients β's a linear model.

For example:

- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ includes two factors.
- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$ includes an interaction term.
- $y = \beta_0 + \beta_1 x + \beta_2 x^2$ is a linear model that includes a second-order term.

Fitting a Quadratic Polynomial

Consider a ball thrown from $(0, 0)$. The height is measured at the following distances: $(1, 3), (10, 8), (15, 6)$. Where do we predict the ball will hit the ground?



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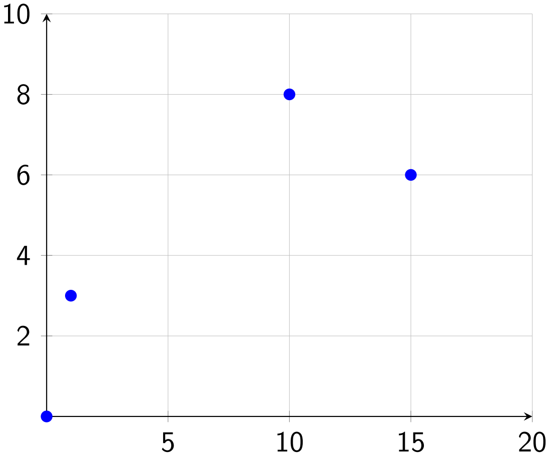

We use a model of $y = \beta_0 + \beta_1 x + \beta_2 x^2$.

$$\begin{bmatrix} 0 \\ 3 \\ 8 \\ 6 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0^2 \\ 1 & 1 & 1^2 \\ 1 & 10 & 10^2 \\ 1 & 15 & 15^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}.$$

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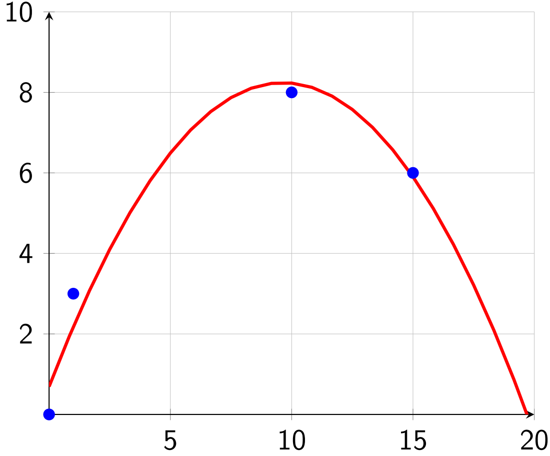

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We solve the normal equations by computing

$$\boldsymbol{\beta} = (A^T A)^{-1} A^T \mathbf{y} = \begin{bmatrix} 0.691 \\ 1.567 \\ -0.0813 \end{bmatrix}.$$

So $y = 0.691 + 1.567x - 0.0813x^2$ is the best fit.

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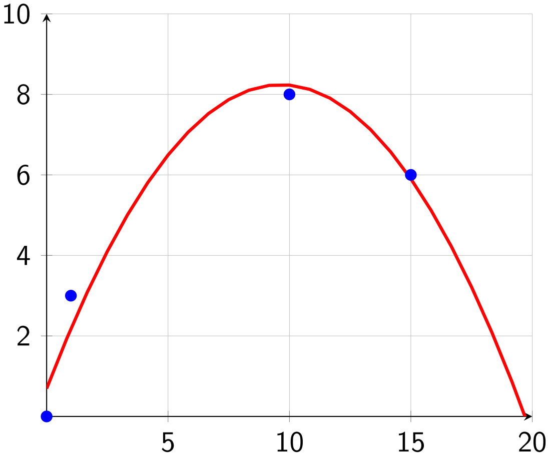

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Using the quadratic formula, height $= 0$ at 19.703.