

## 8. Probabilistic Analysis of Theoretical Linear Regression

**Note:** The following problems are presented as a derivation in the video that follows. We encourage you to attempt them before watching the video.

### Derivation of Theoretical Linear Least Squares Regression I

2/2 points (graded)

Normally, we should be thinking of linear regression being performed on a data set  $\{(x_i, y_i)\}_{i=1}^n$ , which we think of as a **deterministic collection of points in the Euclidean space**. It is helpful to also consider an idealized scenario, where we assume that  $\mathbf{X}$  and  $\mathbf{Y}$  are random variables that follow some joint probability distribution and they have finite first and second moments. In this problem, we will derive the solution to the **theoretical linear regression** problem.

Assume  $\text{Var}(\mathbf{X}) \neq 0$ . The **theoretical linear (least squares) regression of  $\mathbf{Y}$  on  $\mathbf{X}$**  prescribes that we find a pair of real numbers  $\mathbf{a}$  and  $\mathbf{b}$  that minimize  $\mathbb{E}[(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})^2]$  over all possible choices of the pair  $(\mathbf{a}, \mathbf{b})$ .

To do so, we will use a classical calculus technique. Let  $f(\mathbf{a}, \mathbf{b}) = \mathbb{E}[(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})^2]$ , and now we solve for the critical points where the gradient is zero.

*Hint: Here, assume you can switch expectation and differentiation with respect to  $\mathbf{a}$  and  $\mathbf{b}$ . That is,  $\partial_{\mathbf{a}} \mathbb{E}[(\dots)] = \mathbb{E}[\partial_{\mathbf{a}} (\dots)]$ .*

Use  $\mathbf{X}$  and  $\mathbf{Y}$  for random variables  $\mathbf{X}$  and  $\mathbf{Y}$ .

The partial derivatives are:

$$\partial_{\mathbf{a}} f = \mathbb{E} \left[ \boxed{-2(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})} \right] \quad \checkmark \text{ Answer: } -2\mathbf{Y} + 2\mathbf{a} + 2\mathbf{b}\mathbf{X}$$

$$\partial_{\mathbf{b}} f = \mathbb{E} \left[ \boxed{-2\mathbf{X}(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})} \right] \quad \checkmark \text{ Answer: } -2\mathbf{X}\mathbf{Y} + 2\mathbf{a}\mathbf{X} + 2\mathbf{b}\mathbf{X}^2$$

STANDARD NOTATION

**Solution:**

As suggested, it's easier to take the derivative inside the expectation. **Such a step is valid, since the expectation is an integral with respect to  $x$  and  $y$ , while the derivatives are taken with respect to  $a$  and  $b$ .** In fact, keep in mind that we are differentiating with respect to  $\mathbf{a}$  and  $\mathbf{b}$ , so  $\mathbf{X}$  and  $\mathbf{Y}$  should be treated as constants. Using the **chain rule**, we obtain

$$\partial_{\mathbf{a}} f = \mathbb{E}[-2(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})] = \mathbb{E}[-2\mathbf{Y} + 2\mathbf{a} + 2\mathbf{b}\mathbf{X}]$$

$$\partial_{\mathbf{b}} f = \mathbb{E}[-2\mathbf{X}(\mathbf{Y} - \mathbf{a} - \mathbf{b}\mathbf{X})] = \mathbb{E}[-2\mathbf{X}\mathbf{Y} + 2\mathbf{a}\mathbf{X} + 2\mathbf{b}\mathbf{X}^2].$$

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You have used 2 of 2 attempts

**i** Answers are displayed within the problem

### Derivation of Theoretical Linear Least Squares Regression II

1/1 point (graded)

Setting these equal to zero and isolating terms with  $\mathbf{a}$  and  $\mathbf{b}$  to one side, we obtain a system of linear equations

$$\begin{aligned}\mathbb{E}[Y] &= a + \mathbb{E}[X] b \\ \mathbb{E}[XY] &= \mathbb{E}[X] a + \mathbb{E}[X^2] b\end{aligned}$$

Multiplying the first equation by  $\mathbb{E}[X]$  and subtracting from the second equation gives

$$(\mathbb{E}[X^2] - \mathbb{E}[X]^2) b = \mathbb{E}[XY] - \mathbb{E}[X] \mathbb{E}[Y] \implies b = \frac{\text{Cov}(X, Y)}{\text{Var}(X)}$$

Plugging this value back into the first equation to solve for  $a$  gives

$$a = \mathbb{E}[Y] - \frac{\text{Cov}(X, Y)}{\text{Var}(X)} \mathbb{E}[X]$$

We now compute the Hessian

$$H = \begin{pmatrix} f_{aa} & f_{ab} \\ f_{ba} & f_{bb} \end{pmatrix}$$

to make sure that this pair  $(a, b)$  critical point is a local minimum. The determinant of  $H$  at this value  $(a, b)$  is

☐  $-\text{Var}(X)$

☒  $4\text{Var}(X)$  ✓

☐  $\mathbb{E}[X]$

☐  $\text{Cov}(X, Y)$

**Solution:**

The second derivatives can be evaluated using the answers from the first problem, which were:

$$\partial_a f = \mathbb{E}[-2Y + 2a + 2bX], \quad \partial_b f = \mathbb{E}[-2XY + 2aX + 2bX^2].$$

We demonstrate how to compute  $\partial_{aa} f$  as follows:

$$\begin{aligned}\partial_{aa} f &= \partial_a (\partial_a f) \\ &= \mathbb{E}[\partial_a (-2Y + 2a + 2bX)] \\ &= \mathbb{E}[2] = 2.\end{aligned}$$

Similarly, the Hessian evaluates to the matrix

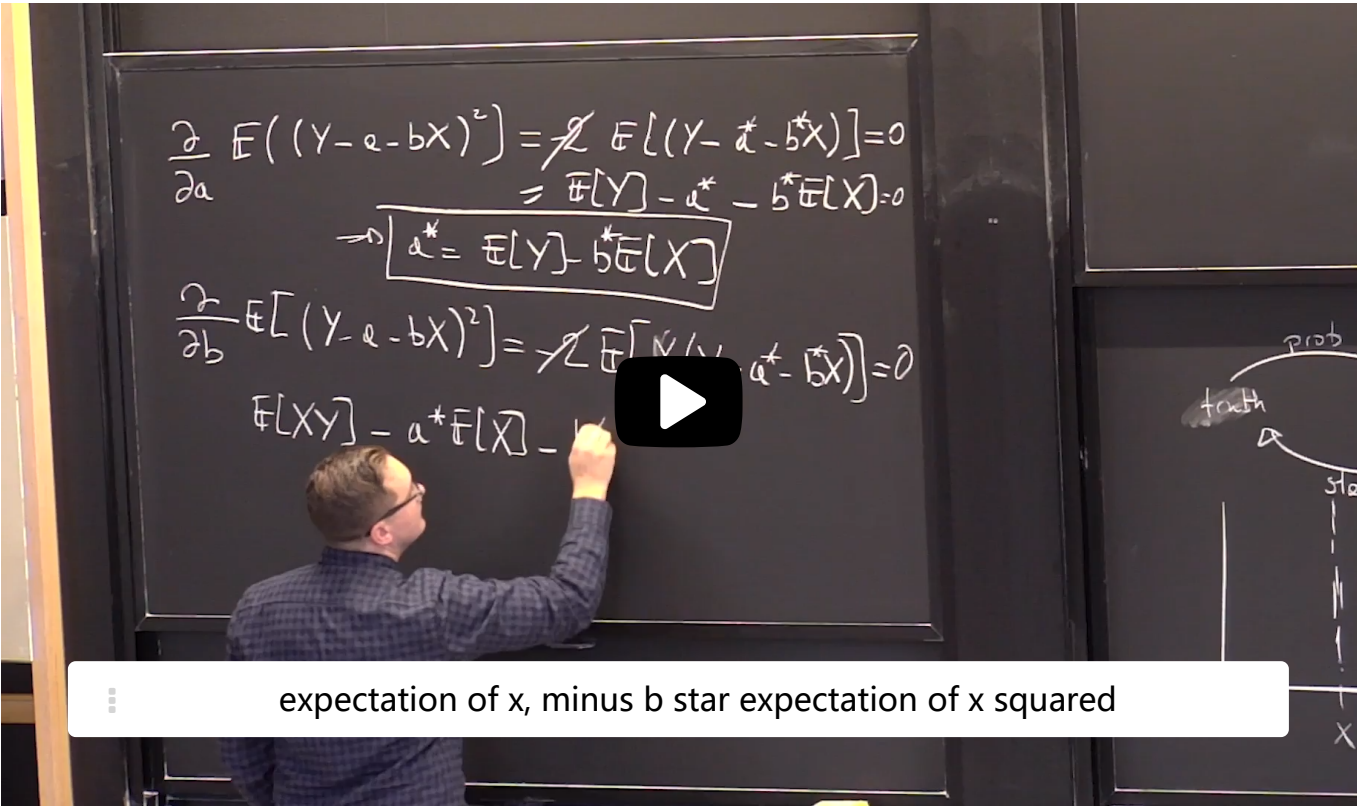
$$H = \begin{pmatrix} 2 & 2\mathbb{E}[X] \\ 2\mathbb{E}[X] & 2\mathbb{E}[X^2] \end{pmatrix}$$

which has determinant  $4\mathbb{E}[X^2] - 4\mathbb{E}[X]^2 = 4\text{Var}(X)$ , independent of the value of  $a$  and  $b$ , and is always positive. This justifies the positive-definiteness of the Hessian everywhere, which means that  $f$  is strictly convex. Therefore,  $(a, b)$  is the global minimizer of  $f$ .

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Optimal Theoretical Regression Line



expectation of x, minus b star expectation of x squared

▶ 5:43 / 9:29

▶ 1.0x 🔊 ⌂ ⌂ ⌂ ⌂

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and so it says the expectation of xy minus a star expectation of x, minus b star expectation of x squared is equal to 0.

So now I have to solve for those two guys-- so I'm just going to plug in my a star equal to this expectation, OK?

So that tells me the expectation of xy is equal to expectation--

sorry, minus expectation of x expectation of y.

So I'm just replacing here by expectation of y, and then I have plus b star expectation of x, and there's two of them, and one that's coming from this guy, and one that's coming from that guy-- minus b star expectation of x squared equals 0.

Now you can start seeing that there's things

Theoretical Linear Regression Visualized I

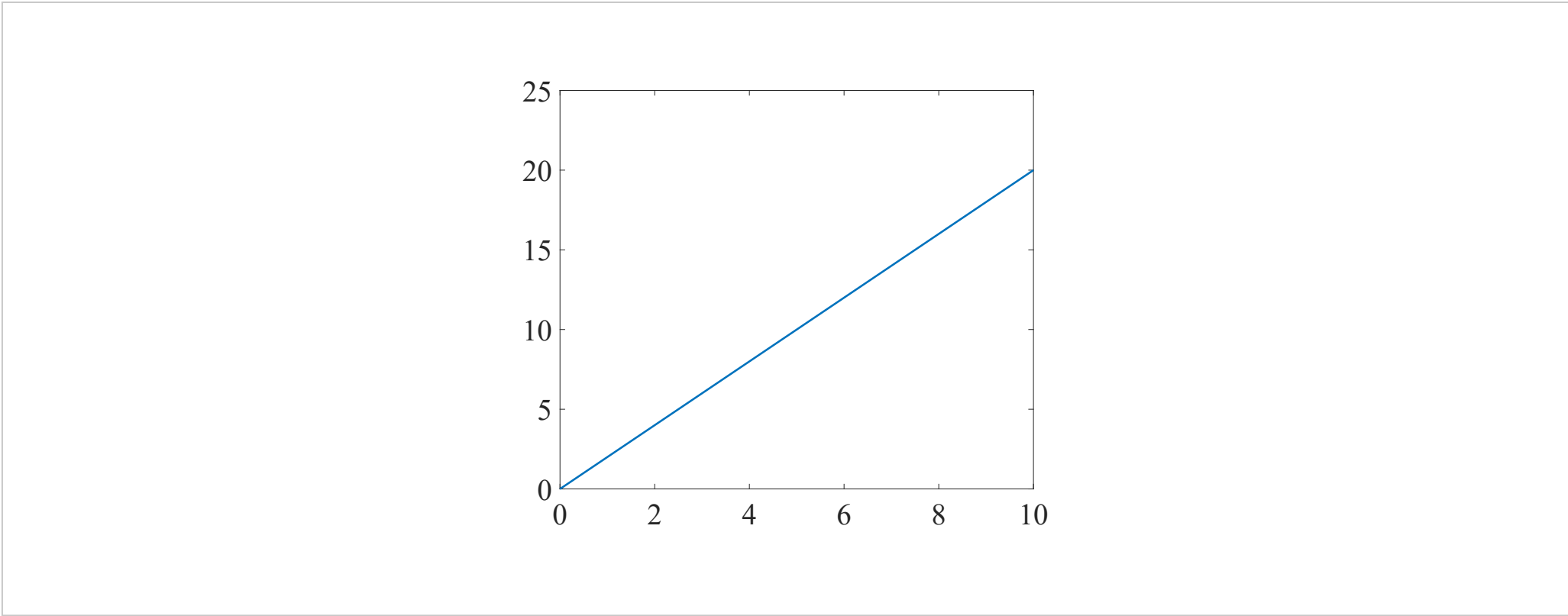
1/1 point (graded)

Consider again the setting of theoretical linear regression, as in the previous problems on this page. Let  $X, Y$  be random variables such that  $\text{Var}(X) \neq 0$ . Assume  $\mathbb{E}[X]$  and  $\mathbb{E}[Y]$  are both zero.

Let  $a, b$  be solutions that minimize the squared error

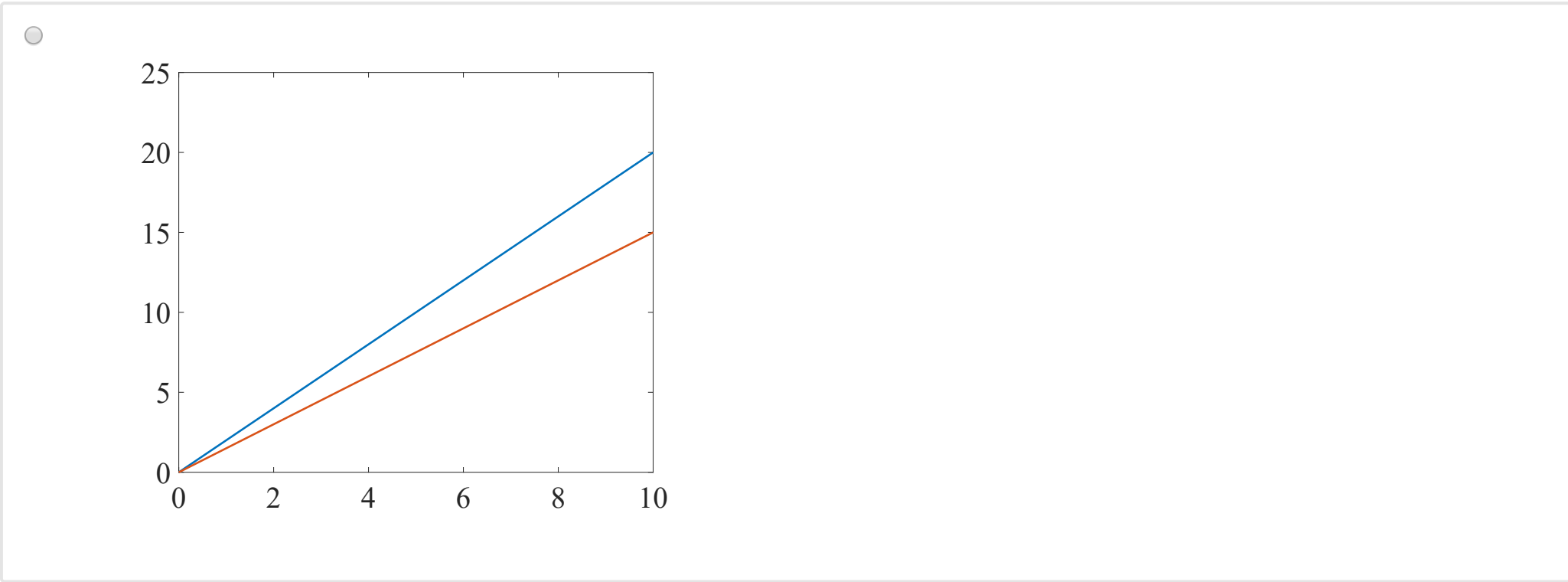
$$a = \mathbb{E}[Y] - \frac{\text{Cov}(X, Y)}{\text{Var}(X)} \mathbb{E}[X], \quad b = \frac{\text{Cov}(X, Y)}{\text{Var}(X)}$$

which gives the best-fitting line  $\mathbb{E}[Y|X = x] \approx a + bx$ . Assume that the line  $y = a + bx$  looks like:



In particular,  $a = 0$  due to our simplifying assumptions.

If  $Y'$  is a different random variable such that  $\mathbb{E}[Y'] = 0$ ,  $\text{Cov}(X, Y') > \text{Cov}(X, Y)$ , which of the following choices best illustrates, via a new line drawn in red, the theoretical linear regression of the pair  $X, Y'$ ?



**Solution:**

Increasing the covariance increases  $b$  and hence the slope increases. Qualitatively, the reason why the slope ought to increase if the covariance increases is revealed in the definition of covariance:

$$\text{Cov}(X, Y) = \mathbb{E}\left[\sum_{y \in \Omega_Y} (x - \mathbb{E}[X]) (y - \mathbb{E}[Y])\right]$$

If  $X$  is held fixed, then the covariance increases if, for each  $x$ :

1.  $y - \mathbb{E}[Y]$  tends to be more positive whenever  $x > \mathbb{E}[X]$ , and

2.  $y - \mathbb{E}[Y]$  tends to be more negative whenever  $x < \mathbb{E}[X]$ .

Which, in our scenario, means that for a typical sample  $(x, y)$ , the  $y$ -coordinate tends to be more positive on average whenever  $x > 0$ , and more negative whenever  $x < 0$ .

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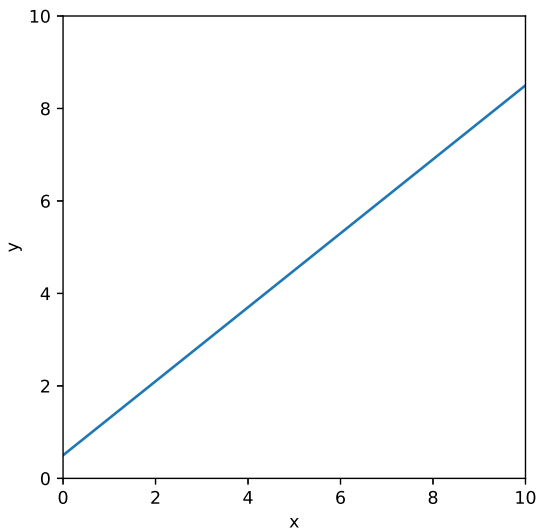
You have used 1 of 1 attempt

**i** Answers are displayed within the problem

Theoretical Linear Regression Visualized II

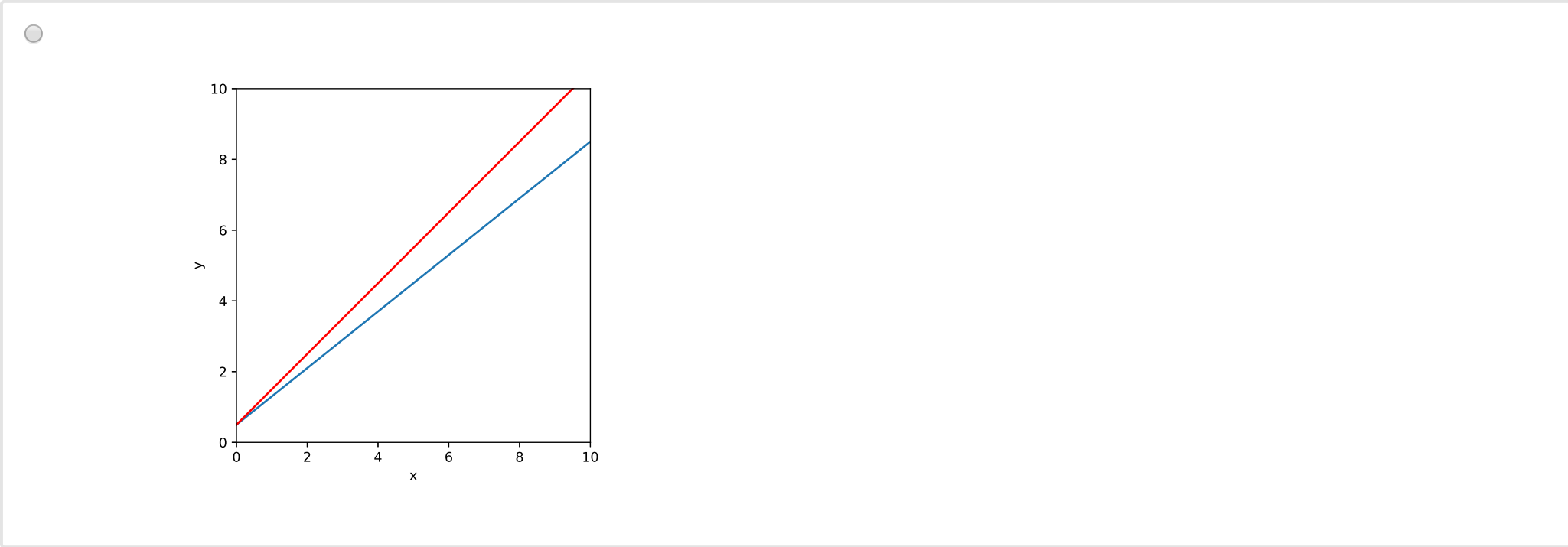
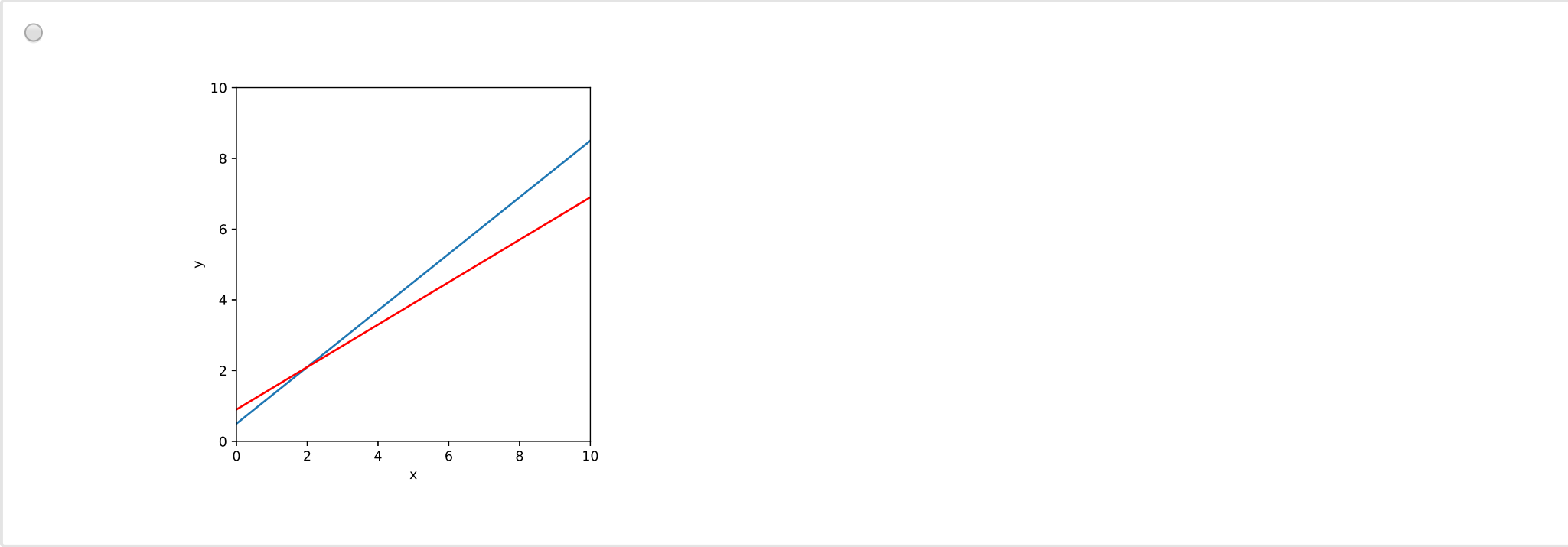
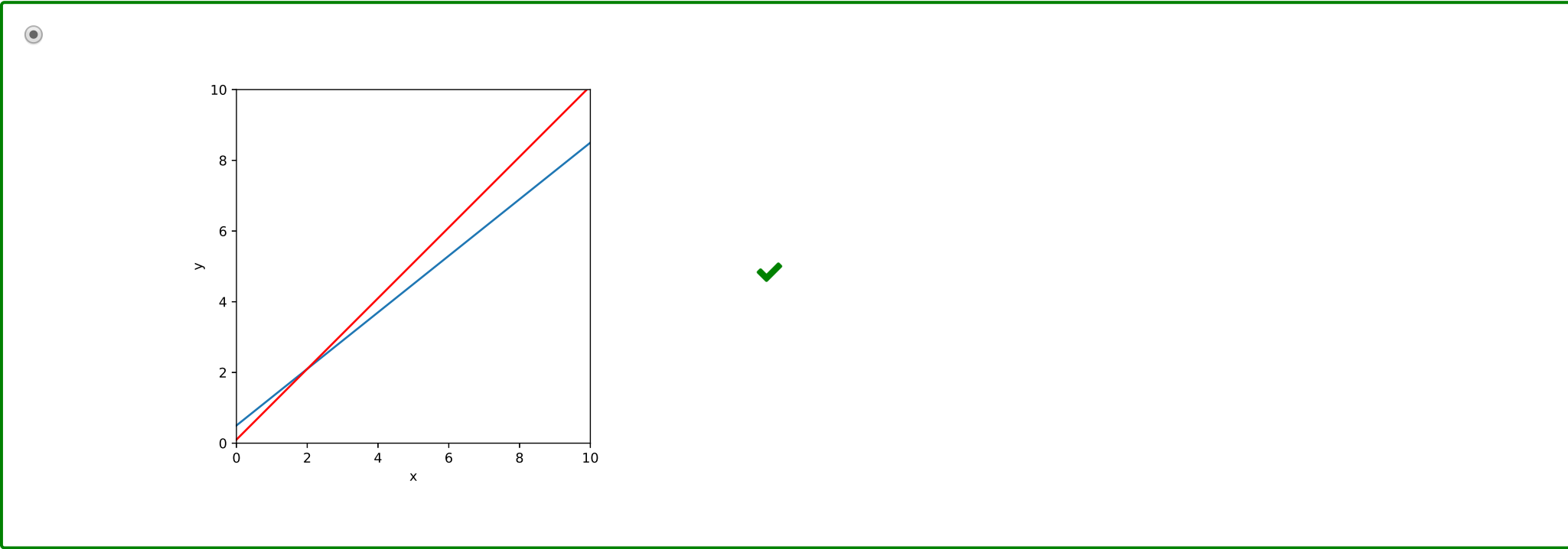
1/1 point (graded)  
Now consider the same setting as in the previous problem, except we drop the assumption  $\mathbb{E}[Y] = 0$ , and we now assume  $\mathbb{E}[X] > 0$ .

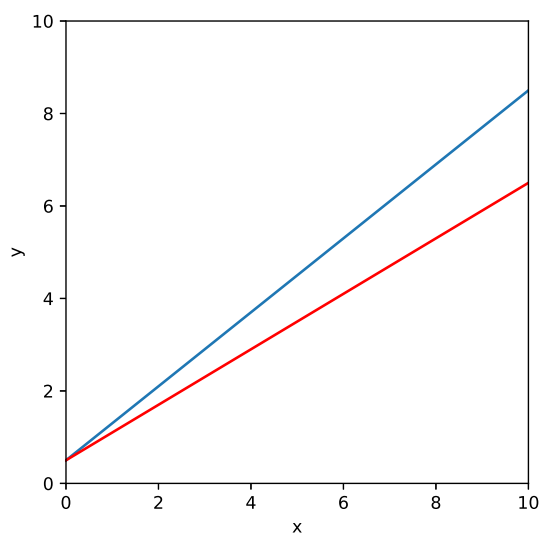
Again, let  $a, b$  be solutions that minimize the squared error, so that the line  $y = a + bx$  looks like:



新的更小

If  $Y'$  is a different random variable such that  $\text{Cov}(X, Y') > \text{Cov}(X, Y)$  and  $\mathbb{E}[Y] \geq \mathbb{E}[Y']$ , which of the following choices best illustrates, via a new line drawn in red, the theoretical linear regression of the pair  $X, Y'$ ?





### Solution:

The reasoning is almost the same as the previous problem's, with an extra step. The slope increases while the intercept decreases.

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You have used 1 of 1 attempt

**i** Answers are displayed within the problem

## Assumptions of Theoretical Linear Regression

1/1 point (graded)

Let us think about what goes wrong when we drop the assumption that  $\text{Var}(X) \neq 0$  in theoretical linear regression.

Let  $X$  and  $Y$  be two real random variables with two moments, and  $\text{Var}(X) = 0$ . (**Note:** the variance of  $X$  is zero whenever  $\mathbf{P}(X = \mathbb{E}[X]) = 1$ .) We make no further assumptions on  $Y$ .

Which one of the following statements is **false**?

☐ There is an infinite family of solutions  $(a, b)$  that minimize the squared mean error,  $\mathbb{E}[(Y - a - bX)^2]$ .

☒ There is no line  $y = a + bx$  that predicts  $Y$  given  $X$  with probability 1, regardless of their distribution. ✓

☐ With probability equal to 1, the random pair  $(X, Y)$  lies on the vertical line  $x = \mathbb{E}[X]$ .

### Solution:

First, a technical remark: one might be tempted to say that the "best fitting line" is the vertical line  $x = \mathbb{E}[X]$ . However, **this is not in the family of lines  $y = a + bx$  parametrized by  $(a, b)$** , which is what the first two choices are asking about.

The only false statement here is " **$Y$  can never be predicted from  $X$ .**". We analyze the choices one by one. For convenience, let  $x_0 = \mathbb{E}[X]$ .

- "**There is an infinite family of solutions  $(a, b)$  that minimize the squared mean error,  $\mathbb{E}[(Y - a - bX)^2]$ .**" There are, indeed, an infinite family of lines from the family  $y = a + bx$  that minimize the mean squared error. Since  $\text{Var}(X) = 0$ , we have

$$\mathbb{E}_{X,Y}[(Y - a - bX)^2] = \mathbb{E}_Y[(Y - a - bx_0)^2]$$

Introduce the variable  $c = a + bx_0$ , which represents the predicted  $y$ -coordinate at  $x = x_0$ . This simplifies the above expectation to  $\mathbb{E}_Y[(Y - c)^2]$ , which is minimized when  $c = \mathbb{E}[Y]$ . This tells us the following important fact: **any line  $y = a + bx$  which crosses the point  $(x_0, \mathbb{E}[Y])$  minimizes the mean error.**

任何斜率的都可以

- “There is no line  $y = a + bx$  that predicts  $Y$  given  $X$  with probability 1, regardless of their distribution.” This is false; consider the case where  $\text{Var}(Y)$  is also zero. Then we can make a prediction for  $Y$ , which is simply  $\mathbb{E}[Y]$ . By the same reasoning about  $\text{Var}(X) = 0$  whenever all of the likelihood is concentrated on a single point, this prediction is correct with probability 1.
- “With probability equal to 1, the random pair  $(X, Y)$  lies on the vertical line  $x = x_0$ .” This is true, because it is simply a re-statement of the remark made in the problem statement:  $\mathbf{P}(X = \mathbb{E}[X]) = 1$ .

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You have used 1 of 1 attempt

**i** Answers are displayed within the problem

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