Optimization

Computational Mathematics and Statistics Camp
University of Chicago
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1. Find the gradient ∇f of the following functions and evaluate them at the given points.

   a. $f(x,y) = \sqrt{x^2+y^2}, \quad (x,y) = (3,4)$

   Let's first rewrite the function so that it is easier to differentiate.

   $$f(x,y) = \sqrt{x^2+y^2} = (x^2+y^2)^{1/2}$$

   Now, taking the partial derivatives with respect to x and y comes more naturally.

   $$\begin{aligned}\frac{\partial f}{\partial x} &= \frac{1}{2}(x^2+y^2)^{-1/2} \cdot \frac{\partial}{\partial x}(x^2+y^2) \\ &= \frac{1}{2}(x^2+y^2)^{-1/2} \cdot (2x) \\ &= x(x^2+y^2)^{-1/2} \\ &= \frac{x}{\sqrt{x^2+y^2}}\end{aligned}$$

   $$\begin{aligned}\frac{\partial f}{\partial y} &= \frac{1}{2}(x^2+y^2)^{-1/2} \cdot \frac{\partial}{\partial y}(x^2+y^2) \\ &= \frac{1}{2}(x^2+y^2)^{-1/2} \cdot (2y) \\ &= y(x^2+y^2)^{-1/2} \\ &= \frac{y}{\sqrt{x^2+y^2}}\end{aligned}$$

   So, the gradient of this function is:

   $$\nabla f(x,y) = \left(\frac{x}{\sqrt{x^2+y^2}}, \frac{y}{\sqrt{x^2+y^2}}\right)$$

   And if we evaluate it at the given point, we get:

   $$\nabla f(3,4) = \left(\frac{3}{\sqrt{3^2+4^2}}, \frac{4}{\sqrt{3^2+4^2}}\right) = \left(\frac{3}{\sqrt{9+16}}, \frac{4}{\sqrt{9+16}}\right) = \left(\frac{3}{\sqrt{25}}, \frac{4}{\sqrt{25}}\right) = \left(\frac{3}{5}, \frac{4}{5}\right)$$

   b. $f(x,y,z) = (x+z)e^{x-y}, \quad (x,y,z) = (1,1,1)$

   This question is slightly more involved; the partial derivative with respect to x will require product rule since x appears in both factors of the product. Recall that the product rule for a generic $h(x) = j(x)k(x)$ is $h'(x) = f'(x)g(x) + f(x)g'(x)$. The partial derivative with respect to y will require the chain rule.

$$\begin{aligned}\frac{\partial f}{\partial x} &= \left(\frac{\partial}{\partial x}(x+z)\right)e^{x-y} + (x+z)\left(\frac{\partial}{\partial x}e^{x-y}\right)\\ &= (1)\cdot e^{x-y} + (x+z)\cdot e^{x-y}\\ &= e^{x-y} + (x+z)\cdot e^{x-y}\\ &= e^{x-y}(x+z+1)\end{aligned}$$

(The partial derivative above technically requires chain rule where you take the derivative of $x-y$ with respect to x, but that's just 1, so we omit that work here.)

$$\begin{aligned}\frac{\partial f}{\partial y} &= (x+z)\cdot e^{x-y}\cdot\left(\frac{\partial}{\partial y}(x-y)\right)\\ &= (x+z)\cdot e^{x-y}\cdot(-1)\\ &= -e^{x-y}(x+z)\end{aligned}$$

$$\begin{aligned}\frac{\partial f}{\partial z} &= \frac{\partial}{\partial z}(xe^{x-y} + ze^{x-y})\\ &= \frac{\partial}{\partial z}(xe^{x-y}) + \frac{\partial}{\partial z}(ze^{x-y})\\ &= 0 + e^{x-y}\\ &= e^{x-y}\end{aligned}$$

The gradient of this function, which we can also write as a vertical vector, is

$$\nabla f(x,y,z) = \begin{bmatrix} e^{x-y}(x+z+1)\\ -e^{x-y}(x+z)\\ e^{x-y}\end{bmatrix}$$

When we evaluate the gradient at the given value, we obtain

$$\nabla f(1,1,1) = \begin{bmatrix} e^{1-1}(1+1+1)\\ -e^{1-1}(1+1)\\ e^{1-1}\end{bmatrix} = \begin{bmatrix} e^0(3)\\ -e^0(2)\\ e^0)\end{bmatrix} = \begin{bmatrix} 1\cdot 3\\ -1\cdot 2\\ 1\end{bmatrix} = \begin{bmatrix} 3\\ -2\\ 1\end{bmatrix}$$

2. Find the Hessian H for the following functions.

   a. $g(x,y) = x^4 - 3x^2y^3$

   In order to find any second partial derivatives, we need the first partial derivatives. These are straightforward. (Here, we'll use the other partial derivative notation just to keep things interesting and to get you accustomed to it.)

$$g_x = 4x^3 - 6xy^3 \qquad g_y = -9x^2y^2$$

Now, we find the second partial derivatives, which are also pretty simple to find.

$$g_{xx} = 12x^2 - 6y^3 \qquad g_{xy} = -18xy^2 \qquad g_{yx} = -18xy^2 \qquad g_{yy} = -18x^2y$$

Note that $f_{xy} = f_{yx}$. We now have everything we need for the Hessian.

$$H = \begin{bmatrix} 12x^2 - 6y^3 & -18xy^2\\ -18xy^2 & -18x^2y\end{bmatrix}$$

b. $f(x, y, z) = xyz - x^2$

Finding this Hessian initially seems daunting because it involves three variables. Fortunately, the second derivatives are all really simple. We start by finding first partial derivatives.

$$f_x = yz - 2x \qquad f_y = xz \qquad f_z = xy$$

Now, we look for the second partial derivatives. Just to keep things orderly, let's start with f_{xx}, f_{yy}, and f_{zz}.

$$f_{xx} = -2 \qquad f_{yy} = 0 \qquad f_{zz} = 0$$

Then we can look for the other second partial derivatives that involve two different variables.

$$f_{xy} = \frac{\partial}{\partial y}(yz - 2x) = z \qquad f_{yz} = \frac{\partial}{\partial z}(xz) = x \qquad f_{zx} = \frac{\partial}{\partial x}(xy) = y$$

$$f_{yx} = \frac{\partial}{\partial x}(xz) = z \qquad f_{zy} = \frac{\partial}{\partial y}(xy) = x \qquad f_{xz} = \frac{\partial}{\partial z}(yz - 2x) = y$$

We have found all second derivatives, so we can now produce the Hessian.

$$H = \begin{bmatrix} f_{xx} & f_{xy} & f_{xz} \\ f_{yx} & f_{yy} & f_{yz} \\ f_{zx} & f_{zy} & f_{zz} \end{bmatrix} = \begin{bmatrix} -2 & z & y \\ z & 0 & x \\ y & x & 0 \end{bmatrix}$$

3. Find the local minimum values, local maximum values, and saddle point(s) of the function. Remember the process we discussed in class: Calculate the gradient, set it equal to zero to solve the system of equations, calculate the Hessian, and assess the Hessian at critical values. Be sure to show your work on each of these steps.

a. $f(x, y) = x^4 + y^4 - 4xy + 2$

The first step, as the problem indicates, is to determine the gradient of the function. Taking the first derivatives here is quite straightforward.

$$\begin{aligned} \frac{\partial}{\partial x}(x^4 + y^4 - 4xy + 2) &= 4x^3 + 0 - 4y + 0 \\ &= 4x^3 - 4y \\ \frac{\partial}{\partial y}(x^4 + y^4 - 4xy + 2) &= 0 + 4y^3 - 4x + 0 \\ &= 4y^3 - 4x \\ \nabla f(x, y) &= (4x^3 - 4y, 4y^3 - 4x) \end{aligned}$$

Now we must set this gradient equal to the zero vector. So we know $4x^3 - 4y = 0$ and $4y^3 - 4x = 0$. The standard method for solving a system of equations is to solve one equation for one variable in terms of the other(s) and substitute that value into the other equations. In this case, let's choose to solve the second equation for x in terms of y. So we have $4y^3 - 4x = 0$. Dividing both sides by 4 gives $y^3 - x = 0$, and adding x to both sides gives $y^3 = x$. Now let's plug this into the other equation. So we have $4(y^3)^3 - 4y = 4y^9 - 4y = 0$. Dividing by 4 gives $y^9 - y = 0$. There are a few ways to go about looking at this equation to get a value for y, but let's take the most rigorous approach. First, let us try to simplify a bit; *if y is not equal to 0*, we can divide by y to get $y^8 - 1 = 0$, or $y^8 = 1$. So taking the square root of both sides gives $y^4 = \pm 1$, but it obviously

cannot be -1, so $y^4 = 1$. Doing so again gives $y^2 = \pm 1$, but again, it cannot be that $y^2 = -1$, so $y^2 = 1$. Taking the square root one last time gives $y = \pm 1$. Both of these values are feasible. Since we know that $x = y^3$, we know that (1,1) and (-1, -1) are critical points of this function.

Are these the only ones, though? Well, not necessarily. Recall that in finding those critical points, we had to divide by y, which we cannot do when $y = 0$. In other words, we made an assumption that y was not 0 - which means we only found the non-zero values of y that produce critical points. Is there a critical point where $y = 0$? In this case, yes - if both y and x are zero, the gradient is zero as well. So (0,0) is also a critical point.

Now let's calulate the Hessian.

$$H(x,y) = \begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x}(4x^3 - 4y) & \frac{\partial}{\partial x}(4y^3 - 4x) \\ \frac{\partial}{\partial y}(4x^3 - 4y) & \frac{\partial}{\partial y}(4y^3 - 4x) \end{bmatrix} = \begin{bmatrix} 12x^2 & -4 \\ -4 & 12y^2 \end{bmatrix}$$

Now we simply have to plug in the x and y values at the critical points and apply the second derivative test.

$$H(1,1) = H(-1,-1) = \begin{bmatrix} 12 & -4 \\ -4 & 12 \end{bmatrix}$$

So for the critical points $(1,1)$ and $(-1,-1)$, $AC - B^2 = 12 * 12 - (-4)^2 = 128 > 0$ and $A = 12 > 0$. So the Hessian at these points is positive definite, and the points $(1,1)$ and $(-1,-1)$ are local minima.

$$H(0,0) = \begin{bmatrix} 0 & -4 \\ -4 & 0 \end{bmatrix}$$

So for the critical point $(0,0)$, $AC - B^2 = 0 * 0 - (-4)^2 = -16 < 0$, so the Hessian is indefinite and the point $(0,0)$ is a saddle point.

b. $k(x,y) = (1 + xy)(x + y)$

As in the first problem, we begin by finding the gradient. To simplify the derivation process, note that $(1 + xy)(x + y) = x^2y + xy^2 + x + y$

$$\frac{\partial}{\partial x}(x^2y + xy^2 + x + y) = 2xy + y^2 + 1$$
$$\frac{\partial}{\partial y}(x^2y + xy^2 + x + y) = x^2 + 2xy + 1$$
$$\nabla f(x,y) = (y^2 + 2xy + 1, x^2 + 2xy + 1)$$

Now we need to set this gradient equal to the zero vector and solve the system of equations (sorry for the awful algebra here!). The standard method of solving one equation for one variable in terms of the other and plugging back into the other equation will work here (and I will write out the algebra below), but there is a much easier way of doing it. Notice that if $x^2 + 2xy + 1 = 0$ and $y^2 + 2xy + 1 = 0$, then it must be the case that $x^2 + 2xy + 1 = y^2 + 2xy + 1$. Now we can subtract $2xy + 1$ from both sides to get $x^2 = y^2$, or $x = \pm y$. This gives us two cases to consider: either $x = y$ or $x = -y$. Let's start with $x = y$. Plugging this value of x into the first equation gives us $y^2 + 2yy + 1 = 3y^2 + 1 = 0$. But then $3y^2 = -1$, which is impossible for any real value of y. So now let's look at $x = -y$. Then the first equation gives us $y^2 + 2(-y)y + 1 = -y^2 + 1 = 0$, which means that $y^2 = 1$, or $y = \pm 1$. If $y = 1$, we know $x = -y = -1$, and if $y = -1$, $x = -y = 1$. So $(-1, 1)$ and $(1, -1)$ are critical points of this function (you can confirm for yourselves that these points are solutions to the other equation as well).

The longer way to do it is as follows. First, let's solve the first equation for x in terms of y. So we begin with $y^2 + 2xy + 1 = 0$. Subtract $2xy$ to get $y^2 + 1 = -2xy$. Clearly, we will want to divide by y, but first, let's check what happens when $y = 0$. If $y = 0$, then $y^2 + 1 = 1$ and $-2xy = 0$ for all x - so there are no solutions. So now, let's divide both sides of $y^2 + 1 = -2xy$ by $-2y$. Then we have $x = -\frac{y^2+1}{2y}$. Plugging this value into the second equation gives us $(-\frac{y^2+1}{2y})^2 + 2y(-\frac{y^2+1}{2y} + 1 = 0$. Distributing out the first term and cancelling out the $2y$ in the second leaves us with $\frac{y^4+2y^2+1}{4y^2} - y^2 = 0$. Now let's multiply both sides by $4y^2$. Then we have $y^4 + 2y^2 + 1 - 4y^4 = -3y^4 + 2y^2 + 1 = 0$. We can then apply the quadratic formula to get

$$y^2 = \frac{-2 \pm \sqrt{2^2 - 4(-3)(1)}}{2(-3} = \frac{-2 \pm \sqrt{16}}{-6} = \frac{-2 \pm 4}{-6}$$

Clearly, if $y^2 = \frac{-2+4}{-6} = -1/3$, y has no real values. So we must have $y^2 = \frac{-2-4}{-6} = 1$, or $y = \pm 1$, as before, with the same x values following.

Now that we have established $(-1, 1)$ and $(1, -1)$ as critical points, we must find the Hessian.

$$H(x,y) = \begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x}(y^2 + 2xy + 1) & \frac{\partial}{\partial x}(x^2 + 2xy + 1) \\ \frac{\partial}{\partial y}(y^2 + 2xy + 1) & \frac{\partial}{\partial y}(x^2 + 2xy + 1) \end{bmatrix} = \begin{bmatrix} 2y & 2x + 2y \\ 2y + 2x & 2x \end{bmatrix}$$

Then we have

$$H(-1,1) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

and

$$H(1,-1) = \begin{bmatrix} -2 & 0 \\ 0 & 2 \end{bmatrix}$$

In both cases, $AC - B^2 = 2(-2) - 0^2 = -4 < 0$, so the Hessian is indefinite and these are saddle points. So there are no local minima or maxima.

4. Suppose we were interested in learning about how years of schooling affect the probability that a person turns out to vote. To simplify things, let's say we're trying to predict whether one individual voted. We did some preliminary work on this yesterday, but suppose we showed a colleague our model from this problem and they complained. "What a lame model", our colleague said, "You definitely have to include an intercept term." So in this problem we'll follow our colleague's advice and do just that.

   Let Y be our single observation of the dependent variable (whether or not a person turned out to vote) and X_1 be our single observation of an independent variable, *education*, the number of years of schooling for this individual. Now though, we're also going to include an intercept term, β_0 in our model along with β_1 a coefficient that's associated with X_1.

   This produces the following model for which we want to find the values of both β_0 and β_1 that minimize the sum of square errors.

$$Y = \beta_0 + \beta_1 X_1 + \epsilon$$

   where ϵ is an error term.

   Use the method of least squares to solve for the values of β_0, β_1 that minimizes the sum of squared errors in the our data. Using the tools of multivariate minimization we've been practicing, find the values of β_0 and β_1 that minimize this quantity.

$$
\begin{aligned}
Y &= \beta_0 + \beta_1 X_1 + \epsilon \\
Y - (\beta_0 + \beta_1 X_1) &= \epsilon \\
(Y - (\beta_0 + \beta_1 X_1))^2 &= \epsilon^2
\end{aligned}
$$

$$
\begin{aligned}
f(\beta_0, \beta_1 | x_i, y_i) &= (Y - \beta_0 - \beta_1 X_1)^2 \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_0} &= -2(Y - \beta_0 - \beta_1 X_1) \\
&= -2Y + 2\beta_0 + 2\beta_1 X_1 \\
0 &= 2Y - 2\beta_0 - 2\beta_1 X_1 \\
\hat{\beta}_0 &= Y - \beta_1 X_1 \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_1} &= -2X_1(Y - \beta_0 - \beta_1 X_1) \\
&= -2YX_1 + 2\beta_0 X_1 + 2\beta_1 X_1^2 \\
0 &= 2YX_1 - 2\beta_0 X_1 - 2\beta_1 X_1^2 \\
\beta_1 X_1^2 &= YX_1 - \beta_0 X_1
\end{aligned}
$$

We then sub in $\hat{\beta}_0$ for β_0 and continue:

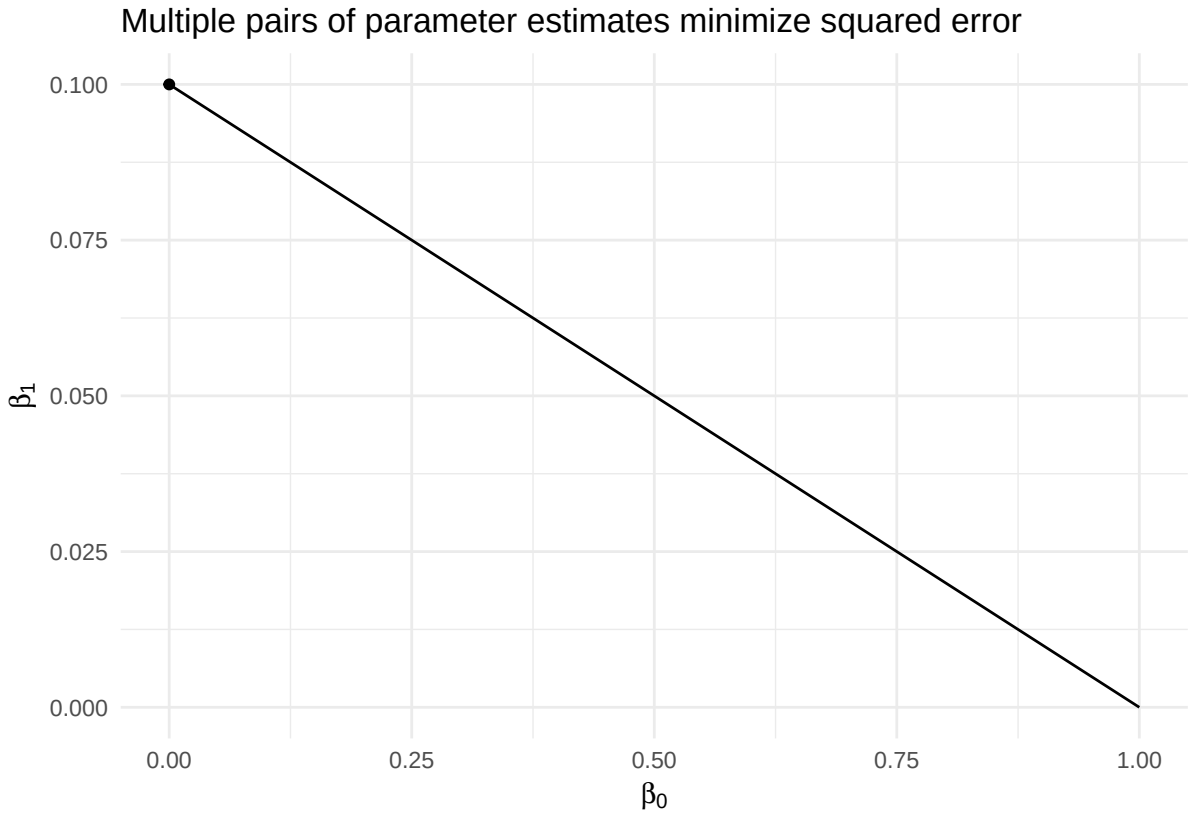
$$
\begin{aligned}
\beta_1 X_1^2 &= YX_1 - (Y - \beta_1 X_1)X_1 \\
\beta_1 X_1^2 &= YX_1 - YX_1 + \beta_1 X_1^2 \\
\beta_1 X_1^2 &= \beta_1 X_1^2 \\
\beta_1 X_1^2 - \beta_1 X_1^2 &= 0 \\
0 &= 0
\end{aligned}
$$

So, what's going on? Why can't we find a solution for $\hat{\beta}_1$?

The problem is that we are trying to use two parameters to describe a single observation of data. This is a case of a problem that occurs when solving systems of equations known as **underdetermination** (i.e., we have two unknown parameters, β_0 and β_1, but only one equation with which to estimate them).

The intuition behind this problem is that, given our data, we don't have enough information to uniquely identify two parameters. With one observation we could minimize the squared error by *either*:

1. Fitting the point exactly with our intercept term, β_0
2. Fitting the point exactly with the parameter on education β_1 or
3. Fitting the point with some linear combination of values for β_0 and β_1. Assuming this individual voted (y=1) and had 10 years of education (x=10), the line shows all the pairs of parameter estimates that would minimize the squared error with the two edge cases as end points (i.e., explain entirely with the intercept term or with the parameter attached to education) and a number of combinations of parameter values that also work in between (e.g., $\beta_0 = .5$ and $\beta_1 = .05$).



Since we have so many different combinations of parameter values that accomplish our goal, to minimize the squared error, equally well, no unique solution exists for this parameter vector. When this occurs we say our model is not identified.

If we start to get more observations than parameters we want to estimate (i.e., we have an overdetermined system of equations), this answer will change and we'll get unique solutions for each.

1. This problem illustrates, in a very simple manner, one symptom of underdetermination: perfect multicollinearity. Because we have a linearly dependent $\hat{\beta} = (X'X)^{-1}X'Y$.

$$\begin{aligned} X &= \begin{bmatrix} 1 & X_1 \end{bmatrix} \\ X'X &= \begin{bmatrix} 1 \\ X_1 \end{bmatrix} \begin{bmatrix} 1 & X_1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & X_1 \\ X_1 & X_1^2 \end{bmatrix} \end{aligned}$$

   Where we can show linear dependence by multiplying the first row in the matrix by X_1 to get an exact copy of the second row. We'll see that perfect multicollinearity can also occur even when we have more observations than variables, if we can write some variables as a linear combination of other variables.

2. If you got values for $\hat{\beta}_0$ and $\hat{\beta}_1$ on this problem you did something wrong (e.g., assumed more than 1 observation, made an algebra mistake).

5. Suppose we were interested in learning about how years of schooling affect the probability that a person turns out to vote. To simplify things, let's say we're trying to predict whether one individual voted. Unlike question 4, let's assume we now have many observations in our data.

   Let Y_i be a vector containing many (n) observations of our dependent variable (whether or not a person i turned out to vote) and X_i be a vector containing many (n) observations of our independent variable,

education, the number of years of schooling for individual i. We're also going to include an intercept term, β_0 in our model along with β_1 a coefficient that's associated with X_i.

This produces the following model for which we want to find the values of both β_0 and β_1 that minimize the sum of square errors.

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

where ϵ_i is an error term for person i.

a. Use the method of least squares to solve for the values of β_0, β_1 that minimizes the sum of squared errors in the our data. Using the tools of multivariate minimization we've been practicing, set the partial derivatives of β_0 and β_1 equal to 0 and determine $\hat{\beta}_0$ and $\hat{\beta}_1$.

$$\sum_{i=1}^{n}(\epsilon_i)^2 = \sum_{i=1}^{n}(Y_i - (\beta_0 + \beta_1 X_i))^2$$

$$\begin{aligned}
f(\beta_0, \beta_1 | x_i, y_i) &= \sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i)^2 \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_0} &= -2(\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i)) \\
&= \sum_{i=1}^{n} -2Y_i + 2\beta_0 + 2\beta_1 X_i \\
0 &= \sum_{i=1}^{n} -2Y_i + 2\beta_0 + 2\beta_1 X_i \\
0 &= -2\sum_{i=1}^{n} Y_i + 2\sum_{i=1}^{n}\beta_0 + 2\beta_1 \sum_{i=1}^{n} X_i \\
0 &= -2\sum_{i=1}^{n} Y_i + (n \times 2\beta_0) + 2\beta_1 \sum_{i=1}^{n} X_i \\
n \times 2\beta_0 &= 2\sum_{i=1}^{n} Y_i - 2\beta_1 \sum_{i=1}^{n} X_i \\
\hat{\beta}_0 &= \frac{2\sum_{i=1}^{n} Y_i}{2n} - \frac{2\beta_1 \sum_{i=1}^{n} X_i}{2n} \\
&= \frac{\sum_{i=1}^{n} Y_i}{n} - \beta_1 \frac{\sum_{i=1}^{n} X_i}{n} \\
\hat{\beta}_0 &= \bar{Y} - \beta_1 \bar{X}
\end{aligned}$$

There are two key moves in the above steps. First, when we take the sum of a constant (e.g., $2\sum_{i=1}^{n}\beta_0$) we can pass it through the summation sign and multiply the constant by n. For intuition think about taking the sum of 1 many times (e.g., $\sum_{i=1}^{n} 1 = n \times 1 = n$). Second, we can write a term like $\frac{\sum_{i=1}^{n} Y_i}{n}$ as a sample mean, $\bar{Y}$.

Ok now let's move on to β_1. Note: In the fourth step below, I sub in $\hat{\beta}_0$, what we just got in the above problem, for β_0.

$$
\begin{aligned}
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_1} &= \sum_{i=1}^{n} -2X_i(Y_i - \beta_0 - \beta_1 X_i) \\
&= \sum_{i=1}^{n} -2Y_i X_i + 2\beta_0 X_i + 2\beta_1 X_i^2 \\
0 &= \sum_{i=1}^{n} -2Y_i X_i + 2\beta_0 \sum_{i=1}^{n} X_i + 2\beta_1 \sum_{i=1}^{n} X_i^2 \\
&= \sum_{i=1}^{n} -2Y_i X_i + 2(\bar{Y} - \beta_1 \bar{X}) \sum_{i=1}^{n} X_i + 2\beta_1 \sum_{i=1}^{n} X_i^2 \\
&= \sum_{i=1}^{n} -2Y_i X_i + 2\bar{Y} \sum_{i=1}^{n} X_i - 2\beta_1 \bar{X} \sum_{i=1}^{n} X_i + 2\beta_1 \sum_{i=1}^{n} X_i^2 \\
2\beta_1 \sum_{i=1}^{n} X_i^2 - 2\beta_1 \bar{X} \sum_{i=1}^{n} X_i &= \sum_{i=1}^{n} 2Y_i X_i - 2\bar{Y} \sum_{i=1}^{n} X_i \\
\beta_1 (\sum_{i=1}^{n} X_i^2 - \bar{X} \sum_{i=1}^{n} X_i) &= \sum_{i=1}^{n} Y_i X_i - \bar{Y} \sum_{i=1}^{n} X_i \\
\hat{\beta}_1 &= \frac{\sum_{i=1}^{n} Y_i X_i - \bar{Y} \sum_{i=1}^{n} X_i}{\sum_{i=1}^{n} X_i^2 - \bar{X} \sum_{i=1}^{n} X_i}
\end{aligned}
$$

Later in the course we'll discuss the variance and covariance of variables. Using this knowledge you will then be able to simplify $\hat{\beta}_1$ to $\frac{Covariance(X,Y)}{Variance(X)}$.

b. **OPTIONAL:** Use what we learned about multivariate optimization to find the the Hessian of $\hat{\beta}$. Does this hessian indicate that $\hat{\beta}_0$ and $\hat{\beta}_1$ minimize the sum of squared errors?

As a final check that these values minimize the sum of squared errors, we need to assess the hessian.

$$
\begin{aligned}
f(\beta_0, \beta_1 | x_i, y_i) &= \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2 \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_0} &= \sum_{i=1}^{n} -2Y_i + 2\beta_0 + 2\beta_1 X_i \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_0 \beta_0} &= \sum_{i=1}^{n} 2 \\
&= 2n \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_0 \beta_1} &= \sum_{i=1}^{n} 2X_i \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_1} &= \sum_{i=1}^{n} -2Y_i X_i + 2\beta_0 X_i + 2\beta_1 X_i^2 \\
\frac{\partial f(\beta_0, \beta_1 | x_i, y_i)}{\partial \beta_1 \beta_1} &= \sum_{i=1}^{n} 2X_i^2
\end{aligned}
$$

This produces the following hessian:

$$H(f(\beta_0, \beta_1|x_i, y_i)) = \begin{bmatrix} \frac{\partial f(\beta_0, \beta_1|x_i, y_i)}{\partial \beta_0 \beta_0} & \frac{\partial f(\beta_0, \beta_1|x_i, y_i)}{\partial \beta_0 \beta_1} \\ \frac{\partial f(\beta_0, \beta_1|x_i, y_i)}{\partial \beta_0 \beta_1} & \frac{\partial f(\beta_0, \beta_1|x_i, y_i)}{\partial \beta_1 \beta_1} \end{bmatrix}$$
$$= \begin{bmatrix} 2n & \sum_{i=1}^{n} 2X_i \\ \sum_{i=1}^{n} 2X_i & \sum_{i=1}^{n} 2X_i^2 \end{bmatrix}$$

Let's use what we learned about hessians yesterday in class to determine whether we are at a minimum. If what we've found minimizes the sum of squares, this hessian must be positive definite.

First, to start with $A = 2n > 0$. Since n can only take positive values, this means the first condition for a positive definite hessian is met.

Second, we need to show that $AD - B^2 > 0$:

$$\begin{aligned} AD &= 2n \times \sum_{i=1}^{n} 2X_i^2 \\ B^2 &= (2\sum_{i=1}^{n} X_i)^2 \\ AD - B^2 &= 2n \times \sum_{i=1}^{n} 2X_i^2 - (2\sum_{i=1}^{n} X_i)^2 \\ &= 4(n\sum_{i=1}^{n} X_i^2 - (\sum_{i=1}^{n} X_i)^2) \\ &= 4n^2(\frac{\sum_{i=1}^{n} X_i^2}{n} - \frac{(\sum_{i=1}^{n} X_i)^2}{n^2}) \\ &= 4n^2(\frac{\sum_{i=1}^{n} X_i^2}{n} - (\frac{\sum_{i=1}^{n} X_i}{n})^2) \\ &= 4n^2(\frac{\sum_{i=1}^{n} X_i^2}{n} - (\bar{X})^2) \\ &= 4n^2 \times \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2 \\ &= 4n\sum_{i=1}^{n}(X_i - \bar{X})^2 \\ 4n\sum_{i=1}^{n}(X_i - \bar{X})^2 &> 0 \\ AD - B^2 &> 0 \end{aligned}$$

The key step is restating $\frac{\sum_{i=1}^{n} X_i^2}{n} - (\bar{X})^2$ as $\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2$. If you're unclear on how we get from this first statement to the second, expand $\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2$ and try and make it look like the first statement.

Once we've stated the relationship this way, it's clear that $AD - B^2$ will always be greater than 0 (barring the pathological case where every X_i equals 0). n is always positive and, because we square the difference of $X_i^2 - \bar{X}$, the second part of the statement will always be positive as well. As a result, the $\hat{\beta}_0$ and $\hat{\beta}_1$ we identified earlier will minimize the sum of squared errors.

- We've worked a lot on taking derivatives, but doing so with when summation is involved makes this different than what we've done before. Algebra tips for working with summation signs are below.
  - If you sum a constant n times, this is equivalent to multiplying that constant by n (e.g., $\sum_{i=1}^{n} 1 = n \times 1 = n$).
  - If you sum a variable that is also multiplied by a constant, you can move the constant outside the summation sign (e.g., $\sum_{i=1}^{n} 2 \times X_i = 2 \sum_{i=1}^{n} X_i$).
  - The summation sign is a linear operator so we can distribute it across variables we add together (e.g., $\sum_{i=1}^{n} (X_i + Y_i) = \sum_{i=1}^{n} X_i + \sum_{i=1}^{n} Y_i$)