Day One: Derivatives, Optimization, and Integrals

SOC Methods Camp

September 3rd, 2019

Outline

- Review and application of derivatives

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    - Chain rule

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  - Derivatives of logs/exponents

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  - Two tools important for optimization

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  - Basic optimization
- Review and application of integrals

Review of topics covered in summer assignment

Interval notation, domain, and range

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- If we use intervals to describe the range of a variable in a dataset, it is okay if the interval encompasses values that don't actually exist in the dataset.
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- The domain and range of functions are often expressed in interval notation. These important intervals represent the range of possible values that x or y can take on.
- Some common sets for domain/range in interval notation:
    - all real numbers (the entire number line): $(-\infty, \infty)$
    - all real numbers except 0: $(-\infty, 0) \cup (0, \infty)$

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Why derivatives?

- Derivatives might seem like a relic from our high school days with unclear relevance for statistics
- But consider the following very applied (stylized) cases

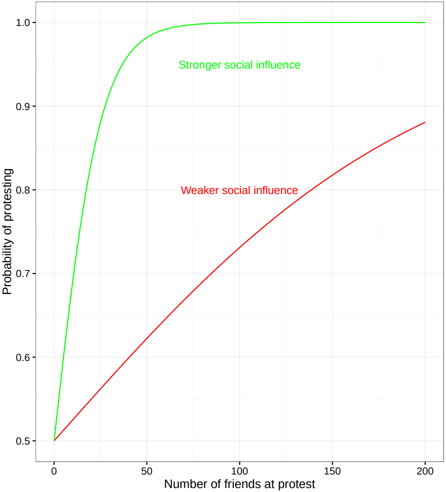
Application one: investigating rates of change under different conditions

Scenario: You want to construct a formal model, similar to the black versus white population change model we reviewed in the summer assignment, where:

- the x axis represents the number of an individual's friends who have joined a protest
- the y axis represents an individual's probability of joining the protest.

You want to see how the rate at which the individual's probability of joining the protest changes (the slope of the curve) at varying number of friends under different assumptions about the strength of influence friends have on protesting

Application one: investigating rates of change under different conditions



Application two: inferring unobserved weights that generate observed patterns

Scenario: You're fitting a model to assign weights to different variables (e.g., education; rural versus urban residence) in predicting whether or not a person will develop an opioid addiction ($1 =$ yes; $0 =$ no). You have a set of data on who developed addiction and their demographic characteristics, and want to find weights for each characteristic in a way that maximizes the probability of observing the correct pattern of 1's and 0's in the addiction variable.

- This is basically what you're trying to do when you run a regression: assign weights to variables to maximize the likelihood of predicting (using the regression model) your observed outcomes given your known inputs.
- **Derivatives help us with maximum likelihood estimation by allowing us to find critical points.**

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  3. Find the derivative more easily!
- For steps two and three, practice with derivatives of logs/exponents is important

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  1. Take the derivative of the "outer layer" of the function ($f(x)$) while keeping the inner layer ($g(x)$) constant while you take the derivative
  2. Then take the derivative of the "inner layer" of the function ($g(x)$)

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  2. Then take the derivative of the "inner layer" of the function $(g(x))$
  3. Then multiply the results from step 1 and step 2 and simplify as needed

Chain rule practice

1. $f(g(x)) = \sqrt{3x^4}$
2. $f(g(x)) = x * \sqrt{1 - x^2}$

Try these on your own and then we'll review as a group...

Chain rule practice: solution one

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   - Outer layer: $f(x) = \sqrt{u} = u^{\frac{1}{2}}$
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$$f'(g(x)) = \frac{1}{2}(3x^4)^{-\frac{1}{2}}$$

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   - Rearrange derivative of outer layer to make more readable:

$$f'(g(x)) = \frac{1}{2} * \frac{1}{\sqrt{3x^4}}$$

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2. **Step two**: take the derivative of the "inner layer" of the function
   - Inner layer: $g(x) = 3x^4$
   - Derivative of inner layer: $g'(x) = 12x^3$

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2. **Step two**: take the derivative of the "inner layer" of the function
   - Inner layer: $g(x) = 3x^4$
   - Derivative of inner layer: $g'(x) = 12x^3$
3. **Step three**: multiply results from steps one and two: $\frac{1}{2} * \frac{12x^3}{\sqrt{3x^4}} = \frac{6x^3}{\sqrt{3x^4}}$

Chain rule practice: solution one

4. **Step four:** Simplify (could have also simplified at an earlier step by taking the constant out of the original equation)

- Break out the x^4 from the square root in the denominator and divide it into the numerator:

$$\frac{6x^3}{\sqrt{3x^4}} = \frac{6x}{\sqrt{3}}$$

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- Break out the x^4 from the square root in the denominator and divide it into the numerator:

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- Multiply both numerator and denominator by $\sqrt{3}$:

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- Simplify:

$$\frac{6x\sqrt{3}}{3} = 2x\sqrt{3}$$

Chain rule practice: solution two

$$f(g(x)) = x * \sqrt{1 - x^2}$$

- Use the **product rule** $\frac{\partial}{\partial x} f(x) * g(x) = f'(x) * g(x) + f(x) * g'(x)$**:**

$$x * (\sqrt{1 - x^2})' + 1 * \sqrt{1 - x^2}$$

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  - Outer layer: $\sqrt{u}$

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  - Outer layer: $\sqrt{u}$
  - Derivative of outer layer while keeping inner layer constant: $\frac{1}{2} * \frac{1}{\sqrt{1-x^2}}$

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  - Outer layer: $\sqrt{u}$
  - Derivative of outer layer while keeping inner layer constant: $\frac{1}{2} * \frac{1}{\sqrt{1-x^2}}$
  - Take the derivative of the "inner layer" of the function: $g(x) = 1 - x^2$; $g'(x) = -2x$

Chain rule practice: solution two

- Multiply inner and outer layer from previous step and simplify:

$$\frac{1}{2} * \frac{-2x}{\sqrt{1-x^2}} = \frac{-x}{\sqrt{1-x^2}}$$

Chain rule practice: solution two

- Multiply inner and outer layer from previous step and simplify:

$$\frac{1}{2} * \frac{-2x}{\sqrt{1-x^2}} = \frac{-x}{\sqrt{1-x^2}}$$

- Plug back into original product rule equation and simplify:

$$x * \frac{-x}{\sqrt{1-x^2}} + \sqrt{1-x^2} = \frac{-x^2}{\sqrt{1-x^2}} + \sqrt{1-x^2}$$

$$= \frac{-x^2}{\sqrt{1-x^2}} + \frac{\sqrt{1-x^2}\sqrt{1-x^2}}{\sqrt{1-x^2}}$$

$$= \frac{-x^2 + \sqrt{1-x^2}\sqrt{1-x^2}}{\sqrt{1-x^2}} = \frac{1-2x^2}{\sqrt{1-x^2}}$$

Why start with chain rule?

The chain rule is often used with derivatives of logs and exponents, which are important tools for making functions easier to work with in maximum likelihood estimation.

Derivatives of logs and exponents

Derivatives:

- $\frac{\partial}{\partial x} ln(x) = \frac{1}{x}$

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Derivatives of logs and exponents

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Some examples to practice on your worksheet

1. $\frac{\partial}{\partial x} ln(x^5)$
2. $\frac{\partial}{\partial x} ln(x^2 + 3)$
3. $\frac{\partial}{\partial x} e^{5x+2}$

Derivatives of logs and exponents: solutions

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   - Inner layer derivative: $2x$

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   - Multiply: $\frac{2x}{x^2+3}$

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    - Inner layer derivative: $2x$
    - Multiply: $\frac{2x}{x^2+3}$
3. $\frac{\partial}{\partial x} e^{5x+2}$
    - Outer layer derivative: e^{5x+2}

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3. $\frac{\partial}{\partial x} e^{5x+2}$
    - Outer layer derivative: e^{5x+2}
    - Inner layer derivative: 5

Derivatives of logs and exponents: solutions

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   - Inner layer derivative: $2x$
   - Multiply: $\frac{2x}{x^2+3}$
3. $\frac{\partial}{\partial x} e^{5x+2}$
   - Outer layer derivative: e^{5x+2}
   - Inner layer derivative: 5
   - Multiply: $5e^{5x+2}$

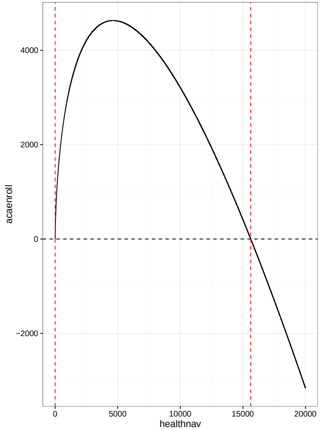
Two useful tools for optimization

Why tools for optimization?

- We've practiced finding the derivative of various functions

Why tools for optimization?

- We've practiced finding the derivative of various functions
- Optimization involves finding the set of points at which the derivative is equal to zero (critical points), which since the derivative is the slope of the function, is the point at which this slope equals zero:



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Why tools for optimization?

- Sometimes we can find these points by actually finding the derivative and setting it equal to zero (analytic optimization: our focus today)
- Other times, an analytic solution is impossible so we instead rely on algorithms that help us "climb the hill" of a curve or jump around the space a function covers to find these points (numerical optimization)
- For both forms of optimization, we need additional tools, which is the focus of the next section

Two useful tools

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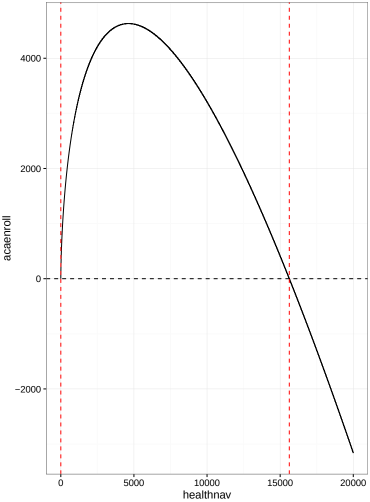
2. *Tool two:* partial derivatives (derivatives for functions with more than one variable)

Tool one: higher order derivatives



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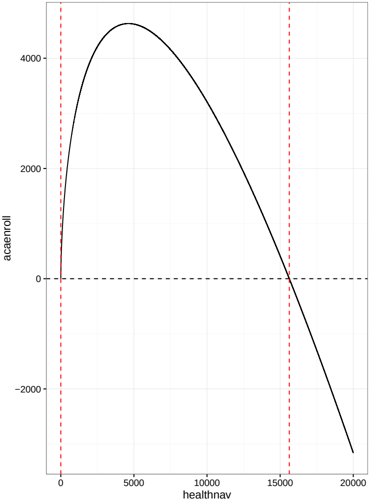

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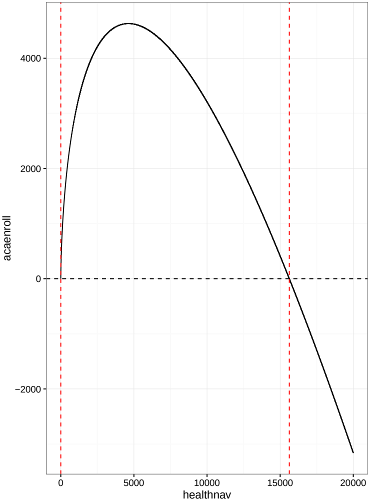

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- But in order to confirm that, we use higher-order derivatives to help us check how the slope changes on either side of that flat point on the curve to assess whether it's a maximum, minimum, or neither

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$$f(x, y) = x^2 y^5 + e^y + ln(x)$$

Find the following on your own:

1. $\frac{\partial f(x,y)}{\partial x}$
2. $\frac{\partial f(x,y)}{\partial y}$
3. $\frac{\partial^2 f(x,y)}{\partial x \partial y}$
4. $\frac{\partial^2 f(x,y)}{\partial x^2}$

Tool two: partial derivatives solutions

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    - Stylized example: finding the number of health navigators to maximize ACA enrollment

Simple case of univariate optimization

Example 1: Health navigators

Suppose a community health center is interested in hiring health navigators to help enroll patients into the ACA. They want to maximize the number of patients they enroll, and are aware that the following relationships hold, letting $h =$ health navigator.

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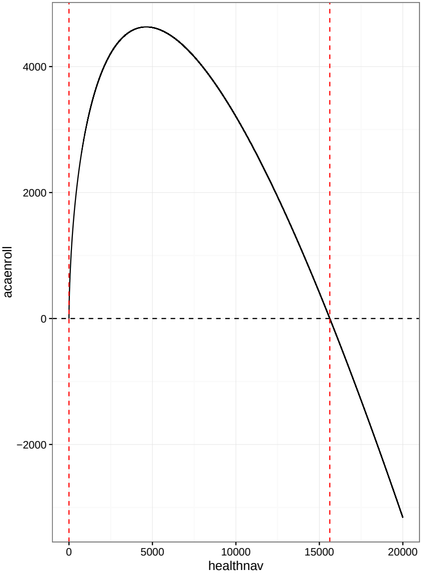
- Putting them together, and letting A = patients enrolled in ACA:

$$A(h) = 50h^{\frac{2}{3}} - 2h$$

Visualizing the function



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- How do we formally (i.e. mathematically) demonstrate these observations?

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1. **Define the domain of interest**: in this case, it is where $h \geq 0$ and $A(h) \geq 0$ (we don't want there to be fewer ACA enrollees as a result of the health navigators)

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$$A(h) = 50h^{\frac{2}{3}} - 2h$$

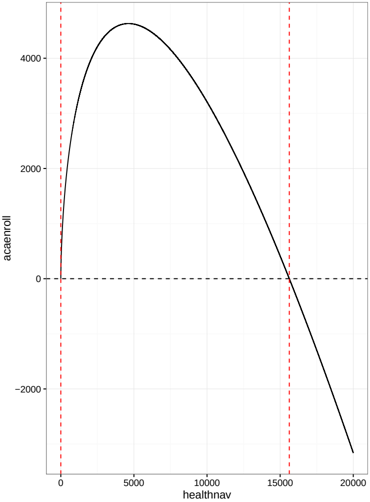
$$A'(h) = \frac{100}{3h^{\frac{1}{3}}} - 2 = 0$$

$$2 = \frac{100}{3h^{\frac{1}{3}}}$$

$$h^{\frac{1}{3}} = \frac{100}{6} = \frac{50}{3}$$

$$(h^{\frac{1}{3}})^3 = \frac{50^3}{3^3} = \frac{125000}{27} = 4629.23$$

Example 1: why do we need a second derivative?



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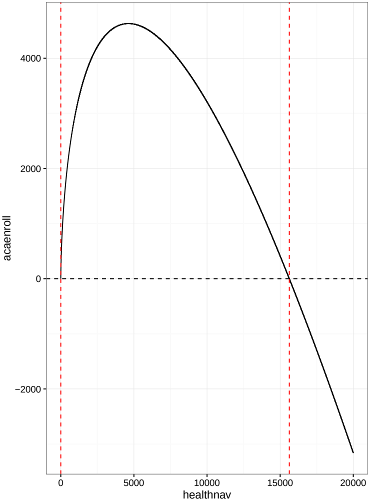

- Now we've been able to formalize the intuition that the slope flattens a little before 5000 navigators, by solving for $\hat{h} \approx 4629$
- How do we formalize (i.e. mathematically demonstrate) that this is indeed a local max and not a local min?

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    3. Signs of second derivative

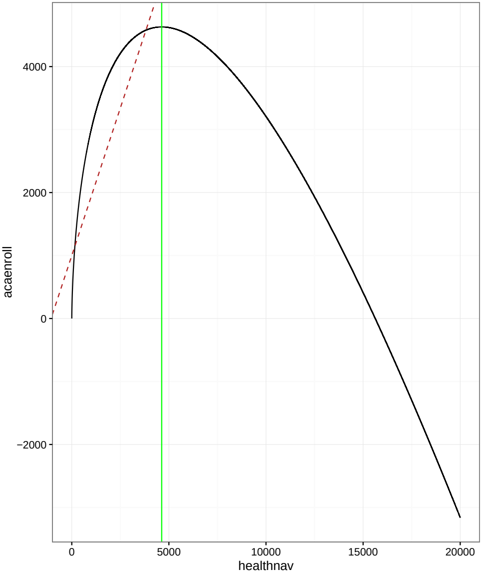
$f'(x)$	$f''(x)$	Classification
0	>0	local min
0	<0	local max
0	0	local min, local max, or inflection point (where f(x) changes concavity)

Graphical represenation

Basic idea: as we approach the maximum, the slope of the curve (first derivative) becomes less and less positive. Because the slope is going, for instance, from 0.937 around health navigators = 1000 to 0.463 around health navigators = 2000 to 0.199 around health navigators = 3000, the *slope of that slope* (the second derivative) is negative

To illustrate graphically. . .

Graphical represenation



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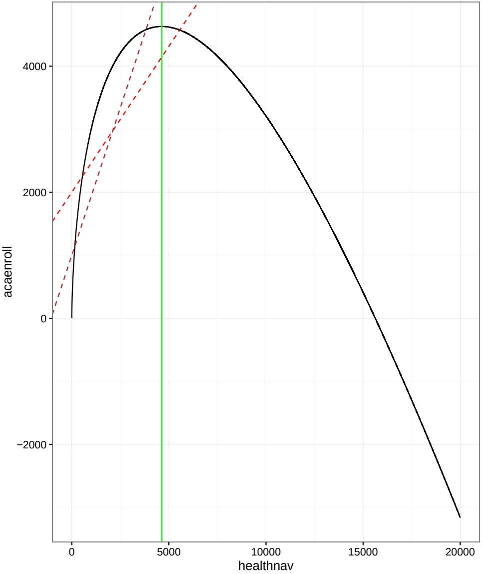

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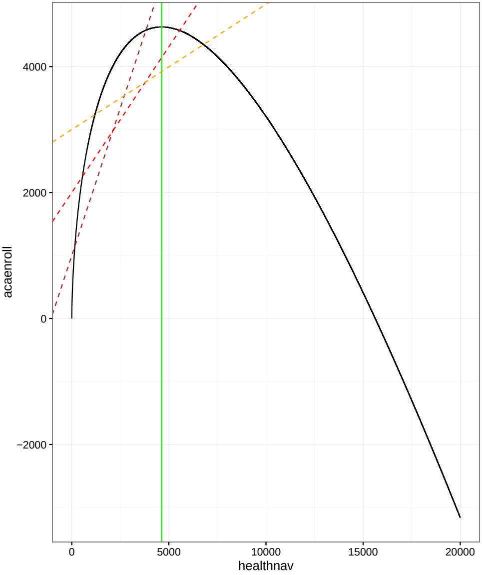

Review and application of integrals

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- We use integrals to find the area under a curve.
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  - For example, if $f(x) = \frac{1}{3}x^3$, the derivative is x^2. The antiderivative of x^2 is $f(x) = \frac{1}{3}x^3$.

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- Integrals are sometimes called called antiderivates, because integration and derivation are opposite procedures.
  - For example, if $f(x) = \frac{1}{3}x^3$, the derivative is x^2. The antiderivative of x^2 is $f(x) = \frac{1}{3}x^3$.
- The integral of a function f(x) is written as:

$$F(x) = \int f(x)\,\mathrm{d}x$$

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- The integral of a function over a set interval [a,b] is called a definite integral and is denoted as follows:

$$F(x) = \int_a^b f(x)\,\mathrm{d}x = F(b) - F(a)$$

Properties of definite integrals

Properties of Definite Integrals

- Constants: $\int_a^b kf(x)dx = k\int_a^b f(x)dx$
- Additive Property: $\int_a^b (f(x)+g(x))dx$

  $= \int_a^b f(x)dx + \int_a^b g(x)dx$
- Linear Functions: $\int_a^b (k_1 f(x) + k_2 g(x))dx$

  $= k_1 \int_a^b f(x)dx + k_2 \int_a^b g(x)dx$
- Intermediate Values: for $a \leq b \leq c$:

  $\int_a^c f(x)dx = \int_a^b f(x)dx + \int_b^c f(x)dx$
- Limit Reversibility: $\int_a^b f(x)dx = -\int_b^a f(x)dx$

Antiderivatives of common functions

Common Functions	Function	Integral
Constant	$\int a\,dx$	$ax + C$
Variable	$\int x\,dx$	$x^2/2 + C$
Square	$\int x^2\,dx$	$x^3/3 + C$
Reciprocal	$\int (1/x)\,dx$	$\ln\lvert x\rvert + C$
Exponential	$\int e^x\,dx$	$e^x + C$
	$\int a^x\,dx$	$a^x/\ln(a) + C$
	$\int \ln(x)\,dx$	$x\ln(x) - x + C$
Trigonometry (x in radians)	$\int \cos(x)\,dx$	$\sin(x) + C$
	$\int \sin(x)\,dx$	$-\cos(x) + C$
	$\int \sec^2(x)\,dx$	$\tan(x) + C$

Integration by Parts

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- Or, another way of looking at it: $\int uv' = uv - \int vu'$

Integration by Parts

- Let's do some practice. Try to solve these examples on scrap paper:
  $\int e^x x \, \mathrm{d}x$
  $\int e^x sin(x) \, \mathrm{d}x$

Integration by Parts: Solutions

For the first problem, let $u = x$ and $v' = e^x$. We know that u' = 1 and $\int e^x \, \mathrm{d}x = v = e^x$. So using our rule for integration by parts, we get:

$$xe^x - e^x$$

$$e^x(x+1) + C$$

For the second problem, we will let $u = sin(x)$ and $v' = e^x$. We then can find that:

$$u' = cos(x)$$

$$\int e^x \, \mathrm{d}x = e^x$$

Putting that together, we get:

$$\int e^x sin(x) \, \mathrm{d}x = sin(x)e^x - \int cos(x)e^x \, \mathrm{d}x$$

While this may look more complicated, we can actually use integration by parts again to get to the solution we need.

Solution continued

So, let $u = cos(x)$ and $v' = e^x$. Then:

$$u' = -sin(x)$$
$$\int e^x \, \mathrm{d}x = e^x$$

Using our intergration by parts rule, we get:

$$\int e^x sin(x) \, \mathrm{d}x = sin(x)e^x - (cos(x)e^x - \int -sin(x)e^x \, \mathrm{d}x)$$
$$\int e^x sin(x) \, \mathrm{d}x = e^x sin(x) - e^x cos(x) - \int e^x sin(x) \, \mathrm{d}x$$
$$2 \int e^x sin(x) \, \mathrm{d}x = e^x sin(x) - e^x cos(x)$$
$$\int e^x sin(x) \, \mathrm{d}x = \frac{e^x sin(x) - e^x cos(x)}{2} + C$$

Why do we care about integrals in statistics?

Integrals help us find the probability of continuous events. You will learn a lot more about this in the stats sequence next year, but for now just take our word on this:

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Integrals help us find the probability of continuous events. You will learn a lot more about this in the stats sequence next year, but for now just take our word on this:

- There are things called probability density functions.
- The areas under these functions help us figure out the probability of given events.

And, as we said at the start, integrals can be used to find the areas under a curve!