ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Computational Methods for Engineering Applications I

Spring semester 2017

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Exam

Issued: August 25, 2017, 15:00

Exam directives. In order to pass the exam, the following requirements have to be met:

- Clear your desk (no cell phones, cameras, etc.): on your desk you should have your Legi, your pen and your notes. We provide you with the necessary paper and the exam sheets.
- Read the first two pages of the exam carefully. Write your name and Legi-ID where requested. Before handing in the exam, **PUT YOUR SIGNATURE ON PAGE 2**.
- The personal summary consists of no more than 4 pages (2 sheets). The personal summary can be handwritten or machine-typed. In case it is machine-typed, the text has to be single-spaced and the font size has to be at least 8 pts. You are not allowed to bring a copy of somebody else's summary.
- The teaching assistants will give you the necessary paper sheets. You are not allowed to use any other paper sheets.
- You are allowed to use a 'non-graphing' and 'non-programmable' calculator, i.e., a calculator that does not have plotting, program-storing, or symbolic capabilities.
- You must always show all the necessary steps required to arrive at your answer, as well as the justification for any answers you select. You will not receive points for merely writing down the final answer.
- You can answer in English or in German; the answers should be handwritten and clearly readable, written in blue or black ink - do NOT write anything in red or green. Unless the question explicitly requires you to pick multiple answers, only one answer per question will be accepted (the first one you attempt). Invalid answers should be clearly crossed out. Whenever you write a C++-compatible pseudo code, also include the relevant comments.
- For questions from 12 to 23, always use a new page for answering each new question (not for sub-questions!). On the top-right corner of every page write your complete name, Legi-ID, and page number. Unless otherwise noted in the question, you should hand-in your answers on paper.
- If something is disturbing you during the exam, or it is preventing you from peacefully solving the exam, please report it immediately to an assistant. Later notifications will not be accepted.
- You must hand in: the exam cover, the sheets with the exam questions and your solutions. The exam cannot be accepted if the cover sheet or the question sheets are not handed back.

Family Name:	
Name:	
Legi-ID:	

Question	Maximum score	Score	TA 1	TA 2
1	3			
2	4			
3	5			
4	6			
5	6			
6	6			
7	8			
8	8			
9	10			
10	6			
11	7			
12	8			
13	8			
14	10			
15	10			
16	12			
17	12			
18	12			
19	18			
20	20			
21	26			
22	15			
23	20			
Total	240			

This exam sums up to 240 points. This is more than the score you are supposed to achieve; your ultimate goal is to reach 180 points. With your signature you confirm that you have read the exam directives; you solved the exam without any unauthorized help and you wrote your answers following the outlined directives.

Signature: ______________________

Short Questions

Question 1: Lagrange interpolation (3 points)

State whether the following statements are true or false.

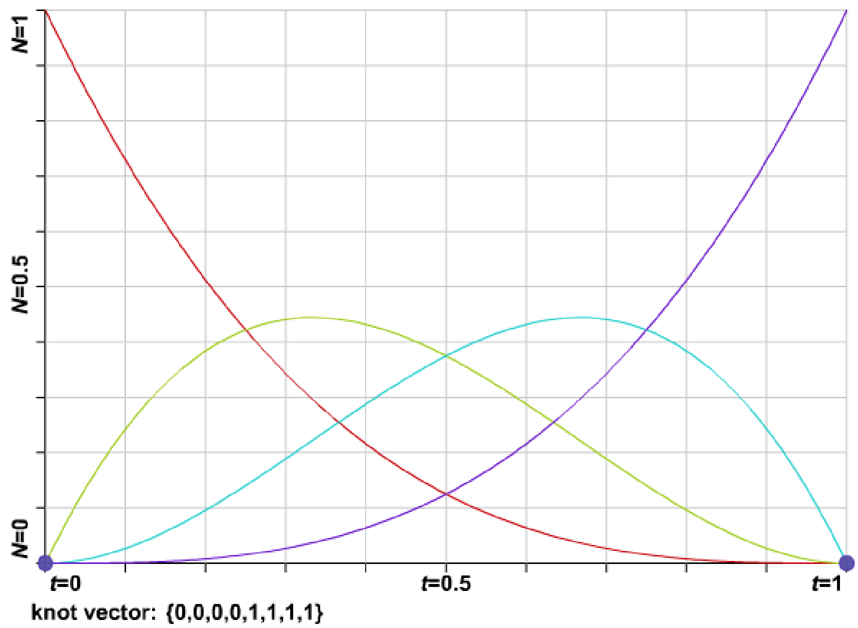
a) For Lagrange interpolation of N data points, the degree of each basis function $L_i(x)$ is N.

b) The Lagrange polynomial passes through every point of the given data set.

c) The Lagrange polynomial is the polynomial of highest degree that assumes the value y_i at each point x_i of a data set $\{x_i, y_i\}, i = 1...N$.

Question 2: B-Splines (4 points)

You are given the set of B-splines shown in the following figure, with the corresponding knot vector $\{0, 0, 0, 0, 1, 1, 1, 1\}$.



a) What is the order of the B-splines? Explain your answer.

b) Are the B-splines "clamped" or "unclamped"? Explain your answer.

Question 3: Orthonormal Basis Functions (4 points)

Let y_1, y_2 be non-zero functions on $[-1, 1]$. Let $\langle f, g\rangle$ denote a scalar dot product. State whether the following statements are true or false:

a) Define $\phi_2 = y_2 - y_1 \cdot \frac{\langle y_1, y_2\rangle}{\langle y_1, y_1\rangle}$. The functions y_1 and ϕ_2 are orthogonal to each other.

b) Assume that $\{y_1, y_2\}$ is an orthonormal basis. Let f be another function that is approximated by $\alpha_1 y_1 + \alpha_2 y_2$. If we want to add another function y_3 to the basis, we have to orthonormalize it with respect to $\{y_1, y_2\}$ and recalculate the coefficients for the approximation.

c) Assume that $\{y_1, y_2\}$ is an orthonormal basis. To augment this orthonormal basis by another function y_3 it is sufficient for it to be orthogonal to y_1 and have norm 1.

d) Let B be a set of orthonormal basis functions of a function space H. Every function ϕ in H may be written as:

$$\phi = \sum_{b \in B} \langle \phi, b \rangle b.$$

Question 4: B-Splines (6 points)

State whether the following statements are true or false. Justify your answer.

a) The knot vector $\{0, 0, 0.2, 0.7, 0.5, 1, 1\}$ is valid to build B-Splines basis functions.

b) The knot vector $\{0, 0.25, 0.5, 0.75, 1\}$ can be used to generate B-Splines of degree 3 at most.

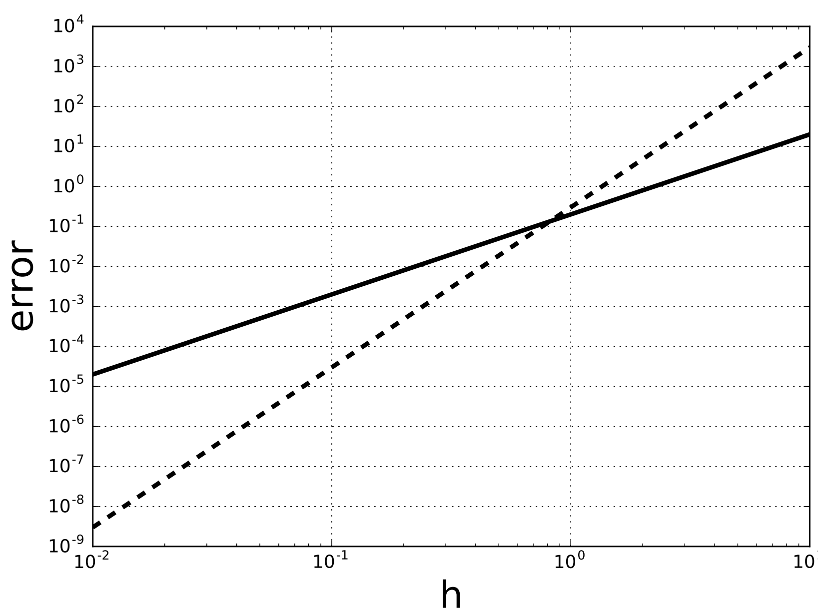
c) The knot vector $\{0, 0, 0.5, 1, 1\}$ can generate at most 4 basis functions.

Question 5: Rate of convergence (6 points)

You integrated $f(x)$ numerically in the interval $[a, b]$ using two different rules: composite Trapezoidal and composite Simpson's rule. Then you performed a convergence study for both rules, and the resulting error plot is shown in the figure below (using logarithmic scale).

a) Which rule (composite Trapezoidal, composite Simpson's) corresponds to which line (continuous, dashed) in the figure? Justify your answer (no need to provide computations).

b) You perform numerical integration with the composite Trapezoidal rule twice, first using N_1 points, and then using 10 times more points ($N_2 = 10N_1$). If the error of your first integration is ϵ_1, give an estimate of the error ϵ_2 when using N_2 points. Justify your answer with rough calculations.



Question 6: Order of accuracy (6 points)

a) Explain one numerical and one analytical way to find the order of accuracy for a numerical method.

b) Let G_1 and G_2 be two numerical methods that both approximate the same quantity. Assume that G_1 is a first-order and G_2 a second-order method. Is the error of G_2 always smaller than the error of G_1? Explain your answer.

Question 7: Least Squares (8 points)

You are given N data points (x_i, y_i). Let α and β be the coefficients of a least squares fit to a linear function $y_i \approx \alpha x_i + \beta$.

a) Find a point such that α and β for the sets of $N+1$ and N points are the same.

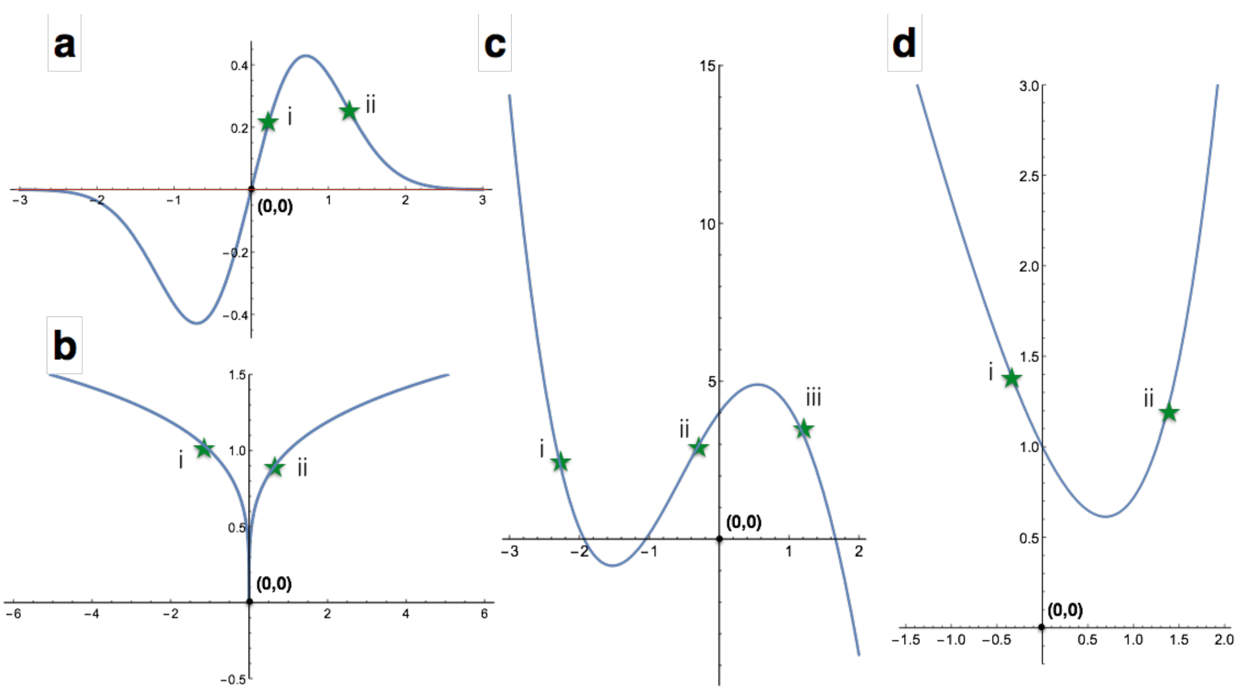
b) Find three points that do not all lie on the same line, such that α and β for the sets of $N+3$ and N points are the same.

Explain your choice.

Question 8: Newton's method (8 points)

You are given the function graphs below. For every function graph state whether it is possible to evaluate one or more roots of the function with Newton's method, starting from the marked points (stars) as initial guesses for the method. Provide a short explanation for your answers.

Note: The x-axis in graph (a) is an asymptote.



Question 9: Numerical integration (10 points)

a) For each of the following situations, select the most appropriate method of integration from the following list: composite Trapezoidal; Romberg; Adaptive; Gauss; Monte Carlo. Explain your choice. You may use the choices provided more than once if necessary.

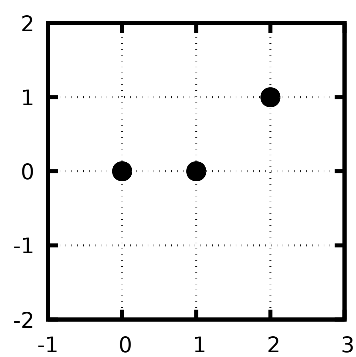
   1. The function is very smooth. Function evaluations are costly.
   2. You want to implement one-dimensional integration quickly for a proof of concept. High accuracy is not so important at this stage.
   3. The function has a non-continuous first derivative at a few known points.
   4. The function has a non-continuous first derivative at a few unknown points.
   5. Function evaluations are cheap and you want to achieve a certain error threshold.
   6. The function is 10-dimensional.

b) To integrate a polynomial of order 11 exactly, Gauss quadrature needs 6 quadrature points while Newton-Cotes formulas need 12 points. Explain why Gauss quadrature needs fewer points than the Newton-Cotes formulas.

Numerical Problems

Question 10: Cross Validation (6 points)

A data set consists of three points $(0, 0)$, $(1, 0)$, $(2, 1)$:



Choose which model $y = b$ or $y = ax + b$ best fits this dataset, using Leave-One-Out Cross validation. Assess the fits using the mean squared error in y.

Question 11: Newton's method (7 points)

a) Derive the formula used for one iteration of Newton's method.
Hint: Taylor series expansion around the starting point x_0.

b) How many iterations does it take for Newton's method to find the root of the function $f(x) = ax + b$ for $a, b \in \mathbb{R}$ and $a \neq 0$? Justify your answer.

c) We are interested in solving the nonlinear equation $\cos(x) = e^x - 1$. Write down the formula for the estimated solution x_1 after one iteration of Newton's method starting from a given x_0.

Question 12: Richardson extrapolation (8 points)

The derivative of a function f can be approximated by the so-called central finite difference method:

$$G_0(h) = \frac{f(x+h) - f(x-h)}{2h} \approx f'(x)$$

where h is a small number.

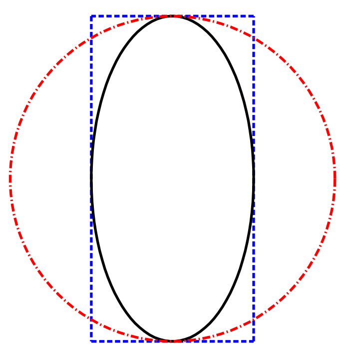
a) Show that this method is second-order accurate using Taylor series expansion. Assume that the function f is infinitely differentiable.

b) Derive a better approximation to $f'(x)$ by applying Richardson's idea to the error formula you derived in subquestion a), i.e., derive the formula for $G_1(h)$.

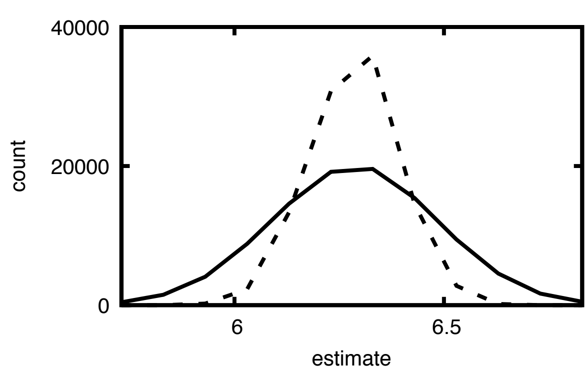
c) What is the order of accuracy of $G_1(h)$? Explain why.

Question 13: Monte Carlo Integration (8 points)

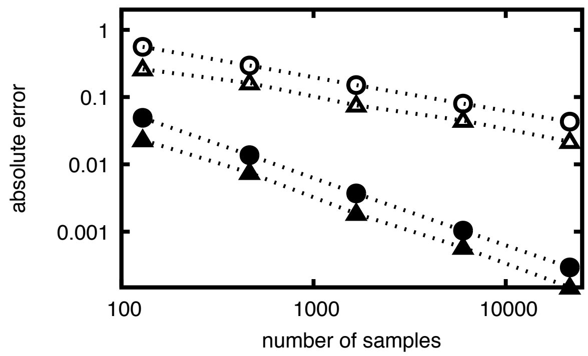
You use the Monte Carlo method to estimate an area of an ellipse. As sampling space you choose two different configurations: a rectangle and a circle.



a) You perform Monte Carlo integration 100000 times using the same number of samples every time, and you record a histogram (Histogram of a quantity: Divide the range of values into a series of intervals and count how often the estimate lies in each of these intervals ("bins")) of the area estimates. The histograms for the two sampling spaces are shown below. Which histogram corresponds to which sampling space? Justify your answers.



b) Out of the four curves plotted below, only two represent convergence plots for the Monte Carlo method. Identify these two curves. Out of these two, which one corresponds to the rectangular sampling space? Which one corresponds to the circular sampling space? Justify your answers.



Question 14: Lagrange Interpolation (10 points)

The time-dependent position of an accelerating car is described by the following relation:

$$x(t) = v_0 \cdot t + \frac{1}{2}\alpha \cdot t^2$$

where α is the constant acceleration and v_0 is the initial velocity. For certain values of α and v_0 we get the following exact data:

t [s]	x(t) [m]
1	4
2	10
4	28
5	40
10	130

a) Calculate the position of the car at $t = 8s$ using Lagrange interpolation. Use the fact that $x(t)$ is a quadratic function.

b) Your friend Alice does not know that $x(t)$ is quadratic, but she is trying to deduce the correct relationship using the data given in the table and Lagrange interpolation. If she uses all the data points given ($N = 5$), what will be the order of the Lagrange basis polynomials? How will the Lagrange interpolating function change if she uses $N = 3, 4$, or 5 data points?

c) What would change if instead of Lagrange Interpolation, Alice used Least Squares to fit a quadratic function to all of the data given in the table?

Question 15: Gauss Quadrature (10 points)

Consider the 2-point Gauss quadrature rule for the interval $[-1, 1]$:

n	points x_i	weights w_i
2	$\pm\sqrt{\frac{1}{3}}$	1

a) Write down the expression of the numerical integral of a function f over the interval $[-1, 1]$ using the above Gauss quadrature rule. How does this expression change for the general interval $[a, b]$?

b) Show that the 2-point Gauss quadrature integrates exactly any polynomial of degree 3 on the interval $[-1, 1]$.

c) Show that in general, the 2-point Gauss quadrature does not integrate exactly polynomials of degree 4.

Question 16: Polygons in circle (12 points)

Consider n-sided regular polygons inscribed in a unit circle. The perimeter of a polygon can be seen as an approximation to the circumference of the circle (2π). Compute the perimeter for $n = 4$ (square) and $n = 8$. Improve the approximation using Richardson extrapolation (assume that the method is second-order accurate), and compute the error.

Question 17: Gram-Schmidt orthonormalization (12 points)

Consider the set of functions $\Phi = \{1, x, \sin(x)\}$ on $[-\pi, \pi]$. Let $\langle f, g\rangle = \int_{-\pi}^{\pi} f(x)g(x)\ \mathrm{d}x$ be the scalar product on the function space spanned by Φ.

a) Prove that Φ is not an orthonormal set of functions.

b) Find the orthonormalized version of Φ using Gram-Schmidt orthonormalization.

Note: Formula for integration by parts for $u(x), v(x)$:

$$\int_a^b u(x)v'(x)dx = [u(x)v(x)]_a^b - \int_a^b u'(x)v(x)dx$$

Question 18: Newton-Cotes formulas (12 points)

The Newton-Cotes formula with $n+1$ quadrature points $x_0, \ldots, x_n$ is given by

$$\int_a^b f(x)\ \mathrm{d}x \ \approx\ I_{\mathsf{NC}} = (b-a)\sum_{k=0}^{n} C_k^n f(x_k).$$

a) What is the connection between Lagrange polynomials and Newton-Cotes formulas?

b) Assume that the quadrature points are arranged symmetrically in the interval $[a, b]$ (i.e., $|a - x_k| = |b - x_{n-k}|$). Show that the corresponding weights are symmetric as well, i.e., show that

$$C_k^n = C_{n-k}^n.$$

Hint: $\int_a^b f(x)\ \mathrm{d}x = \int_b^a (-f)(x)\ \mathrm{d}x$.

c) Derive a Newton-Cotes quadrature rule that is exact for polynomials of order 3 on the interval [0,1].
Hint: $\sum_{k=0}^{n} C_k^n = 1$.

Question 19: Cubic splines (18 points)

We associate to a curve $f : [a,b] \to \mathbb{R}$ the following curvature energy:

$$U[f] = \int_a^b [f''(x)]^2 \, dx.$$

We want to show that the cubic spline S with natural boundary conditions is the interpolating curve that minimizes the above energy, i.e., we want to show that

$$U[S] \le U[f] \text{ for all interpolating functions } f \in \mathcal{C}^2([a,b]).$$

Let $f \in \mathcal{C}^2([a,b])$ ($\mathcal{C}^2([a,b])$ is the set of all functions $f : [a,b] \to \mathbb{R}$ with continuous second derivative.) be an arbitrary interpolating function and S be a cubic spline that both interpolate the same data points.

a) Introduce $g = f - S$ and show that

$$U[f] = U[S] + U[g] + 2\int_a^b S''(x)g''(x)dx.$$

b) Show that

$$\int_a^b S''(x)g''(x)dx = -\int_a^b S'''(x)g'(x)dx.$$

Hint: Use integration by parts.

c) Show that

$$\int_a^b S'''(x)g'(x)dx = 0.$$

Hint: Split the integral into subdomains, use the properties of the cubic splines and of the function g.

d) Using your previous results, show that the cubic spline interpolation is the one minimizing the curvature energy.

Question 20: Cubic splines (20 points)

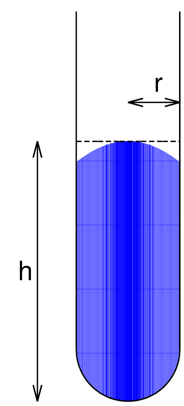
The 'not-a-knot' boundary condition for cubic splines means that the third derivative of the spline is continuous at the nodes x_1 and x_{N-1} (assuming the nodes are $x_0, x_1, \cdots, x_{N-2}, x_{N-1}, x_N$). Let f be the interpolating spline and $f_i'' = f''(x_i), i = 0, \ldots, N$.

a) Derive the additional equations for the f_i'' that follow from this boundary condition.

b) Write down the full matrix system of equations that has to be solved when constructing the cubic spline with $N = 4$.

Question 21: Volume of a liquid column (26 points)

Mercury in a test tube (German: Reagenzglas) forms a convex meniscus, i.e., a curved surface. The cross-section of the test tube is shown below.



Here $h = 2$cm and $r = 0.4$cm. The bottom of the test tube is a hemisphere. By choosing a suitable coordinate system, the meniscus can be described by a paraboloid of the form $z = -x^2 - y^2 + c$.

a) Choose a coordinate system so that the meniscus can be described by the given formula. What is the value of c?

b) Compute the area of the cross-section of the mercury in the test tube analytically.

c) Compute the area of the cross-section of the mercury in the test tube numerically using a method that is at least second-order accurate. Use at least 4 sub-intervals.

d) Find the volume of the column using using the midpoint rule (rectangle rule). Use at least 4×4 sub-domains for setting up your problem, and then exploit any useful geometrical features to reduce your computational effort.

Pseudocode

Question 22: Gram-Schmidt orthonormalization (15 points)

Write a pseudocode to orthonormalize a given set of vectors using the Gram-Schmidt method.

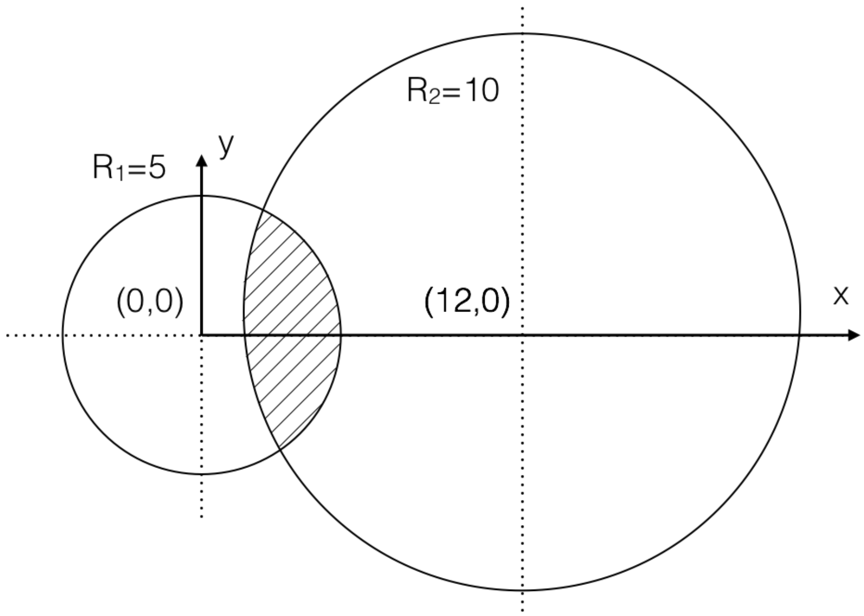
Question 23: Monte Carlo Sampling (20 points)

a) Write a pseudocode to calculate the overlapping area of the two circles shown below using Monte Carlo Sampling. Assume that you have a function `random()`, which returns a uniformly distributed random number in the interval $[0, 1]$.

b) What would you have to change in your pseudocode if you wanted to estimate the error of the Monte Carlo sampling? Answer qualitatively, do not write any pseudocode.

c) How does the error of the method change if you use 10 times more samples?

d) How does the error of the method change if you use a two times larger sampling space?



Good luck!