Project Milestone 4 – Algorithm Refinement and Final Deliverable

Instructions

- 1. Read this document carefully. You are responsible for following all instructions in this document.
- 2. Read the Learning Objectives at the end of the document to understand how your work will be graded.
- 3. Use professional language in all written responses and format all plots for technical presentation. See EPS01 and EPS02 for guidelines.
- 4. Good programming standards apply to all m-files.
- 5. Submit deliverables to Gradescope. Name your files to match the format in the table below, where SSS_TT is your section and team ID (e.g., 001_03 is Section 001, Team 3)

Item	Deliverables		
M4 Answer Sheet	M4_AnswerSheet_SSS_TT.pdf		
M4 Algorithm	M4_Algorithm_SSS_TT.m		
M4 Main Function	M4_Main_ <i>SSS_TT</i> .m		
Technical Brief	M4_TechnicalBrief_SSS_TT.pdf		

See submission requirements on the last page of this answer sheet.

6. Complete the Assignment Header before starting the answer sheet.

Assignment Header

Team Member Name	Purdue Career Account Login
Creigh Dircksen	cdirckse@purdue.edu
Joe Pahoresky	Jpahores@purdue.edu
Winston Lin	wylin@purdue.edu
Taylor Duchinski	tduchins@purdue.edu

Role of Each Team Member

In this section, put each team member's name who worked on this milestone. In the Detailed Description of Work, each person on the team should write their own description of how they contributed to this milestone. Be very detailed here. Then in the last column, your team should estimate the percentage of the work that each team member did on the milestone. This column needs to add up to 100%. We know that on any given milestone that this will vary, but one person in the team should not be doing significantly more than the others throughout the whole project. Use this column as a way for you to make sure your workload is balanced throughout the project.

Team Member Name	Detailed Description of Work	Percent of Work
Creigh Dircksen	Technical Brief, Vmax function, Refinement	25%

Joe Pahoresky	Feedback Review, Resume, Refinement, Figures	25%
Winston Lin	Main Function, V0i function, Technical Brief	25%
Taylor Duchinski	Refinement, Technical Brief	25%

Part 0: M3 Feedback Review

Reflect on your M3 feedback for the purpose of improvement. Your reflection should provide a clear, useful summary of your M3 feedback and provide a clear and practical plan to address the issues. Complete Table 1 below.

Table 1. Feedback summary and plan

Part A: Based on your feedback from M3, identify at least one strength and one limitation of your team's work in M3. Consider how the feedback you received on M3 could lead to improvements in your work.

The strength of the team's work in this project was how we worked together in creating the algorithm. We created an algorithm that did what it was supposed to do well. A specific strength of the algorithm was the calculation portion. While working on it. We commented well enough to know what was calculated below so we knew where to figure out the mistakes when we ran into problems. A weakness of our group in the answer sheet was understanding what type of graph the answer sheet called for and implementing it properly. A weakness in our code was accurately describing actions through comments. While we were properly commented for calculation type. We did not describe the calculation inputs and outputs well to an outsider.

Part B: Explain how you will incorporate the M3 feedback to improve your parameter identification (do not just reword your response from Part A; include concrete actions you will take).

Based on our feedback from M3 we need to make sure we are properly formatting the graphs we make for a technical presentation. We are working to ensure that our figures with multiple subplots are properly labeled and displayed to be most helpful. To do this we are putting titles on the subplots to make sure it is technically presented to be most helpful. Moreover, we are adding grid lines where needed to show the scale of our figures better.

Part 1: Algorithm Improvements Plan

Respond to each of the prompts below in the space provided. Your goal is to introduce the **two improvements** to your M3 algorithm. Use your ideas from Part 3 of M3 to help formulate ideas. Briefly describe, in words (not code), the nature of the improvements you will implement in your MATLAB code. Provide a brief, but thoughtful, description of your refinement, using evidence-based rationales for why the refinement is necessary and should improve your solution. Read the rest of this document carefully **before** you begin your work on this milestone. Once you are ready to begin Part 1, put your refinements and your rationale in Table 2.

Table 2. Algorithm refinement plans

Refinement 1

Parameter(s) Targeted: V0i

Description

Instead of using the rise over run method that we used previously, we could use a more defined method. We used to simply take the average slope of the first twenty values and use that as the V0i. Now we will implement least squared regression (Kenton) for the first number of data points to find the best fit line for those first number of points and use the slope of that model as the value for V0i. We would determine that number of points by testing using every number of the first datapoints and checking all their percent errors and choosing the number with the least percent error. Percent error is what percentage the calculated value is from the actual value (Anne Marie Helmenstine). That way, we can truly know what matrix we should pass into the V0i function to get the most accurate result.

We can see the improvement by taking the new percent error of the V0is that comes out of the equation. If the method is improved, then the percent error should be lower. We can also test SSE with all the V0is compared to a benchmark Michealis-Menten equation with reference Vmax and Kms and see if the new V0is have a lower SSE.

Rationale for Refinement

Because our previous method is not an actual method used by engineers it is not as reliable or accurate as the least squares method. This method is used and taught to engineers because it works and by implementing it, we should see a decrease in precent error. Also, as stated before, the number of values chosen to calculate V0i is completely arbitrary. With this method, we will have a defined number of values that we know are going to give the most accurate results.

Refinement 2

Parameter(s) Targeted: V0i

Description

We want to refine the sample size and scope used to calculate V0i to get more accurate Km and Vmax values. We do this by running our algorithm and checking which data length reduces the percent error the most in our data based off the test data given. Once we find the best sample size to reduce percent error, we implement the sample size for the 5 Enzymes given to find a more accurate representation of V0i.

Rationale for Refinement

This refinement is valid because we test based off the known values to see what the best sample size is to reduce error. Once we know that, we can implement it to see the reduction of error for Km and Vmax error.

Part 2: Algorithm Refinements Implementation

Before you make any changes to your code, resave your M3 code files as

- M4_Algorithm_SSS_TT.m
- M4_Main_SSS_TT.m

Implement improvements in M4_Algorithm_SSS_TT.m. Clearly comment where you made improvements within the code, using the text 'Improvement 1' or 'Improvement 2' and a concise, meaningful description of the change for each improvement.

Do not delete any code as you implement the improvements: comment out unnecessary code and comment on the change. Clearly indicate where new code is added with the commenting described above.

Evaluate the improvements in your algorithm by using the data for the reference enzyme PGO-X50 from M3. Compare the parameters identified for the PGO-X50 data using the algorithm you submitted in M3 and your refined algorithm for M4. This step ensures that you can compare the percent error of your algorithm known values of the data. Report your results in Table 3. Use appropriate decimal places.

Table 3. Algorithm refinement comparison

Parameter (μM/s)	PGO-X50 Reference Values	M3_Algorithm	Percent Error between PGO-X50 and M3_Algorithm	M4_Algorithm	Percent Error between PGO-X50 and M4_Algorithm
v_{0_1}	0.025	0.0303	21.263%	0.025	0.034%
v_{0_2}	0.049	0.0617	25.832%	0.0502	2.404%
v_{0_3}	0.099	0. 1152	16.332%	0.0989	0.099%
v_{0_4}	0.176	0. 2086	18.529%	0.1765	0.262%
v_{0_5}	0.329	0. 3930	19.456%	0.3342	1.595%
v_{0_6}	0.563	0. 6167	9.530%	0.5606	0.419%
v_{0_7}	0.874	0. 8609	1.497%	0.8440	3.434%
v_{0_8}	1.192	1. 2153	1.956%	1.1701	1.841%
v_{0_9}	1.361	1. 3799	1.388%	1.3480	0.959%
$v_{0_{10}}$	1.603	1. 5986	0.274%	1.5639	2.442%
V_{max}	1.806	1.6265		1.7326	
K_m (μ M)	269.74	196.2		254.9545	

Next, use your M4 algorithm to analyze the full 100 enzyme test data sets and obtain the parameters V_{max} and K_m . Here you will run your M3 algorithm and your updated M4 algorithm on the full data set. You may need to make adjustments to both algorithms to account for the replicate data sets and 5

enzymes. In Table 4, record your results from both your M3 and M4 algorithm. Use appropriate decimal places.

Table 4. M3 and M4 algorithm comparison of experimental data parameters

	M3 Algorithm		M4 Algorithm		
Enzyme	Enzyme Parameters		Enzyme Parameters		
	V _{max} (μM/s)	<i>K_m</i> (μM)	V _{max} (μM/s)	<i>K_m</i> (μM)	
NextGen-A	.969	143.34	0.983	164.78	
NextGen-B	.939	357.64	0.910	364.08	
NextGen-C	1.379	202.24	1.324	218.79	
NextGen-D	1.642	286.13	1.532	292.83	
NextGen-E	1.526	138.44	1.608	178.60	

In Table 5, include any references you used throughout this answer sheet for Parts 0-2. Use APA format. Make sure there is an in-text citation for all references listed and vice versa.

Table 5. References used in Parts 0-2 (if any)

Anne Marie Helmenstine, P. D. (2020, November 2). *This is how to calculate percent error*. ThoughtCo. Retrieved April 15, 2022, from https://www.thoughtco.com/how-to-calculate-percent-error-609584

Kenton, W. (2022, March 29). *Understanding the least squares method*. Investopedia. Retrieved April 15, 2022, from https://www.investopedia.com/terms/l/least-squares-method.asp

Part 3: Technical Brief

Consult the M4 memo from NaturalCatalysts, Inc. for the details concerning your technical brief. Use the provided template M4_TechnicalBrief_template.docx to respond to the memo. You may find the original introduction memo and the project background documents helpful when composing your technical brief.

Part 4: Resumé Insert

In response to the opportunity presented in the NaturalCatalysts memo, create an insert for your resumé by completing the following on this answer sheet:

Guidance:

Summarizing your ENGR 132 project for your resumé

Choose a header and specific language to describe your project. Possible Headers for Engineering 132 Project Descriptions include: Engineering Projects, Design Projects, Related Experience, Engineering Experience. The specific language should be "action" oriented and highlight both the project and your contributions to it. Your project title should be something that describes this project.

Template:

HEADER

Project Title, Purdue University

Semester YYYY

- Power Verb (Skill) + Identifiable task + Purpose/Method/or Result
- Power Verb (Skill) + Identifiable task + Purpose/Method/or Result
- Power Verb (Skill) + Identifiable task + Purpose/Method/or Result

Example:

DESIGN PROJECTS

Autonomous Lawn Mower, Purdue University

Spring 2020

- Improved sensor technology resulting in increased safety and reduced cost
- Developed MATLAB code to optimize sensor performance and to perform constraint analysis
- Constructed and tested a functional prototype that surpassed industry standards

Things to keep in mind:

- Headers should stand out (Bold/Underlined/Larger Font and/or CAPS).
- Do not use "Engineering 132" Project as the project title. Prospective employers will not know what that title means. Give the project a descriptive name.
- Differentiate between project title and location using style change or location variance.
- Separate the location and the date of the project. Placing the date on the right side of the page is common, but not required.
- Your 3-5 bulleted statements should all maintain the *same tense* (past if previously completed, or present if currently working on).
- Begin each bullet with a different power verb.
- For these 3-5 statements, try to answer the questions "What did you do?", "How did you do it?", and "What was your result?"

NaturalCatalysts Project

Resumé Text: In the space below, write a summary of your project suitable for inclusion on your resumé. Be sure to use the guidelines above regarding formatting and language. A resumé typically includes 3-5 bullet items describing a project. The stems for your bullet points should be power verbs that convey what you did on the project (i.e., implemented, led, developed, analyzed, etc.). Use your individual versions from the video activity to create a team version here.

Engineering Design Project

Enzyme Data Modeling, Purdue University

Spring 2022

- Wrote code to create a usable model representing the initial speed of a given Enzyme Reaction
- Researched and Tested code off actual values to find errors and how to improve them.
- Produced constants that can be used in the equation to find initial velocity given a specific Concentration of the enzyme.

Finally, you should each add this insert or your individual one from the video activity into your own resumé.

How to Submit

- 1. Save this answer sheet as a PDF named **M4_AnswerSheet_SSS_TT.pdf** where **SSS** is your section number (e.g., 001 for section 001) and **TT** is your team number (e.g., 07 for team 7).
- Save your technical brief document as a PDF named M4_TechnicalBrief_SSS_TT.pdf.
- 3. Select one person to submit the deliverables for the team. That person should
 - a. Log into Gradescope and submit all deliverables to the M4 assignment.
 - i. M4_AnswerSheet_SSS_TT.pdf
 - ii. M4_Algorithm_SSS_TT.m
 - iii. M4_Main_*SSS_TT*.m
 - iv. M4_TechnicalBrief_SSS_TT.pdf
 - b. Select all team members for the group assignment and submit.
 - c. Double-check that all team members are assigned to the submission.
- 4. Each team member should confirm that they are part of the submission.
- 5. After submission, distribute the submitted files to all team members. *Ensure all members of the team have copies of the submitted files.*

Learning Objectives

Teamwork (TW)

Contribute to team products and discussions

TW02. Document all contributions to the team performance with evidence that these contributions are significant.

Process Awareness (PA)

Reflect on both personal and team's problem solving/design approach and process for the purpose of continuous improvement.

PA01. Identify strengths in the approach used.

PA02. Identify limitations in the approach used.

PA03. Identify potential behaviors to improve approach in future problem solving/design projects.

Idea Fluency (IF)

Generate ideas fluently. Take risks when necessary.

IFO3. Generate testable prototypes (including process steps) for a set of potential solutions.

Evidence-Based Decision Making (EB)

Use evidence to develop and optimize solution. Evaluate solutions, test and optimize chosen solution based on evidence.

- EB01. Test prototypes and analyze results to inform comparison of alternative solutions.
- EB03. Clearly articulate reasons for answers with explicit reference to data to justify decisions or to evaluate alternative solutions.
- EB05. Present findings from iterative testing or optimization efforts used to further improve aspect or performance of a solution.
- EB06. Clearly articulate reasons for answers when making decisions or evaluating alternative solutions.

Solution Quality (SQ)

Design final solution to be of high technical quality. Design final solution to meet client and user needs.

SQ01. Use accurate, scientific, mathematical, and/or technical concepts, units, and/or data in solutions.

Information Literacy (IL)

Seek, find, use and document appropriate and trustworthy information sources.

- ILO4. Include citations within the text (in-text citations) that show how the references at the end of the text are used as evidence to support decisions.
- ILO5. Format reference list of used sources that is traceable to original sources (APA or MLA are recommended)

Engineering Professional Skills

- PC05. Fully address all parts of assignment by following instructions and completing all work.
- EPS01. Use professional written and oral communication.
- EPS02. Format plots for technical presentation.

Programming

MAT01. Develop code that follows good programming standards.

MAT05. Create and use MATLAB scripts and functions.

MAT08. Debug scripts and functions to ensure programs execute properly, perform all required

tasks, and produce expected results.