

Project report: Gauss-Newton optimization method

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1 Introduction

This project investigates fitting a function such as

$$\varphi(\mathbf{x}; t) = x_1 e^{-x_2 t} + x_3 e^{-x_4 t},$$

where $\mathbf{x} = (x_1, x_2, x_3, x_4)^T$ are parameters, to a given set of data points $(t_i, y_i), i = 1, \dots, m$.

In particular, we seek to minimize the sum of the squared distances from each data point (t_i, y_i) to the point $(t_i, \varphi(\mathbf{x}; t_i))$. If we denote the distance by $r_i(\mathbf{x}) = \varphi(\mathbf{x}; t_i) - y_i$, then our goal is to

$$\underset{\mathbf{x} \in \mathbb{R}^4}{\text{minimize}} f(\mathbf{x}) \quad \text{where} \quad f(\mathbf{x}) = \sum_{i=1}^m r_i(\mathbf{x})^2.$$

To solve this minimization problem, we use the Gauss-Newton method.

2 Methods

2.1 Gauss-Newton method

Let $r(\mathbf{x}) = (r_1(\mathbf{x}), \dots, r_m(\mathbf{x}))^T$. We claim that

$$r(\mathbf{x} + \boldsymbol{\delta}) \approx r(\mathbf{x}) + J(\mathbf{x})\boldsymbol{\delta},$$

where $J(\mathbf{x})$ is the Jacobian matrix of $r(\mathbf{x})$ and $\boldsymbol{\delta}$ is an increment vector, also a direction vector.

This can be thought of as extending the concept of using the tangent line to estimate nearby values to higher dimensions.

We then observe that

$$\begin{aligned} f(\mathbf{x} + \boldsymbol{\delta}) &= \sum_{i=1}^m r_i(\mathbf{x} + \boldsymbol{\delta})^2 \\ &= r(\mathbf{x} + \boldsymbol{\delta})^T r(\mathbf{x} + \boldsymbol{\delta}) \\ &\approx (r(\mathbf{x}) + J(\mathbf{x})\boldsymbol{\delta})^T (r(\mathbf{x}) + J(\mathbf{x})\boldsymbol{\delta}). \end{aligned}$$

Since we want the output of f to be the minimum possible, the gradient of this approximation should be 0. Writing that as an equation and simplifying, we end up with

$$-J(\mathbf{x})^T J(\mathbf{x})\boldsymbol{\delta} = J(\mathbf{x})^T r(\mathbf{x}).$$

This presents the following iterative algorithm. First, we make an initial guess \mathbf{x}_0 for \mathbf{x} , and then we:

1. Solve the linear system $-J(\mathbf{x})^T J(\mathbf{x})\boldsymbol{\delta} = J(\mathbf{x})^T r(\mathbf{x})$ for $\boldsymbol{\delta}$.
2. Determine an optimal step length λ for direction $\boldsymbol{\delta}$ using a line search algorithm.
3. Update \mathbf{x} to $\mathbf{x} + \lambda\boldsymbol{\delta}$.

We repeat these actions until the step $\lambda\boldsymbol{\delta}$ is smaller than some chosen tolerance. Step size tolerance is a good choice for the stop criterion because we already have to compute $\lambda\boldsymbol{\delta}$ as part of each iteration.

As a practical consideration, we have added a small regularization term to the linear system in our implementation, as in

$$-(J(\mathbf{x})^T J(\mathbf{x}) + \varepsilon I)\boldsymbol{\delta} = J(\mathbf{x})^T r(\mathbf{x}),$$

to help prevent numerical instability.

2.2 Line search algorithm

For the line search mentioned in the second step of the Gauss-Newton iteration algorithm, we use Armijo's rule on $F(\lambda) = f(\mathbf{x} + \lambda\boldsymbol{\delta})$.

Let $T(\lambda) = F(0) + \varepsilon F'(0)\lambda$ be a straight line through $(0, F(0))$ with less negative slope than the point's tangent, so $0 < \varepsilon < 1$.

Armijo's rule is made up of two (upper and lower) conditions, which are

$$F(\lambda) \leq T(\lambda) \quad \text{and} \quad F(\alpha\lambda) \geq T(\alpha\lambda) \quad \text{for fixed } \alpha > 1.$$

This rule ensures λ will be in an *interval* of points where F is substantially smaller. Computationally, this is faster than looking for a perfect choice for λ . This makes an Armijo's rule based algorithm a good choice for this project.

So that λ satisfies Armijo's rule, we choose it as follows:

1. Make an initial guess for λ .
2. Repeatedly scale λ up by α until it satisfies the lower condition.
3. Repeatedly scale λ down by α until it satisfies the upper condition.

3 Project work

3.1 Structure

The project is [stored on GitHub as a repository](#). It is made up of:

- phi1.m, phi2.m, data1.m, data2.m, grad.m as provided,
- gaussnewton.m, the implementation of the Gauss-Newton method,
- line_search.m, the line search algorithm based on Armijo's rule,
- script.m, the main script containing tests and tasks,
- report.tex and report.pdf, forming this report,
- metadata and configuration files.

3.2 Responsibilities

Nicolas handled most of the MATLAB programming for the project, including implementing the Gauss-Newton method and creating the main script file.

Artis was responsible for maintaining the project repository, and also helped with implementing the line search algorithm in MATLAB.

Vidar and Artis worked together on creating the \LaTeX report for the project. In particular, Vidar worked on the analysis of different initial guesses and strategies for choosing the initial point.

3.3 Results

We fit the two functions from `phi1.m` and `phi2.m`,

$$\varphi_1(\mathbf{x}; t) = x_1 e^{-x_2 t}, \quad \mathbf{x} = (x_1, x_2)^T$$

and

$$\varphi_2(\mathbf{x}; t) = \varphi(\mathbf{x}; t) = x_1 e^{-x_2 t} + x_3 e^{-x_4 t}, \quad \mathbf{x} = (x_1, x_2, x_3, x_4)^T,$$

to the two sets of data points `data1` and `data2` from `data1.m` and `data2.m`. Throughout, $x_n = n$ is used for the initial guess. The results are:

Case	Optimal point \mathbf{x}	$\ \nabla f(\mathbf{x})\ _2$	$\ r(\mathbf{x})\ _\infty$
<code>data1</code> , φ_1	$(10.8108, 2.4786)^T$	$3.7450 \cdot 10^{-4}$	1.6287
<code>data2</code> , φ_1	$(12.9789, 1.7861)^T$	$8.0031 \cdot 10^{-2}$	1.0397
<code>data1</code> , φ_2	$(6.3445, 10.5866, 6.0959, 1.4003)^T$	$4.0651 \cdot 10^{-5}$	0.4334
<code>data2</code> , φ_2	$(4.1741, 0.8747, 9.7390, 2.9208)^T$	$9.5220 \cdot 10^{-3}$	0.1182

3.4 Initial points

We consider multiple initial guesses for the `data1`, φ_2 case, with the tolerance set to 10^{-4} .

It is easily seen that x_2 and x_4 must be non-negative for this function, as a negative value causes the function to blow up. The considered initial guesses follow this restriction.

We use the number of iterations and function evaluations to define how fast the system converges.

Initial guess \mathbf{x}_0	Total iterations	Function evaluations	Optimal point \mathbf{x}
$(0, 0, 0, 0)^T$	15	49	$(6.3446, 10.5865, 6.0959, 1.4003)^T$
$(100, 100, 100, 100)^T$	14	80	$(6.0959, 1.4003, 6.3445, 10.5865)^T$
$(10, 10, 10, 10)^T$	11	64	$(6.0959, 1.4003, 6.3445, 10.5866)^T$
$(1, 1, 1, 1)^T$	8	49	$(6.0959, 1.4003, 6.3445, 10.5867)^T$
$(-10, 0, -10, 0)^T$	21	81	$(6.3446, 10.5864, 6.0958, 1.4003)^T$
$(10, 0, 10, 0)^T$	16	59	$(6.3445, 10.5866, 6.0959, 1.4003)^T$
$(-5, 0, -5, 0)^T$	11	53	$(6.3445, 10.5865, 6.0959, 1.4003)^T$
$(5, 0, 5, 0)^T$	11	54	$(6.3446, 10.5864, 6.0959, 1.4003)^T$
$(-1, 0, -1, 0)^T$	16	98	$(6.0959, 1.4003, 6.3446, 10.5864)^T$
$(1, 0, 1, 0)^T$	12	60	$(6.3446, 10.5863, 6.0958, 1.4003)^T$
$(-1, 0, -5, 0)^T$	23	296	$(3.3205, 4013.4884, 9.1190, 3631.4299)^T$

The most efficient initial guess with the fastest convergence appears to be

$$\mathbf{x}_0 = (1, 1, 1, 1)^T.$$

3.5 Initial guess strategy

We introduce a strategy for picking the initial guess for φ_2 .

To find an accurate initial guess for

$$\varphi_2(\mathbf{x}; t) = x_1 e^{-x_2 t} + x_3 e^{-x_4 t},$$

we may make use of

$$\varphi_1(\mathbf{x}; t) = x_1 e^{-x_2 t}.$$

Comparing these two functions, we can use prior results from fitting φ_1 in order to get a good initial guess for φ_2 . By running the program multiple times to fit φ_1 with `data2`, we can get initial values for x_1 and x_2 that we can then use in the `data2`, φ_2 case.

As we have $-x_4$ in the exponential, we can restrict x_4 values to being non-negative. Meanwhile, x_3 still needs to be sought through a range of values, based on, for example, minimizing the amount of iterations or function evaluations.

3.6 Detailed result

For the `data2`, φ_2 case, we present a full printout. The initial point for this example is $(1, 2, 3, 4)^T$.

```
Gauss-Newton Iteration 1: Starting line search...
  Line Search Backtrack Iteration: lambda = 5.0000e-01, F(lambda) = 2.8163e+22
  Line Search Backtrack Iteration: lambda = 2.5000e-01, F(lambda) = 8.4145e+10
  Line Search Backtrack Iteration: lambda = 1.2500e-01, F(lambda) = 1.5305e+05
  Line Search Backtrack Iteration: lambda = 6.2500e-02, F(lambda) = 2.7764e+04
Gauss-Newton Iteration 1:
x = [-0.1860, 0.3882, 4.7977, 3.2363]
max(abs(r)) = 1.0019e+01, norm(grad) = 6.8024e+03, lambda = 6.2500e-02
Gauss-Newton Iteration 2: Starting line search...
  Line Search Backtrack Iteration: lambda = 5.0000e-01, F(lambda) = 2.7633e+06
  Line Search Backtrack Iteration: lambda = 2.5000e-01, F(lambda) = 1.4590e+04
Gauss-Newton Iteration 2:
x = [0.7098, -0.8628, 6.2213, 2.9969]
max(abs(r)) = 9.4068e+00, norm(grad) = 1.1161e+04, lambda = 2.5000e-01
Gauss-Newton Iteration 3: Starting line search...
Gauss-Newton Iteration 3:
x = [0.8378, -0.3380, 12.8793, 1.4757]
max(abs(r)) = 7.0874e+00, norm(grad) = 1.5113e+04, lambda = 1.0000e+00
Gauss-Newton Iteration 4: Starting line search...
Gauss-Newton Iteration 4:
x = [3.4844, 1.2798, 10.2036, 2.5278]
max(abs(r)) = 2.3072e+00, norm(grad) = 2.1603e+04, lambda = 1.0000e+00
Gauss-Newton Iteration 5: Starting line search...
Gauss-Newton Iteration 5:
x = [1.6255, 0.2138, 12.2776, 2.7719]
max(abs(r)) = 6.2761e-01, norm(grad) = 1.5974e+03, lambda = 1.0000e+00
Gauss-Newton Iteration 6: Starting line search...
Gauss-Newton Iteration 6:
x = [2.6973, 0.7203, 11.1893, 2.7070]
max(abs(r)) = 5.4273e-01, norm(grad) = 9.6006e+02, lambda = 1.0000e+00
Gauss-Newton Iteration 7: Starting line search...
  Line Search Iteration: lambda = 2.0000e+00, F(lambda) = 2.0939e+01
Gauss-Newton Iteration 7:
x = [5.5035, 1.1028, 8.4286, 3.0652]
max(abs(r)) = 3.2980e-01, norm(grad) = 8.9192e+02, lambda = 2.0000e+00
Gauss-Newton Iteration 8: Starting line search...
Gauss-Newton Iteration 8:
x = [3.7177, 0.8468, 10.1922, 2.8388]
max(abs(r)) = 2.4740e-01, norm(grad) = 2.7354e+02, lambda = 1.0000e+00
Gauss-Newton Iteration 9: Starting line search...
Gauss-Newton Iteration 9:
x = [4.1808, 0.8779, 9.7318, 2.9178]
max(abs(r)) = 1.9147e-01, norm(grad) = 3.4489e+02, lambda = 1.0000e+00
Gauss-Newton Iteration 10: Starting line search...
Gauss-Newton Iteration 10:
x = [4.1741, 0.8747, 9.7390, 2.9208]
max(abs(r)) = 1.2141e-01, norm(grad) = 7.5698e+00, lambda = 1.0000e+00
Gauss-Newton Iteration 11: Starting line search...
  Line Search Iteration: lambda = 2.0000e+00, F(lambda) = 8.9616e+00
Gauss-Newton Iteration 11: Converged with tol 1.0000e-04, max(abs(r)) 1.1817e-01.

Final Results:
x = [4.1741, 0.8747, 9.7390, 2.9208]
Final norm(grad) = 9.5220e-03
Total iterations = 11
Total function evaluations = 30
Total elapsed time: 0.2712 seconds
```

Appendix

gaussnewton.m

[illegible]

```

% 3.5. Update parameters
x = x + lambda * d;

% 3.6. Check for convergence
if norm(lambda * d) < tol
    % Compute the maximum absolute residual
    max_residual = max(abs(residual));

    fprintf(['Gauss-Newton Iteration %d: Converged with tol %.4e,' ...
            ' max(abs(r)) %.4e.\n'], N_iter, tol, max_residual);
    break; % Exit loop if update step is below the tolerance
end

% Print intermediate results if printout flag is set
if printout
    % Compute the maximum absolute residual
    max_residual = max(abs(residual));

    % Compute the gradient norm
    normg = norm(2 * J' * residual);

    % Print the iteration details
    fprintf('Gauss-Newton Iteration %d:\n', N_iter);
    fprintf('x = [%.4f, %.4f, %.4f, %.4f]\n', x);
    fprintf('max(abs(r)) = %.4e, norm(grad) = %.4e, lambda = %.4e\n', ...
            max_residual, normg, lambda);
end

% Print final results
normg = norm(2 * J' * residual); % Final gradient norm
fprintf('\nFinal Results:\n');
fprintf('x = [%.4f, %.4f, %.4f, %.4f]\n', x);
fprintf('Final norm(grad) = %.4e\n', normg);
fprintf('Total iterations = %d\n', N_iter); % Number of Gauss-Newton iterations
fprintf('Total function evaluations = %d\n', N_eval); % Evaluations in Gauss-Newton
                                                    % and line search

elapsed_time = toc; % Stop timing
fprintf('Total elapsed time: %.4f seconds\n', elapsed_time); % Display elapsed time

% Plot results if requested
if plotout
    figure; % Create a new figure
    plot(t, y, 'ro', 'MarkerSize', 6, 'DisplayName', 'Data'); % Plot data points
    hold on;
    % Plot fitted curve:
    plot(t, phi(x, t), 'b-', 'LineWidth', 1.5, 'DisplayName', 'Fitted Curve');
    legend show; % Add a legend
    title('Gauss-Newton Fit');
    xlabel('t'); % Label x-axis
    ylabel('y'); % Label y-axis
    grid on; % Add grid -> better visualization
end
end

```


line_search.m

```
function [lambda, N_eval] = line_search(F, lambda0, N_eval)

% Inputs:
% F      - Function handle for F(lambda)
% lambda0 - Initial guess for lambda
% N_eval - Function evaluation counter to be updated

% Outputs:
% lambda - Step length that minimizes F(lambda)
% N_eval - Updated function evaluation counter

% Parameters
alpha = 2;           % Alpha from Alg 3, p.53
lambda = lambda0;    % Initial lambda
F0 = F(0);           % Initial F(lambda) value
gf = grad(F,0);      % F'(0)
ep = 0.1;            % Epsilon from Alg 3, p.53

% Increment function evaluations for F(0)
N_eval = N_eval + 1;

% Increase lambda while sufficient reduction is not met
while F(alpha*lambda) < F0 + ep * gf * alpha * lambda
    lambda = alpha * lambda;
    N_eval = N_eval + 1;
    fprintf([' Line Search Iteration: lambda = %.4e, ' ...
            'F(lambda) = %.4e\n'], lambda, F(lambda));
end

% Decrease lambda while F(lambda) is still too large
while F(lambda) > F0 + ep * gf * lambda
    lambda = lambda / alpha;
    N_eval = N_eval + 1;
    fprintf([' Line Search Backtrack Iteration: lambda = %.4e, ' ...
            'F(lambda) = %.4e\n'], lambda, F(lambda));
end

% Warning to handle invalid or problematic results
if isnan(F(lambda)) || F(lambda) > F0
    warning(['Potential issue with the line search: ' ...
            'F(lambda) = %.4e, F(0) = %.4e'], F(lambda), F0);
end

return;
end
```

script.m

```
%% Line Search Subroutine Test
a_values = [2, -2, 5, -5, 10, -10]; % Test cases for a
initial_guess = 0.1; % Initial guess for lambda

% Initialize total function evaluations counter
total_N_eval = 0;

for i = 1:length(a_values)
    a = a_values(i); % Assign the current test case
    fprintf('Test %d, a = %d\n', i, a); % Print current test info

    F = @(lambda) (1 - 10^a * lambda)^2; % Define the test function

    % Initialize test-specific function evaluation counter
    test_N_eval = 0;

    % Perform line search and track function evaluations
    % Start evaluations from 0 for this test:
    [lambda, test_N_eval] = line_search(F, initial_guess, 0);
    % Add to the total evaluation count:
    total_N_eval = total_N_eval + test_N_eval;

    % Calculate expected lambda
    expected_lambda = 1 / 10^a;
    error = abs(lambda - expected_lambda);
    F_lambda = F(lambda);

    % Print results
    fprintf('Computed lambda = %.5f\n', lambda);
    fprintf('Expected lambda = %.5f\n', expected_lambda);
    fprintf('Error = %.5e\n', error);
    fprintf('F(lambda) = %.5e (should be close to 0)\n', F_lambda);
    fprintf('Function evaluations in this test = %d\n', test_N_eval);
end

fprintf('Total function evaluations in all tests = %d\n', total_N_eval);

%% Test 1
[t,y] = data1;
[x,N_eval,N_iter,normg] = gaussnewton(@phi2,t,y,[1;2;3;4],1e-4,1,1);

%% Diverse initial guessss test
[t,y] = data1;
t1 = [0; 0; 0; 0]; % Neutral start
t2 = [100; 100; 100; 100]; % Far-from-solution guess
t3 = [-10; 0; -10; 0]; % Negative values
% (x2 and x4 must >=0 for phi2, x2 must >= 0 for phi1)

t_choice = t3; % Current test

[x,N_eval,N_iter,normg] = gaussnewton(@phi2,t,y,t_choice,1e-4,1,1);

%% Task - phi1, data1
[t,y] = data1;
[x,N_eval,N_iter,normg] = gaussnewton(@phi1,t,y,[1;2;3;4],1e-4,1,1);

%% Task - phi1, data2
[t,y] = data2;
[x,N_eval,N_iter,normg] = gaussnewton(@phi1,t,y,[1;2;3;4],1e-4,1,1);

%% Task - phi2, data1 (Test 1)
[t,y] = data1;
[x,N_eval,N_iter,normg] = gaussnewton(@phi2,t,y,[1;2;3;4],1e-4,1,1);
```

```

%% Task - phi2, data2
[t,y] = data2;
[x,N_eval,N_iter,normg] = gaussnewton(@phi2,t,y,[1;2;3;4],1e-4,1,1);

%% Fit phi1 to data1/data2 for multiple starting points
% Format results_phi_data: initial guesses, final values, N_eval, N_iter, normg
[t1, y1] = data1;
[t2, y2] = data2;

% Define range of starting points
num_start_points = 4; % Number of different starting points
x1_range = linspace(0.1, 20, num_start_points);
x2_range = linspace(0.01, 10, num_start_points); % Reminder: x2>0 required

% Loop over different starting points for data1
results_phi1_data1 = [];
fprintf('Fitting phi1 to data1:\n');
for x1 = x1_range
    for x2 = x2_range
        x0 = [x1; x2]; % Initial guess
        [x, N_eval, N_iter, normg] = gaussnewton(@phi1, t1, y1, x0, 1e-4, 0, 0);
        results_phi1_data1 = [results_phi1_data1; x0', x', N_eval, N_iter, normg];
        fprintf(['Initial: [%.2f, %.2f], Final: [%.2f, %.2f], ' ...
            'Iterations: %d, Normg: %.2e\n'], ...
            x1, x2, x(1), x(2), N_iter, normg);
    end
end

% Loop over different starting points for data2
results_phi1_data2 = [];
fprintf('\nFitting phi1 to data2:\n');
for x1 = x1_range
    for x2 = x2_range
        x0 = [x1; x2]; % Initial guess
        [x, N_eval, N_iter, normg] = gaussnewton(@phi1, t2, y2, x0, 1e-4, 0, 0);
        results_phi1_data2 = [results_phi1_data2; x0', x', N_eval, N_iter, normg];
        fprintf(['Initial: [%.2f, %.2f], Final: [%.2f, %.2f], ' ...
            'Iterations: %d, Normg: %.2e\n'], ...
            x1, x2, x(1), x(2), N_iter, normg);
    end
end

%% Fit phi2 to data1/data2 for multiple starting points
% Format results_phi_data: initial guesses, final values, N_eval, N_iter, normg
[t1, y1] = data1;
[t2, y2] = data2;

% Define the range of starting points
num_start_points = 4; % Number of different starting points
x1_range = linspace(0.1, 20, num_start_points);
x2_range = linspace(0.01, 10, num_start_points); % Reminder x2>0 required
x3_range = linspace(0.1, 20, num_start_points);
x4_range = linspace(0.01, 10, num_start_points); % Reminder: x4>0 required

% Loop over different starting points for data1
results_phi2_data1 = [];
fprintf('\nFitting phi2 to data1:\n');
for x1 = x1_range
    for x2 = x2_range
        for x3 = x3_range
            for x4 = x4_range
                x0 = [x1; x2; x3; x4]; % Initial guess
                [x, N_eval, N_iter, normg] = gaussnewton(@phi2, t1, y1, x0, 1e-4, 0, 0);
                results_phi2_data1 = [results_phi2_data1; ...
                    x0', x', N_eval, N_iter, normg];
            end
        end
    end
end

```

```

        fprintf(['Initial: [%.2f, %.2f, %.2f, %.2f], ' ...
                'Final: [%.2f, %.2f, %.2f, %.2f], ' ...
                'Iterations: %d, Normg: %.2e\n'], ...
                x0(1), x0(2), x0(3), x0(4), x(1), x(2), x(3), x(4), N_iter, normg);
    end
end
end
end

% Fit phi2 to data2 using the best results from phi1 on data2
fprintf('\nFitting phi2 to data2:\n');
results_phi2_data2 = [];

% Find the best x1 and x2 from phi1 on data2 (minimum normg)
[min_value, best_index] = min(results_phi1_data2(:, end));
best_x1_x2 = results_phi1_data2(best_index, 3:4); % Extract best [x1, x2]
best_x1 = best_x1_x2(1);
best_x2 = best_x1_x2(2);

% Iterate over x3 and x4 while keeping x1 and x2 fixed
for x3 = x3_range
    for x4 = x4_range
        x0 = [best_x1; best_x2; x3; x4]; % Use best x1 and x2, vary x3 and x4
        [x, N_eval, N_iter, normg] = gaussnewton(@phi2, t2, y2, x0, 1e-4, 0, 0);
        results_phi2_data2 = [results_phi2_data2; x0', x', N_eval, N_iter, normg];
        fprintf(['Initial: [%.2f, %.2f, %.2f, %.2f], ' ...
                'Final: [%.2f, %.2f, %.2f, %.2f], ' ...
                'Iterations: %d, Normg: %.2e\n'], ...
                x0(1), x0(2), x0(3), x0(4), x(1), x(2), x(3), x(4), N_iter, normg);
    end
end
end

```