Department of Mathematics, IIT Madras

MA-5105-Scientific Computing & Advanced Programming Lab

Practice Problems 6

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1 Curve Fitting Using Unconstrained Optimization

The data in "curve_fitting_data.txt" represent measurements of an unknown response y as a function of t. Assume that the data can be approximated by a quadratic model

$$f(t;\theta) = \theta_1 + \theta_2 t + \theta_3 t^2,$$

where $\theta = (\theta_1, \theta_2, \theta_3)^T$ is the vector of unknown parameters.

1. **Formulation:** Construct a least-squares objective $J(\theta)$ that measures the discrepancy between the model predictions and the given observations.
2. **Optimization:** Implement the steepest descent method and Newton's method to minimize $J(\theta)$. Derive the gradient and Hessian of the objective and use them in your algorithms.
3. **Numerical experiment:** Run both methods from the same initial guess. Compare the number of iterations, final objective values, and gradient norms.
4. **Interpretation:** Plot the fitted quadratic curve together with the observations. Briefly discuss the quality of the fit and the difference in convergence between the two methods.

Hints:

- Define the residual at each observation as the difference between the model prediction and the measured value.
- Construct the objective by aggregating the squared residuals.
- For Newton's method, solve the linear system involving the Hessian rather than explicitly computing its inverse.
- The choice of initial guess and step size can strongly affect steepest descent.

2 Constrained Optimization Using the Penalty Method

Consider the constrained optimization problem

$$\begin{aligned} \min_{(x,y)\in\mathbb{R}^2} \quad & f(x,y) = (x-2)^2 + (y-3)^2, \\ \text{subject to} \quad & x + y \leq 2. \end{aligned}$$

The objective favours points near $(2, 3)$, but this point does not satisfy the constraint.

1. **Penalty formulation:** Convert the constrained problem into an unconstrained optimization problem using a quadratic penalty term. Introduce a penalty parameter $\mu > 0$.
2. **Implementation:** Implement the penalty objective and minimize it using steepest descent or Newton's method. Start from the same initial guess for each choice of μ.
3. **Numerical investigation:** Repeat the experiment for several increasing values of μ. Record the minimizer, the original objective value, and the constraint violation.
4. **Discussion:** Explain how increasing μ affects constraint satisfaction and the numerical behaviour of the unconstrained optimization algorithm.

Hints:

- The penalty should be zero when the constraint is satisfied and positive when it is violated.
- For an inequality constraint, penalize only the violating part.
- A very large penalty parameter may enforce the constraint more strongly but can also make the optimization problem harder to solve numerically.