Homework #1

Due: February 14, 2025 at 11:59 PM

Regression

Introduction

This homework is on different three different forms of regression: nearest neighbors regression, kernelized regression, and linear regression. We will discuss implementation and examine their tradeoffs by implementing them on the same dataset, which consists of temperature over the past 800,000 years taken from ice core samples.

The folder `data` contains the data you will use for this problem. There are two files:

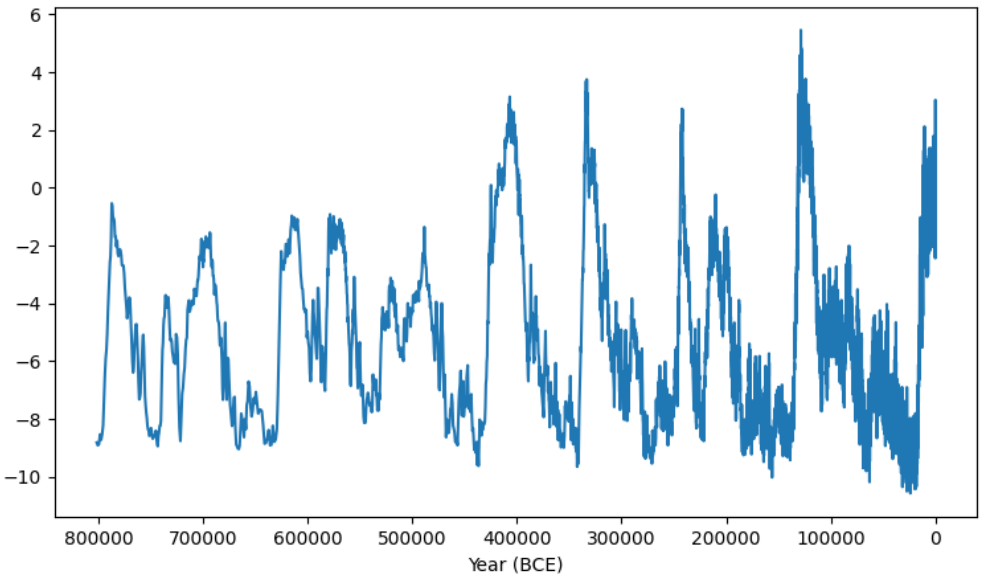
- `earth_temperature_sampled_train.csv`
- `earth_temperature_sampled_test.csv`

Each has two columns. The first column is the age of the ice core sample. The second column is the approximate difference in a year's temperature (K) from the average temperature of the 1,000 years preceding it. The temperatures were retrieved from ice cores in Antarctica (Jouzel et al. 2007)[1].

The following is a snippet of the data file:

```
# Age, Temperature
399946,0.51
409980,1.57
```

And this is a visualization of the full dataset:



Due to the large magnitude of the years, we will work in terms of thousands of years BCE in these problems. This is taken care of for you in the provided notebook.

[1] Retrieved from https://www.ncei.noaa.gov/pub/data/paleo/icecore/antarctica/epica_domec/edc3deuttemp2007.txt
Jouzel, J., Masson-Delmotte, V., Cattani, O., Dreyfus, G., Falourd, S., Hoffmann, G., ... Wolff, E. W. (2007). Orbital and Millennial Antarctic Climate Variability over the Past 800,000 Years. *Science, 317*(5839), 793–796. doi:10.1126/science.1141038

Resources and Submission Instructions

If you find that you are having trouble with the first couple problems, we recommend going over the fundamentals of linear algebra and matrix calculus (see links on website). The relevant parts of the cs181-textbook notes are Sections 2.1 - 2.7. We strongly recommend reading the textbook before beginning the homework.

We also encourage you to first read the Bishop textbook, particularly: Section 2.3 (Properties of Gaussian Distributions), Section 3.1 (Linear Basis Regression), and Section 3.3 (Bayesian Linear Regression). (Note that our notation is slightly different but the underlying mathematics remains the same!).

Please type your solutions after the corresponding problems using this LaTeX template, and start each problem on a new page.

Please submit the writeup PDF to the Gradescope assignment 'HW1'. Remember to assign pages for each question. **You must include any plots in your writeup PDF.** . Please submit your LaTeXfile and code files to the Gradescope assignment 'HW1 - Supplemental.' The supplemental files will only be checked in special cases, e.g. honor code issues, etc. Your files should be named in the same way as we provide them in the repository, e.g. `hw1.pdf`, etc.

Problem 1 (kNN and Kernels, 35pts)

You will now implement two non-parametric regressions to model temperatures over time.

Make sure to include all required plots in your PDF. Passing all test cases does not guarantee that your solution is correct, and we encourage you to write your own.

1. Recall that kNN uses a predictor of the form

$$f(x^*) = \frac{1}{k} \sum_n y_n \mathbb{I}(x_n \texttt{ is one of k-closest to } x^*),$$

where $\mathbb{I}$ is an indicator variable.

   (a) The kNN implementation **has been provided for you** in the notebook. Run the cells to plot the results for $k = \{1, 3, N-1\}$, where N is the size of the dataset. Describe how the fits change with k. Please include your plot in your solution PDF.

   (b) Now, we will evaluate the quality of each model *quantitatively* by computing the error on the provided test set. Write Python code to compute the test MSE for each value of k. Report the values here. Which solution has the lowest MSE?

2. *Kernel-based regression* techniques are another form of non-parametric regression. Consider a kernel-based regressor of the form

$$f_\tau(x^*) = \frac{\sum_n K_\tau(x_n, x^*) y_n}{\sum_n K_\tau(x_n, x^*)}$$

where $\mathcal{D}_{\texttt{train}} = \{(x_n, y_n)\}_{n=1}^N$ are the training data points, and x^* is the point for which you want to make the prediction. The kernel $K_\tau(x, x')$ is a function that defines the similarity between two inputs x and x'. A popular choice of kernel is a function that decays as the distance between the two points increases, such as

$$K_\tau(x, x') = \exp\left(-\frac{(x - x')^2}{\tau}\right)$$

where τ represents the square of the lengthscale (a scalar value that dictates how quickly the kernel decays).

   (a) First, implement the `kernel_regressor` function in the notebook, and plot your model for years in the range 800,000 BC to 400,000 BC at 1000 year intervals for the following three values of τ: $1, 50, 2500$. Since we're working in terms of thousands of years, this means you should plot $(x, f_\tau(x))$ for $x = 400, 401, \ldots, 800$. **In no more than 10 lines**, describe how the fits change with τ. Please include your plot in your solution PDF.

   (b) Denote the test set as $\mathcal{D}_{\texttt{test}} = \{(x'_m, y'_m)\}_{m=1}^M$. Write down the expression for the MSE of f_τ over the test set as a function of the training set and test set. Your answer may include $\{(x'_m, y'_m)\}_{m=1}^M$, $\{(x_n, y_n)\}_{n=1}^N$, and K_τ, but not f_τ.

   (c) Compute the MSE on the provided test set for the three values of τ. Report the values here. Which model yields the lowest MSE? Conceptually, why is this the case? Why would choosing τ based on $\mathcal{D}_{\texttt{train}}$ rather than $\mathcal{D}_{\texttt{test}}$ be a bad idea?

   (d) Describe the time and space complexity of both kernelized regression and kNN with respect to the size of the training set N. How, if at all, does the size of the model—everything that needs to be stored to make predictions—change with the size of the training set N? How, if at all, do the number of computations required to make a prediction for some input x^* change with the size of the training set N?.

   (e) What is the exact form of $\lim_{\tau \to 0} f_\tau(x^*)$?

Solution: Your solution here.

Problem 2 (Deriving Linear Regression, 20pts)

We now seek to model the temperatures with a parametric method: linear regression. Before we implement anything, let's revisit the mathematical formulation of linear regression. Specifically, the solution for the least squares linear regression "looks" kind of like a ratio of covariance and variance terms. In this problem, we will make that connection more explicit.

Suppose we have some 2-D data where each observation has the form (x, y) and is independent and identically distributed according $x \sim p(x)$, $y \sim p(y|x)$. We will consider the process of fitting these data from this distribution with the best linear model possible, that is a linear model of the form $\hat{y} = wx$ that minimizes the expected squared loss $E_{x,y}[(y - \hat{y})^2]$.

Note: The notation $E_{x,y}$ indicates an expectation taken over the joint distribution $p(x, y)$. This essentially just means to treat x and y as random.

1. Derive an expression for the optimal w, that is, the w that minimizes the expected squared loss above. You should leave your answer in terms of moments of the distribution, e.g. terms like $E_x[x]$, $E_x[x^2]$, $E_y[y]$, $E_y[y^2]$, $E_{x,y}[xy]$ etc.

2. Note that while x, y are data that we have access to, $E_{x,y}[yx]$ is a theoretical constant. Keeping in mind the interpretation of expectations as average values, how could you use observed data $\{(x_n, y_n)\}_{n=1}^N$ to estimate $E_{x,y}[yx]$ and $E_x[x^2]$?

3. In general, moment terms like $E_{x,y}[yx]$, $E_{x,y}[x^2]$, $E_{x,y}[yx^3]$, $E_{x,y}[\frac{x}{y}]$, etc. can easily be estimated from the data (like you did above). If you substitute in these empirical moments, how does your expression for the optimal w^* in this problem compare with the optimal $\hat{\boldsymbol{w}}$ from Problem 4.3 of HW0?

4. Many common probabilistic linear regression models assume that variables x and y are jointly Gaussian. Did any of your above derivations rely on the assumption that x and y are jointly Gaussian? Why or why not?

Solution: Your solution here.

Problem 3 (Basis Regression, 30pts)

Having reviewed the theory, we now implement some linear regression models for the temperature. If we just directly use the data as given to us, we would only have a one dimensional input to our model, the year. To create a more expressive linear model, we will introduce basis functions.

Make sure to include all required plots in your PDF.

1. We will first implement the four basis regressions below. Note that we introduce an addition transform f (already into the provided notebook) to address concerns about numerical instabilities.

   (a) $\phi_j(x) = f(x)^j$ for $j = 1, \ldots, 9$. $f(x) = \frac{x}{1.81 \cdot 10^2}$.

   (b) $\phi_j(x) = \exp\left\{-\frac{(f(x) - \mu_j)^2}{5}\right\}$ for $\mu_j = \frac{j+7}{8}$ with $j = 1, \ldots, 9$. $f(x) = \frac{x}{4.00 \cdot 10^2}$.

   (c) $\phi_j(x) = \cos(f(x)/j)$ for $j = 1, \ldots, 9$. $f(x) = \frac{x}{1.81}$.

   (d) $\phi_j(x) = \cos(f(x)/j)$ for $j = 1, \ldots, 49$. $f(x) = \frac{x}{1.81 \cdot 10^{-1}}$. [a]

   * Note: Please make sure to add a bias term for all your basis functions above in your implementation of the `make_basis`.

   Let

   $$\phi(\mathbf{X}) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix} \in \mathbb{R}^{N \times D}.$$

   You will complete the `make_basis` function which must return $\phi(\mathbf{X})$ for each part (a) - (d). You do NOT need to submit this code in your LaTeXwriteup.

   Then, create a plot of the fitted regression line for each basis against a scatter plot of the training data. Boilerplate plotting code is provided in the notebook—you will only need to finish up a part of it. **All you need to include in your writeup for this part are these four plots.**

2. Now we have trained each of our basis regressions. For each basis regression, compute the MSE on the test set. Discuss: do any of the bases seem to overfit? Underfit? Why?

3. Briefly describe what purpose the transforms ϕ serve: why are they helpful?

4. As in Problem 1, describe the space and time complexity of linear regression. How does what is stored to compute predictions change with the size of the training set N and the number of features D? How does the computation needed to compute the prediction for a new input depend on the size of the training set N? How do these complexities compare to those of the kNN and kernelized regressor?

5. Briefly compare and constrast the different regressors: kNN, kernelized regression, and linear regression (with bases). Are some regressions clearly worse than others? Is there one best regression? How would you use the fact that you have these multiple regression functions?

Note: Recall that we are using a different set of inputs $\mathbf{X}$ for each basis (a)-(d). Although it may seem as though this prevents us from being able to directly compare the MSE since we are using different data, each transformation can be considered as being a part of our model. Contrast this with transformations (such as standardization) that cause the variance of the target $\mathbf{y}$ to be different; in these cases the MSE can no longer be directly compared.

[a] For the trigonometric bases (c) and (d), the periodic nature of cosine requires us to transform the data such that the lengthscale is within the periods of each element of our basis.

Solution: Your solution here.

Problem 4 (Probablistic Regression and Regularization, 30pts)

Finally, we will preview Bayesian regression and explore its connection to regularization for linear models. Then, we will fit a regularized model to the temperature data. Although the content is related, you do not need to know the material from the lectures on frequentist model selection and Bayesian model selection to solve this problem.

Recall that the probabilistic version of linear regression states that

$$y_n = \mathbf{w}^\top \mathbf{x}_n + \epsilon_n, \quad \epsilon_n \sim \mathcal{N}(0, \sigma^2)$$

In Bayesian regression, we impose a prior $p(\mathbf{w})$ on the weights and fit the weights $\mathbf{w}$ through maximizing the posterior likelihood

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{w}, \mathbf{X})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})}$$

Note: since we maximize with respect to $\mathbf{w}$, it suffices to just maximize the numerator.

1. Suppose $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \frac{\sigma^2}{\lambda}\mathbf{I})$. Show that maximizing the posterior likelihood is equivalent to minimizing
$$\mathcal{L}_{ridge}(\mathbf{w}) = \frac{1}{2}||\mathbf{y} - \mathbf{X}\mathbf{w}||_2^2 + \frac{\lambda}{2}||\mathbf{w}||_2^2.$$
Note that minimizing $\mathcal{L}_{ridge}(\mathbf{w})$ is exactly what ridge regression does.
Hint: You don't need to solve for the maximizer/minimizer to show that the optimization problems are equivalent.

2. Solve for the value of $\mathbf{w}$ that minimizes $\mathcal{L}_{ridge}(\mathbf{w})$.

3. The Laplace distribution has the PDF
$$L(a, b) = \frac{1}{2b}\exp\left(-\frac{|x - a|}{b}\right)$$
Show that if all $w_d \sim L\left(0, \frac{2\sigma^2}{\lambda}\right)$, maximizing the posterior likelihood is equivalent to minimizing
$$\mathcal{L}_{lasso}(\mathbf{w}) = \frac{1}{2}||\mathbf{y} - \mathbf{X}\mathbf{w}||_2^2 + \frac{\lambda}{2}||\mathbf{w}||_1.$$
Note that minimizing $\mathcal{L}_{lasso}(\mathbf{w})$ is exactly what LASSO regression does.

4. Why is there no general closed form for the LASSO estimator, i.e. the value of $\mathbf{w}$ that minimizes $\mathcal{L}_{ridge}(\mathbf{w})$?

5. Since there is no general closed form for LASSO, we use numerical methods for estimating $\mathbf{w}$. One approach is to use *coordinate descent*, which works as follows:
   (a) Initialize $\mathbf{w} = \mathbf{w}_0$.
   (b) For each $d = 1, \ldots, D$ do the following 2 steps consecutively:
      i. Compute $\rho_d = \tilde{\mathbf{x}}_d^\top(\mathbf{y} - (\mathbf{X}\mathbf{w} - w_d\tilde{\mathbf{x}}_d))$. We define $\tilde{\mathbf{x}}_d$ as the d-th column of $\mathbf{X}$.
      ii. If $d = 1$, set $w_1 = \frac{\rho_1}{||\tilde{\mathbf{x}}_1||_2^2}$. Otherwise if $d \neq 1$, compute $w_d = \frac{\text{sign}(\rho_d)\max\left\{|\rho_d| - \frac{\lambda}{2}, 0\right\}}{||\tilde{\mathbf{x}}_d||_2^2}$.
   (c) Repeat step (b) until convergence or the maximum number of iterations is reached.

   Implement the `find_lasso_weights` function according to the above algorithm, letting $\mathbf{w}_0$ be a vector of ones and the max number of iterations be 5000. Then, fit models with $\lambda = 1, 10$ to basis (d) from Problem 3 and plot the predictions on the train set. Finally, compute the test MSE's. You will need to do some preprocessing, but a completed helper function for this is already provided. How do the graphs and errors compare to those for the unregularized basis (d) model?

Solution: Your solution here.

Name:
Collaborators and Resources: