Recitation 3

Gradient Descent

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CDS

February 12, 2020

Announcement

- New TA office hour
- 5:30 pm - 6:30 pm, room 650, 60 5th Ave

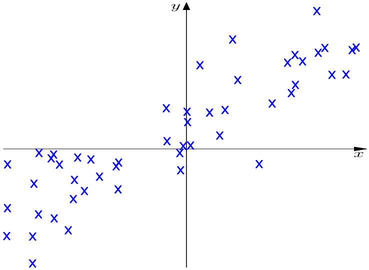
Agenda

- Motivation
- Calculating the gradient
- Gradient descent algorithm
- Coding exercise: gradient descent implementation

Intro Question

Question

We are given the data set $(x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. We want to fit a **linear function** to this data by performing **empirical risk minimization**. More precisely, we are using the hypothesis space $\mathcal{F} = \{h_\theta(x) = \theta^T x \mid \theta \in \mathbb{R}^d\}$ and the loss function $\ell(a, y) = (a - y)^2$. Given an initial guess $\tilde{\theta}$ for the empirical risk minimizing parameter vector, how could we improve our guess?



Intro Solution

Solution

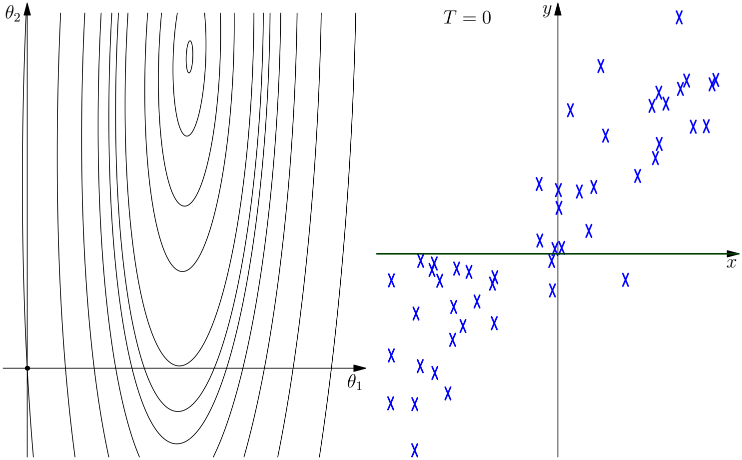
- The empirical risk is given by

$$J(\theta) := \hat{R}_n(h_\theta) = \frac{1}{n}\sum_{i=1}^{n}\ell(h_\theta(x_i), y_i) = \frac{1}{n}\sum_{i=1}^{n}(\theta^T x_i - y_i)^2 = \frac{1}{n}\|X\theta - y\|_2^2,$$

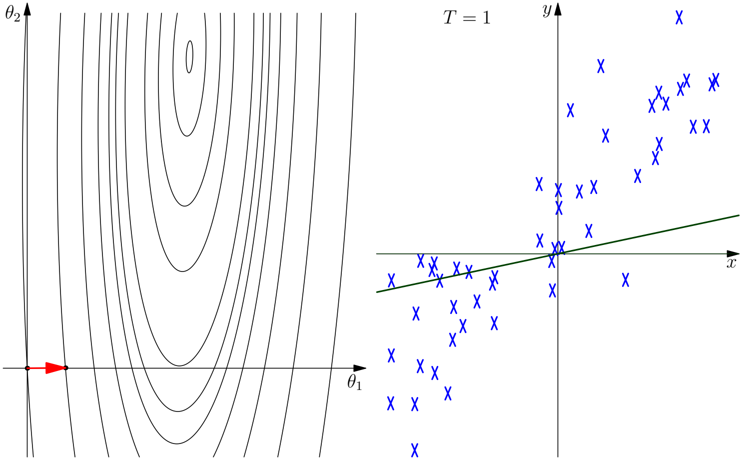
where $X \in \mathbb{R}^{n\times d}$ is the matrix whose ith row is given by x_i^T.

- Can improve a non-optimal guess $\tilde{\theta}$ by taking a small step in the direction of the negative gradient $-\nabla J(\theta)$.

Negative Gradient Steps



Negative Gradient Steps



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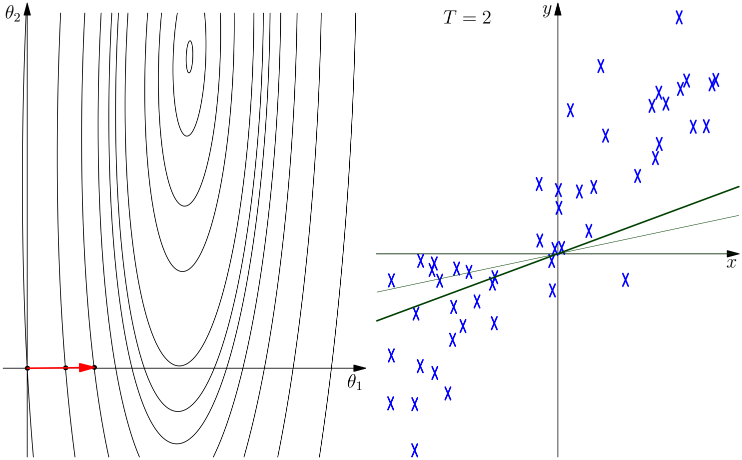

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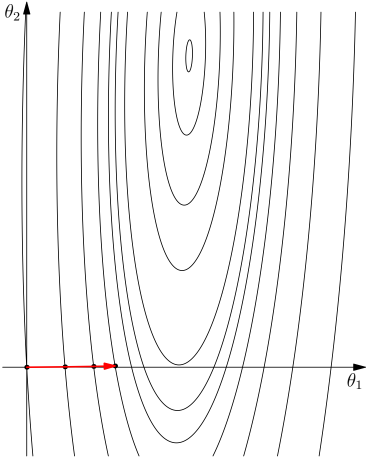

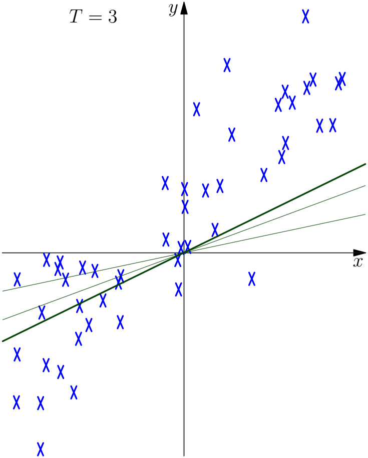

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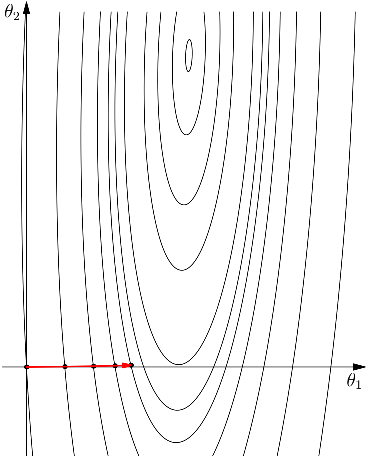

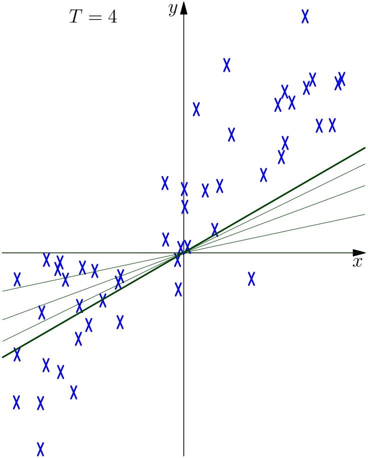

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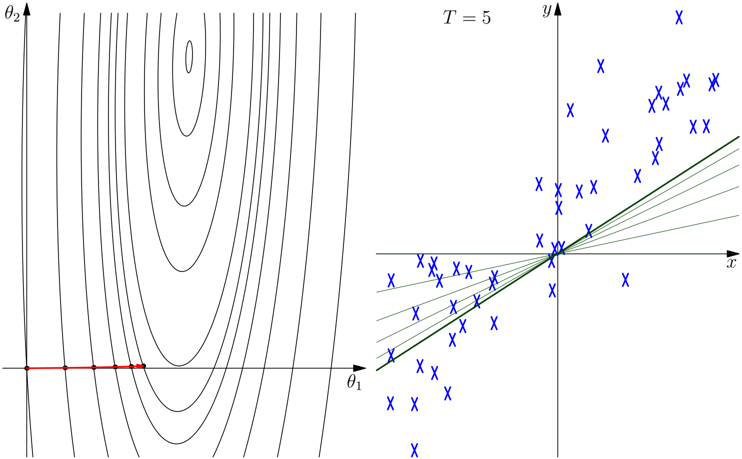

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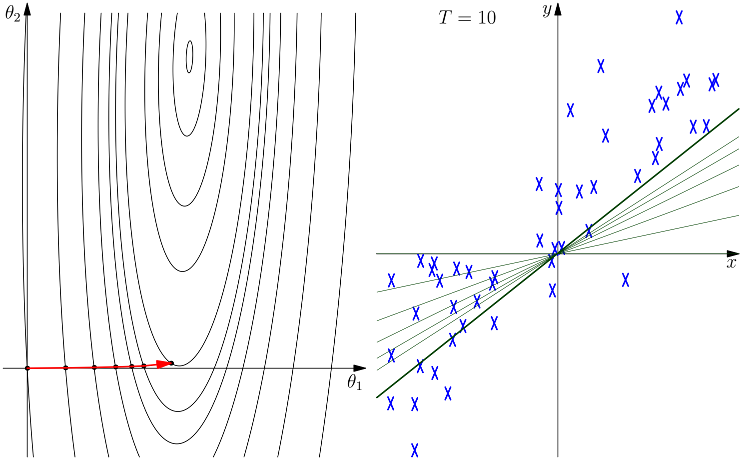

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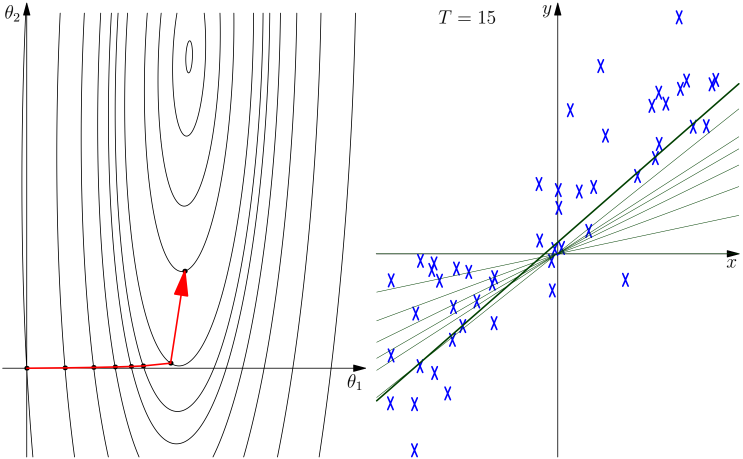

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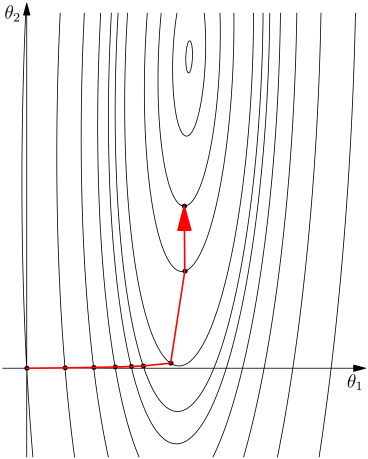

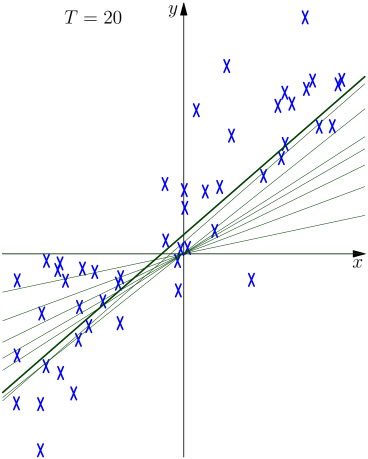

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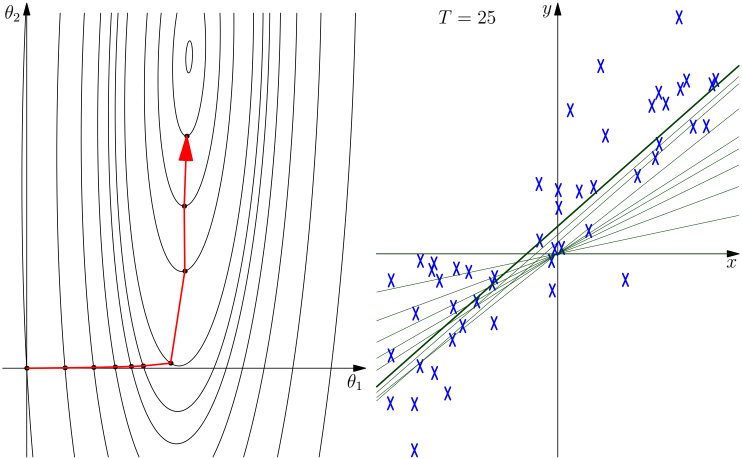

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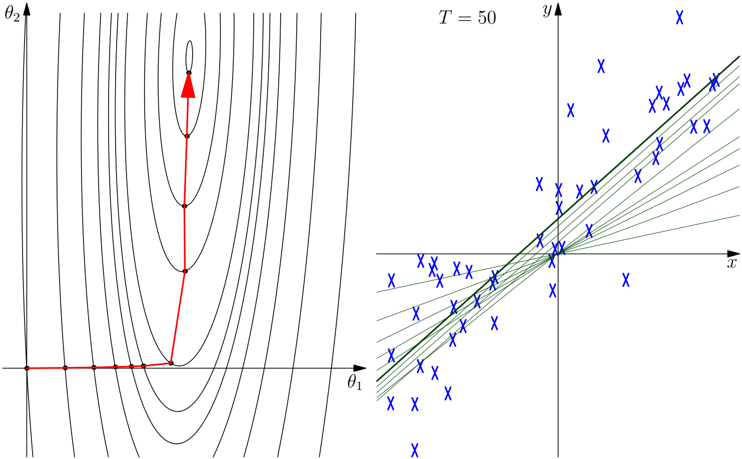


Intuition

- Why don't we directly compute the derivative $\frac{\partial}{\partial\theta}J(\theta, y)$ and solve for θ^* that makes $\frac{\partial}{\partial\theta}J(\theta^*, y) = 0$.
  - But what if the analytical solution for $\frac{\partial}{\partial\theta}J(\theta^*, y) = 0$ is computationally intractable?
- We can improve the an initial guess θ_0 by iteratively "updating" it using the gradient of the loss $\nabla J(\theta)$.
- This process will give us a "good enough" approximation for θ^*.
- To do so, we need to know how to calculate the gradient $J(\theta^*, y)$.

Directional Derivative

Definition

Let $f : \mathbb{R}^n \to \mathbb{R}$. The directional derivative $f'(x; u)$ of f at $x \in \mathbb{R}^n$ in the direction $u \in \mathbb{R}^n$ is given by

$$f'(x; u) = \lim_{h \to 0} \frac{f(x + hu) - f(x)}{h}.$$

- We say that u is a *descent direction* of f at x if $f'(x; u) < 0$.
- Taking a small enough step in a descent direction causes the function value decreases.

Partial Derivative

- Let $e_i = (\overbrace{0, 0, \ldots, 0}^{i-1}, 1, 0, \ldots, 0)$ denote the ith standard basis vector.
- The ith *partial derivative* is defined to be the directional derivative along e_i.
- It can be written many ways:

$$f'(x; e_i) = \frac{\partial}{\partial x_i} f(x) = \partial_{x_i} f(x) = \partial_i f(x).$$

- What is the intuitive meaning of $\partial_{x_i} f(x)$? For example, what does a large value of $\partial_{x_3} f(x)$ imply?

Differentiability and Gradients

- We say a function $f : \mathbb{R}^n \to \mathbb{R}$ is *differentiable* at $x \in \mathbb{R}^n$ if

$$\lim_{v \to 0} \frac{f(x+v) - f(x) - g^T v}{\|v\|_2} = 0,$$

  for some $g \in \mathbb{R}^n$.
- If it exists, this g is unique and is called the *gradient* of f at x with notation

$$g = \nabla f(x).$$

- It can be shown that

$$\nabla f(x) = \begin{pmatrix} \partial_{x_1} f(x) \\ \vdots \\ \partial_{x_n} f(x) \end{pmatrix}.$$

Computing Gradients

Question

Compute the gradient $\nabla f(\theta) \in \mathbb{R}^2$ for the following function:

$$f(\theta) = \theta_0^2 + 2\theta_0\theta_1^3$$

The gradient of this function can be computed as following:

$$\frac{\partial}{\partial \theta_0} = 2\theta_0 + 2\theta_1^3$$

$$\frac{\partial}{\partial \theta_1} = 6\theta_0\theta_1^2$$

$$\nabla f(\theta) = \begin{bmatrix} 2\theta_0 + 2\theta_1^3 \\ 6\theta_0\theta_1^2 \end{bmatrix}$$

Computing Gradients

Question

Compute the gradient $\nabla J(\theta) \in \mathbb{R}^d$ for

$$J(\theta) = \|X\theta - y\|_2^2$$

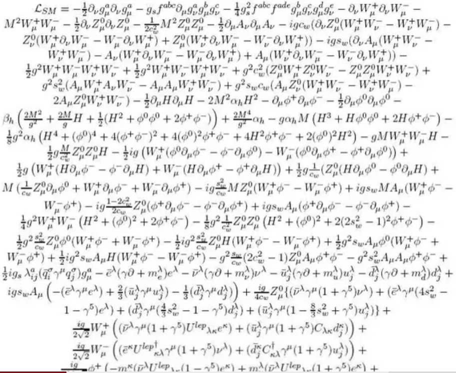
where $X \in \mathbb{R}^{n \times d}, y \in \mathbb{R}^n, \theta \in \mathbb{R}^d$.

In homework2, we will show that

$$\nabla J(\theta) = 2(X^T X\theta - X^T y) = 2X^T(X\theta - y)$$

Gradient Checker

- So far we have worked with relatively simple functions where it is straight-forward to compute the gradient.
- For more complex functions, the gradient computation can be notoriously difficult to debug and get right. Example from `www.quora.com/What-is-the-most-complex-equation-in-the-world`.
- How can we test if our gradient computation is correct?



Gradient Checker

- Recall the mathematical definition of the derivative as:

$$\frac{\partial}{\partial \theta} f(\theta) = \lim_{\epsilon \to 0} \frac{f(\theta + \epsilon) - f(\theta - \epsilon)}{2\epsilon}$$

- We can approximate the gradient (left hand side) using the equation on the right hand side by setting ϵ to a small constant, say $\epsilon = 10^{-4}$.
- Now let's expand this method to deal with vector input $\theta \in \mathbb{R}^d$. Let's say we want to verify out gradient at dimension i $(\nabla f(\theta))_i$. We can make use of one-hot vector e_i in which all dimension except the ith are 0 and the ith dimension has a value of 1: $e_i = [0, 0, ..., 1, ..., 0]^T$
- The gradient at ith dimension can be then approximated as

$$[\nabla f(\theta)]^{(i)} \approx \frac{f(\theta + \epsilon e_i) - f(\theta - \epsilon e_i)}{2\epsilon}$$

Recap

- To find a good decision function we will minimize the empirical loss on the training data.
- Having fixed a hypothesis space parameterized by θ, finding a good decision function means finding a good θ.
- Given a current guess for θ, we will use the gradient of the empirical loss (w.r.t. θ) to get a local linear approximation.
- If the gradient is non-zero, taking a small step in the direction of the negative gradient is guaranteed to decrease the empirical loss.
- This motivates the minimization algorithm called gradient descent.

Gradient Descent

Gradient descent Algorithm

- Goal: find $\theta^* = \arg\min_\theta f(\theta)$
- θ^0 :=[initial condition]
- $i := 0$
- while not [termination condition]:
  - compute $\nabla f(\theta_i)$
  - ϵ_i :=[choose learning rate at iteration i]
  - $\theta^{i+1} := \theta^i - \epsilon_i \nabla f(\theta_i)$
  - $i := i + 1$
- return θ^i

Gradient Descent

- How to initialize θ^0?
  - sample from some distribution
  - compose θ_0 using some heuristics
- How to choose termination conditions?
  - run for a fixed number of iteration
  - the value of $f(\theta)$ stabilizes
  - θ_i converges
- What is a good learning rate?

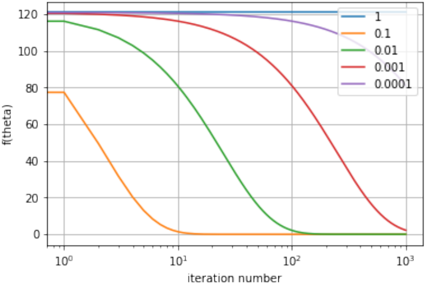
Learning Rate

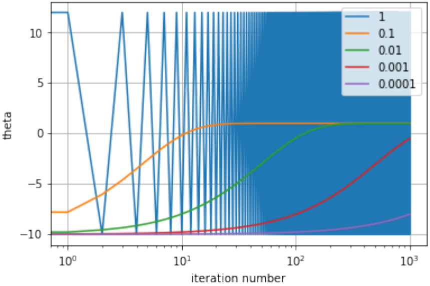
Application

Suppose we would like to find $\theta^* \in \mathbb{R}$ that minimizes $f(\theta) = \theta^2 - 2\theta + 1$. The gradient (in this case, the derivative) $\nabla f(\theta) = 2\theta - 2$. We can easily see that $\theta^* = \text{argmin}_\theta f(\theta) = 1$.

Learning Rate

- We applied gradient descent for 1000 iterations on $f(\theta) = \theta^2 - 2\theta + 1$ with varying learning rate $\epsilon \in \{1, 0.1, 0.01, 0.001, 0.0001\}$.
- When the learning rate is too large ($\epsilon = 1$), $f(\theta)$ does not decrease through iterations. The value of θ_i at each iteration significantly fluctuates.
- When the learning rate is too small ($\epsilon = 0.0001$), $f(\theta)$ decreases very slowly.





Adaptive Learning Rate

- Instead of using a fixed learning rate through all iterations, we can adjust our learning rate in each iteration using a simple algorithm.
- At each iteration i:
  - $\tilde{\theta} := \theta_{i-1} - \epsilon_{i-1} \nabla f(\theta_{i-1})$
  - $\delta := f(\theta_{i-1}) - f(\tilde{\theta})$
  - if $\delta \geq$ threshold:
    - we achieve a satisfactory reduction on $f(\theta)$
    - $\theta_i = \tilde{\theta}$
    - maybe we can consider increasing the learning rate for next iteration $\epsilon_i := 2\epsilon_{i-1}$
  - else:
    - the reduction is unsatisfactory
    - $\theta_i = \theta_{i-1}$
    - the learning rate is too large, so we reduce the learning rate
    - $\epsilon_i := \frac{1}{2}\epsilon_{i-1}$

Adaptive Learning Rate

How to decide a proper threshold for $f(\theta_{i-1}) - f(\tilde{\theta})$?

Armijo rule

If learning rate ϵ satisfies

$$f(\theta_{i-1}) - f(\tilde{\theta}) \geq \frac{1}{2}\epsilon\|\nabla f(\theta_{i-1})\|^2 \tag{1}$$

then $f(\theta)$ is guaranteed to converge to a (local) maximum under certain technical assumptions.

You can find more details at **this link**.

Coding Exercise

In the provided notebook, we will use Python to:

- calculate the gradient for two example functions
- implement the gradient checker
- implement the gradient descent algorithm with Armijo's rule
- apply gradient descent on the UCI Automobile dataset