‘cs229’—Notes

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Chapter 1

Supervised learning

Given a dataset of n *training examples* $\{(x^{(i)}, y^{(i)}); i = 1\}, \ldots, n\}$—a *training set*—where $\boldsymbol{x}$ represents the *features* and $\boldsymbol{y}$ the "output" or *target* variable we are trying to predict. If not already obvious, we denote the vector space of $\boldsymbol{x}$ as $\mathcal{X}$ and that of the outputs $\boldsymbol{y}$ as $\mathcal{Y}$.

Our goal is, given a training set, to learn a function $h : \mathcal{X} \mapsto \mathcal{Y}$ so that $h(x)$ is a "good" predictor for the corresponding y. This function h is called a *hypothesis*.

When trying to predict a continuous target variable, we call this a *regression* problem; whereas when y can take on only a small number of discrete values we call that a *classification* problem.

1.1 Linear Regression

Say we decide to approximate y as a linear function of x:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots$$

Where $\boldsymbol{\theta}$ represents the *parameters/weights* (parametrising the space of linear functions mapping from $\mathcal{X}$ to $\mathcal{Y}$). We can simplify our notation as such: (by convention letting $x_0 = 1$, aptly named the *intercept* term)

$$h(x) = \sum_{i=0}^{d} \theta_i x_i = \boldsymbol{\theta}^T \boldsymbol{x}$$

In order to formalise a measure of proximity between the predicted value $h(x)$ and the target y, we define a *cost function*:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{n} (h_\theta(x^{(i)}) - y^{(i)})^2$$

This particular cost function implies an *ordinary least squares* regression model.

1.1.1 LMS algorithm

Our cost function $J(\theta)$ gives us a measure of prediction accuracy. We want to choose θ so as to minimise $J(\theta)$. Starting with an initial set of θ, we need a search algorithm that repeatedly changes θ in an attempt to minimise $J(\theta)$. Here we consider the *gradient descent* algorithm, which, given some initial θ, repeatedly performs the update:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

Where the update is simultaneously performed for all values of $j = 0, \ldots, d$. α is called the *learning rate* (how much we move in the direction the gradient points in).

Intuition
Consider attempting to minimise the least mean squares (LMS) cost function for a single training example:

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{d} \theta_i x_i - y \right) \\
&= (h_\theta(x) - y)\, x_j
\end{aligned}$$

This gives us the update rule:

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$

(we use the notation $a := b$ to denote (in a script) overwriting a with b) Notice the property of the LMS update rule that the magnitude of the update is proportional to the *error* term $\left(y^{(i)} - h_\theta(x^{(i)})\right)$; this means that predictions further off the mark result in a greater correction to θ.
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Batch Gradient Descent
We had the LMS rule for when there was only a single training example. One way to modify this method for a training set of more than one example is the following algorithm:

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}, \text{ (for every } j)$$

}

Written more succinctly (θ_j and x_j as vectors):

$$\theta := \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)}) \right) x^{(i)}$$

This method looks at every example in the entire training set on every step, and is called *batch gradient descent*.

Stochastic gradient descent
Now consider another algorithm:

Loop {
  for $i = 1$ to n, {

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}, \quad \text{(for every } j)$$

  }
}

Written more compactly:

$$\theta := \theta + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x^{(i)}, \text{ (update } \theta \text{ } n \text{ times)}$$

Here we update θ for each training example during each run of the training set. This is called *stochastic/incremental gradient descent*.

Whereas batch gradient descent has to scan through the entire training set before taking a single step—which is costly if n is large—stochastic gradient descent continues to make progress with each example it looks at. Stochastic gradient descent gets θ "close" to the minimum much faster than batch gradient descent. Note that "convergence" doesn't really occur—the parameters θ will keep oscillating around the minimum of $J(\theta)$. (though most values near minimum would be reasonably good approximations to the true minimum)

1.1.2 Gradient/Hessian of $b^T x$, $x^T A x$

Matrix Derivatives
For a function $f : \mathbb{R}^{n \times d} \mapsto \mathbb{R}$ mapping from n-by-d matrices to real numbers, we define the derivative of f with respect to A to be

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \cdots & \frac{\partial f}{\partial A_{1d}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial A_{n1}} & \cdots & \frac{\partial f}{\partial A_{nd}} \end{bmatrix}$$

Gradient of $b^T x$:
For $x \in \mathbb{R}^n$ and $f(x) = b^T x$ for known $b \in \mathbb{R}^n$, we have

$$f(x) = \sum_{i=1}^{n} b_i x_i$$

and so

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} b_i x_i = b_k$$

Consider repeating this for the partial of each element of x. See that $\nabla_x b^T x = b$ (analagous to single variable calculus).

Gradient of $f(x) = x^T A x$:
Now consider the quadratic function $f(x) = x^T A x$ for $A \in \mathbb{S}^n$ (meaning symmetric). First see that

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

this can be seen from considering that

$$b = Ax \in \mathbb{R}^{n \times 1}$$

can be written as

$$\begin{aligned} b_1 &= \sum_{i=1}^{n} A_{1i} x_i \\ &\vdots \\ b_n &= \sum_{i=1}^{n} A_{ni} x_i \end{aligned}$$

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so we can write

$$\begin{aligned} x^T Ax = x^T b &= \sum_{j=1}^{n} x_j b_j \in \mathbb{R} \\ &= \sum_{j=1}^{n} x_j \left(\sum_{i=1}^{n} A_{ji} x_i \right) \end{aligned}$$

Rewriting gives us

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

which was what we wanted. Now we take the partial derivative by considering the terms including x_k an x_k^2 factors separately:

$$\begin{aligned} \frac{\partial f(x)}{\partial x_k} &= \frac{\partial f(x)}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\ &= \frac{\partial f(x)}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\ &= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2A_{kk} x_k \\ &= \sum_{i=1} A_{ik} x_i + \sum_{j=1} A_{kj} x_j = 2 \sum_{i=1}^{n} A_{ki} x_i \end{aligned}$$

where the last equality follows since A is assumed to be *symmetric*. Since

$$\sum_{i=1}^{n} A_{ki} x_i$$

is just the inner product of a single row of A and x—the kth entry of $\nabla_x f(x)$ is the just the inner product of the kth row of A and x; therefore

$$\nabla_x x^T Ax = 2Ax$$

also analagous to single variable calculus.
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Hessian
Finally we consider the Hessian of the quadratic function $f(x) = x^T Ax$ (it should be obvious that the Hessian of a linear function $b^T x$ is zero):

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial}{\partial x_k}\left[\frac{\partial f(x)}{\partial x_\ell}\right] = \frac{\partial}{\partial x_k}\left[2\sum_{i=1}^{n} A_{\ell i} x_i\right] = 2A_{\ell k} = 2A_{k\ell}$$

See therefore that $\nabla_x^2 x^T Ax = 2A$.

Recapitulation:

- $\nabla_x b^T x = b$
- $\nabla_x x^T Ax = 2Ax$
- $\nabla_x^2 x^T Ax = 2A$

1.1.3 Least Squares matrix representation

Here we consider $J(\theta)$—the least squares cost function—in matrix-vectorial notation.

Given a training set, we define the *design matrix* X to be the $n \times d$ matrix ($n \times d+1$ if we include the intercept term) that contains the training examples' inputs values in its rows:

$$X = \begin{bmatrix} —(x^{(1)})^T— \\ —(x^{(2)})^T— \\ \vdots \\ —(x^{(n)})^T— \end{bmatrix}$$

and y the n-dimensional vector containing the target values:

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

Now we try to represent the least squares function over the entire dataset; see that since

$$h_\theta(x^{(i)}) = (x^{(i)})^T\theta$$

we can write

$$\begin{aligned} X\theta - y &= \begin{bmatrix} (x^{(1)})^T\theta \\ \vdots \\ (x^{(n)})^T\theta \end{bmatrix} - \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix} \\ &= \begin{bmatrix} h_\theta(x^{(1)}) - y^{(1)} \\ \vdots \\ h_\theta(x^{(n)}) - y^{(n)} \end{bmatrix} \in \mathbb{R}^n \end{aligned}$$

Using the fact that for a vector z, $z^T z = \sum_i z_i^2$:

$$\begin{aligned} \frac{1}{2}(X\theta - y)^T(X\theta - y) &= \frac{1}{2}\sum_{i=1}^{n}(h_\theta(x^{(i)}) - y^{(i)})^2 \\ &= J(\theta) \end{aligned}$$

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Minimising the LMS
To minimise the cost function $J(\theta)$ we want its derivatives with respect to θ:

$$\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - y)^T(X\theta - y) \\
&= \frac{1}{2}\nabla_\theta \left((X\theta)^T - y^T\right)(X\theta - y) \\
&= \frac{1}{2}\nabla_\theta(\theta^T X^T X\theta - y^T X\theta - (X\theta)^T y - y^T y) \\
&= \frac{1}{2}\nabla_\theta(\theta^T X^T X\theta - y^T X\theta - y^T X\theta) \\
&= \frac{1}{2}\nabla_\theta(\theta^T X^T X\theta - 2(X^T y)\theta) \\
&= \frac{1}{2}(2X^T X\theta - 2X^T y) \\
&= X^T X\theta - X^T y
\end{aligned}$$

Of note:

- The third equality comes from $(Ab)^T = b^T A^T$
- The fourth equality comes from $a^T b = b^T a$
- To differentiate we use the facts $\nabla_x b^T x = b$ and $\nabla_x x^T Ax = 2Ax$. Note the second fact assumes A is symmetric, which is true here since $X^T X$ is symmetric.

To minimise J we set the derivative to zero and obtain the *normal equations*:

$$X^T X\theta = X^T y$$

Thus we have, in closed-form, the value of θ that minimises $J(\theta)$, given by

$$\theta = (X^T X)^{-1} X^T y$$

Note that this final step implicitly assumes that $X^T X$ is invertible. This can be checked before calculating the inverse; if either the number of linearly independent examples is fewer than the number of features, or if the features are not linearly independent:

See that a matrix $A \in \mathbb{R}^{n \times m}$ can have rank m $(= \min(n, m))$ only if $n \geq m$ (thus more linearly independent examples than features are required—m representing features and n samples.) If the features (m) were not linearly independent, the matrix A would not have rank m. See that

$$\begin{aligned}
A^T Ax = 0 \implies x^T A^T Ax = 0 \implies (Ax)^T Ax = 0 \\
\implies ||Ax||^2 = 0 \implies Ax = 0
\end{aligned}$$

Intuitively, only if $Ax = 0$ is the trivial solution (meaning A is a one-to-one mapping for m sized vectors), then would $A^T Ax$ also be one-to-one and also invertible.

1.1.4 Probabalistic interpretation of linear regression simplifies to LMS

Hypothesis
Here we make some probabalistic assumptions, under which least-squares regression is derived as a very natural algorithm. Assume that the target variables and the inputs are related via the equation:

$$y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)}$$

were ϵ is an error term that captures either unmodeled effects or random noise. Let us further assume that the $\epsilon^{(i)}$ are distributed IID (independently and identically distributed) according to a Gaussian/Normal distribution with mean zero and some variance σ^2. We can write this assumption as $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$, where $\epsilon^{(i)}$ has the probability density function:

$$p(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\epsilon^{(i)})^2}{2\sigma^2}\right)$$

This implies that

$$p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right)$$

The distribution of $y^{(i)}$ can also be written as $y^{(i)}|x^{(i)};\theta \sim \mathcal{N}(\theta^T x^{(i)}, \sigma^2)$

Likelihood
Given all our data in X (the design matrix) and θ, our distribution of all the $y^{(i)}$, when viewed for a fixed value of θ (we don't actually know θ, but we come up with a function given a value), we have the *likelihood function*

$$L(\theta) = L(\theta; X, y) = p(y|X;\theta)$$

(the combined probability of all these $y^{(i)}$ occuring given X and a value of θ) By the independence assumption on the $\epsilon^{(i)}$ this can be written as

$$\begin{aligned} L(\theta) &= \prod_{i=1}^{n} p(y^{(i)}|x^{(i)};\theta) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \end{aligned}$$

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Maximum Likelihood
Given this probabilistic model relating the $y^{(i)}$ and $x^{(i)}$, we should choose θ so as to maximise the probability of the data—we want to maximise $L(\theta)$—the *maximum likelihood*.

Given the monotonicity of the logarithm, and that we are simply looking for the θ to maximise the function, and not the value of the function itself, maximising over the *log likelihood* $\ell(\theta)$ simplifies things:

$$\begin{aligned}
\ell(\theta) &= \log L(\theta) \\
&= \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\
&= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\
&= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma} + \sum_{i=1}^{n} \log \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\
&= n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2 \\
&= \underbrace{n \log \frac{1}{\sqrt{2\pi}\sigma}}_{\text{constant}} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2
\end{aligned}$$

see therefore that maximising $\ell(\theta)$ is the same as maximising

$$\frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2$$

which is our original least-squares cost function. Note that the final choice of θ did not depend on what σ^2 was.

1.1.5 Locally Weighted Linear Regression

LWR

In the original linear regression algorithm, to make a *prediction* at a query point x (to evaluate $h(x)$), we would

1. Fit θ to minimise $\sum_i (y^{(i)} - \theta^T x^{(i)})^2$
2. Output $\theta^T x$

In contrast, the *locally weighted linear regression* algorithm does the following:

1. Fit θ to minimise $\sum_i w^{(i)} (y^{(i)} - \theta^T x^{(i)})^2$
2. Output $\theta^T x$

Here the $w^{(i)}$ are non-negative valued *weights*. Intuitively, if $w^{(i)}$ is large for a particular value of i then that particular example $x^{(i)}$ will have a larger effect on the optimisation of θ. If $w^{(i)}$ is small, then that example carries less impact on our selection of θ. A fairly standard choice for the weights is

$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right)$$

See that the weights depend on the particular point x at which we're trying to predict at—our entire selection of θ *changes with each predicton*—we re-train the model each time we make a prediction.

If $|x^{(i)} - x|$ is small, then $w^{(i)}$ is close to 1; if $|x^{(i)} - x|$ is large, then $w^{(i)}$ is small—θ is chosen giving a much higher 'weight' to the (errors on) training examples close to the query point (the point we want to predict) x. The parameter τ is called the *bandwith* parameter; it controls how quickly the weight of a training example falls off with distance from the query point x.

Non-parametric vs parametric algorithms

Locally weighted linear regression is an example of a *non-parameteric* algorithm, as opposed to (unweighted) linear regression which is a *parametric* learning algorithm. Parametric learning algorithms have a fixed, finite number of parameters θ which are fit to the data and stored, after which we no longer require the training data (since all predictions are made on the same θ). In contrast, for LWR we need to keep the entire training set around (since w changes with our prediction input and we need to optimise θ again). 'Non-parametric' refers to the idea that the amound of stuff we need to keep in order to represent the hypothesis h grows with the size of the training set.

1.1.6 Binary Classification and Logistic Regression

Classification

Classification problems are applicable in situations where the values y we want to predict take on only a small number of discrete values. Here we consider *binary classification*, where y can take on only two values—0 and 1. 0 is called the *negative class* and 1 the *positive class*. For a given $x^{(i)}$, the corresponding $y^{(i)}$ is also called the *label* for the training example.

Logistic Regression

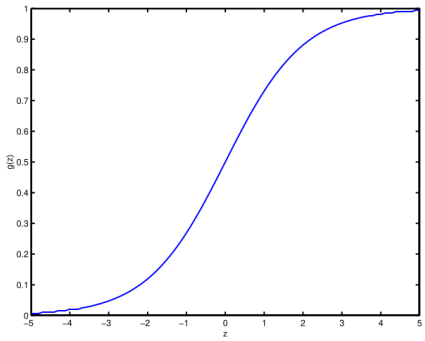
A linear regression algorithm in this case would perform poorly given the nature of the problem—intuitively it doesn't make sense for $h_\theta(x)$ to take values larger than 1 or smaller than 0 when we already know that $y \in \{0, 1\}$. To fix this we consider a different hypothesis h:

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

where

$$g(z) = \frac{1}{1 + e^{-z}}$$

is called the *logistic/sigmoid* function:



See that $g(z)$ tends toward 1 as $z \to \infty$, and to 0 as $z \to -\infty$. Also see that it is always bounded between 0 and 1. As before we keep the convention of $x_0 = 1$, so that $\theta^T x = \theta_0 + \sum_{j=1}^{d} \theta_j x_j$.

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Derivative of the Sigmoid function
Defining g as the sigmoid function, we note its derivative:

$$\begin{aligned} g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\ &= \frac{1}{(1+e^{-z})^2}(e^{-z}) \\ &= \frac{1}{(1+e^{-z})} \cdot \left(1 - \frac{1}{(1+e^{-z})}\right) \\ &= g(z)(1-g(z)) \end{aligned}$$

Probabalistic assumptions and maximum likelihood