Chapter 1

Linear regression

To make our housing example more interesting, let's consider a slightly richer dataset in which we also know the number of bedrooms in each house:

Living area (feet^2)	#bedrooms	Price (1000$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
$\vdots$	$\vdots$	$\vdots$

Here, the x's are two-dimensional vectors in $\mathbb{R}^2$. For instance, $x_1^{(i)}$ is the living area of the i-th house in the training set, and $x_2^{(i)}$ is its number of bedrooms. (In general, when designing a learning problem, it will be up to you to decide what features to choose, so if you are out in Portland gathering housing data, you might also decide to include other features such as whether each house has a fireplace, the number of bathrooms, and so on. We'll say more about feature selection later, but for now let's take the features as given.)

To perform supervised learning, we must decide how we're going to represent functions/hypotheses h in a computer. As an initial choice, let's say we decide to approximate y as a linear function of x:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 = \begin{pmatrix}\theta_0 & \theta_1 & \theta_2\end{pmatrix}\begin{pmatrix}1\\ x_1\\ x_2\end{pmatrix}$$

Here, the θ_i's are the **parameters** (also called **weights**) parameterizing the space of linear functions mapping from $\mathcal{X}$ to $\mathcal{Y}$. When there is no risk of

$$\vec{\theta} = \begin{pmatrix}\theta_0\\ \theta_1\\ \theta_2\end{pmatrix} \quad \vec{x} = \begin{pmatrix}x_0\\ x_1\\ x_2\end{pmatrix} = \begin{pmatrix}1\\ x_1\\ x_2\end{pmatrix}$$

where $x_0 = 1$

confusion, we will drop the θ subscript in $h_\theta(x)$, and write it more simply as $h(x)$. To simplify our notation, we also introduce the convention of letting $x_0 = 1$ (this is the **intercept term**), so that

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

where on the right-hand side above we are viewing θ and x both as vectors, and here d is the number of input variables (not counting x_0).

Now, given a training set, how do we pick, or learn, the parameters θ? One reasonable method seems to be to make $h(x)$ close to y, at least for the training examples we have. To formalize this, we will define a function that measures, for each value of the θ's, how close the $h(x^{(i)})$'s are to the corresponding $y^{(i)}$'s. We define the **cost function**:

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

If you've seen linear regression before, you may recognize this as the familiar least-squares cost function that gives rise to the **ordinary least squares** regression model. Whether or not you have seen it previously, let's keep going, and we'll eventually show this to be a special case of a much broader family of algorithms.

1.1 LMS algorithm

We want to choose θ so as to minimize $J(\theta)$. To do so, let's use a search algorithm that starts with some "initial guess" for θ, and that repeatedly changes θ to make $J(\theta)$ smaller, until hopefully we converge to a value of θ that minimizes $J(\theta)$. Specifically, let's consider the **gradient descent** algorithm, which starts with some initial θ, and repeatedly performs the update:

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

(This update is simultaneously performed for all values of $j = 0, \ldots, d$.) Here, α is called the **learning rate**. This is a very natural algorithm that repeatedly takes a step in the direction of steepest decrease of J.

In order to implement this algorithm, we have to work out what is the partial derivative term on the right hand side. Let's first work it out for the

$\frac{\partial}{\partial\theta_j} J(\theta) = \frac{\partial}{\partial\theta_j} \frac{1}{2}(h_\theta(x)-y)^2$ $\quad h_\theta(x) = \sum_{i=0}^{d} \theta_i x_i$ where $x_0 = 1$

$= \frac{1}{2} \frac{\partial}{\partial\theta_j} (h_\theta(x)-y)^2$ $\quad = (h_\theta(x)-y)\, x_j$

$= (h_\theta(x)-y) \cdot \frac{\partial}{\partial\theta_j} (h_\theta(x)-y)$ $\quad \Rightarrow \theta_j := \theta_j - \alpha x_j (h_\theta(x)-y)$

$= (h_\theta(x)-y) \cdot \frac{\partial}{\partial\theta_j} \left(\sum_{i=0}^{d} \theta_i x_i - y\right)$ $\quad \Leftrightarrow \theta_j := \theta_j + \alpha (h_\theta(y^{(i)}) - h_\theta(x^{(i)})) x_j^{(i)}$

case of if we have only one training example (x, y), so that we can neglect the sum in the definition of J. We have:

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

For a single training example, this gives the update rule:[1]

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

The rule is called the **LMS** update rule (LMS stands for "least mean squares"), and is also known as the **Widrow-Hoff** learning rule. This rule has several properties that seem natural and intuitive. For instance, the magnitude of the update is proportional to the **error** term $(y^{(i)} - h_\theta(x^{(i)}))$; thus, for instance, if we are encountering a training example on which our prediction nearly matches the actual value of $y^{(i)}$, then we find that there is little need to change the parameters; in contrast, a larger change to the parameters will be made if our prediction $h_\theta(x^{(i)})$ has a large error (i.e., if it is very far from $y^{(i)}$).

We'd derived the LMS rule for when there was only a single training example. There are two ways to modify this method for a training set of more than one example. The first is replace it with the following algorithm:

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}, \text{(for every } j) \tag{1.1}$$

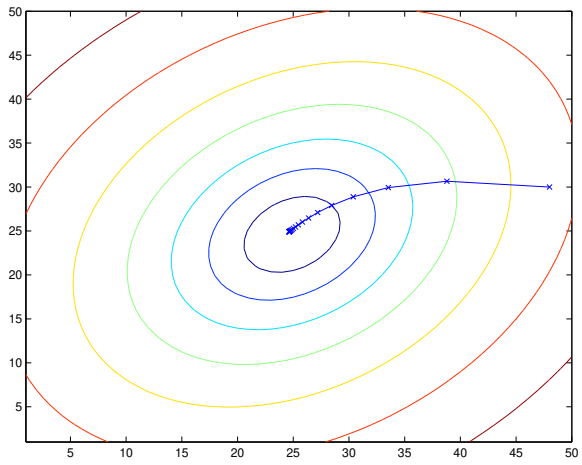
}

[1] We use the notation "$a := b$" to denote an operation (in a computer program) in which we *set* the value of a variable a to be equal to the value of b. In other words, this operation overwrites a with the value of b. In contrast, we will write "$a = b$" when we are asserting a statement of fact, that the value of a is equal to the value of b.

By grouping the updates of the coordinates into an update of the vector θ, we can rewrite update (1.1) in a slightly more succinct way:

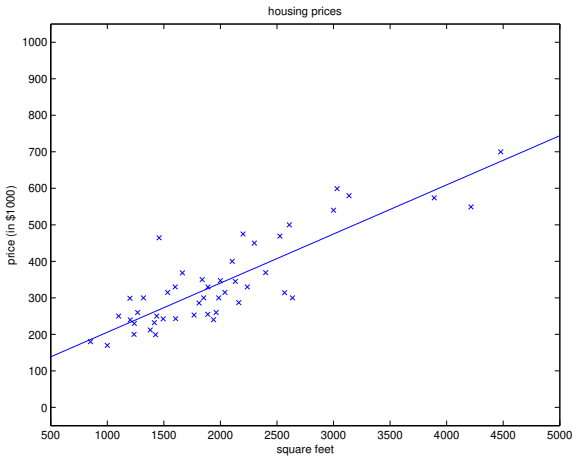
$$\theta := \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)})\right) x^{(i)}$$

The reader can easily verify that the quantity in the summation in the update rule above is just $\partial J(\theta)/\partial \theta_j$ (for the original definition of J). So, this is simply gradient descent on the original cost function J. This method looks at every example in the entire training set on every step, and is called **batch gradient descent**. Note that, while gradient descent can be susceptible to local minima in general, the optimization problem we have posed here for linear regression has only one global, and no other local, optima; thus gradient descent always converges (assuming the learning rate α is not too large) to the global minimum. Indeed, J is a convex quadratic function. Here is an example of gradient descent as it is run to minimize a quadratic function.



The ellipses shown above are the contours of a quadratic function. Also shown is the trajectory taken by gradient descent, which was initialized at (48,30). The x's in the figure (joined by straight lines) mark the successive values of θ that gradient descent went through.

When we run batch gradient descent to fit θ on our previous dataset, to learn to predict housing price as a function of living area, we obtain $\theta_0 = 71.27$, $\theta_1 = 0.1345$. If we plot $h_\theta(x)$ as a function of x (area), along with the training data, we obtain the following figure:



If the number of bedrooms were included as one of the input features as well, we get $\theta_0 = 89.60, \theta_1 = 0.1392$, $\theta_2 = -8.738$.

The above results were obtained with batch gradient descent. There is an alternative to batch gradient descent that also works very well. Consider the following algorithm:

Loop {

for $i = 1$ to n, {

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)}, \quad \text{(for every } j\text{)} \tag{1.2}$$

}

}

By grouping the updates of the coordinates into an update of the vector θ, we can rewrite update (1.2) in a slightly more succinct way:

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

In this algorithm, we repeatedly run through the training set, and each time we encounter a training example, we update the parameters according to the gradient of the error with respect to that single training example only. This algorithm is called **stochastic gradient descent** (also **incremental gradient descent**). Whereas batch gradient descent has to scan through the entire training set before taking a single step—a costly operation if n is large—stochastic gradient descent can start making progress right away, and

continues to make progress with each example it looks at. Often, stochastic gradient descent gets θ "close" to the minimum much faster than batch gradient descent. (Note however that it may never "converge" to the minimum, and the parameters θ will keep oscillating around the minimum of $J(\theta)$; but in practice most of the values near the minimum will be reasonably good approximations to the true minimum.[2]) For these reasons, particularly when the training set is large, stochastic gradient descent is often preferred over batch gradient descent.

1.2 The normal equations

Gradient descent gives one way of minimizing J. Let's discuss a second way of doing so, this time performing the minimization explicitly and without resorting to an iterative algorithm. In this method, we will minimize J by explicitly taking its derivatives with respect to the θ_j's, and setting them to zero. To enable us to do this without having to write reams of algebra and pages full of matrices of derivatives, let's introduce some notation for doing calculus with matrices.

1.2.1 Matrix derivatives

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

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

Thus, the gradient $\nabla_A f(A)$ is itself an n-by-d matrix, whose (i, j)-element is $\partial f / \partial A_{ij}$. For example, suppose $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ is a 2-by-2 matrix, and the function $f : \mathbb{R}^{2 \times 2} \mapsto \mathbb{R}$ is given by

$$f(A) = \frac{3}{2} A_{11} + 5A_{12}^2 + A_{21} A_{22}.$$

[2] By slowly letting the learning rate α decrease to zero as the algorithm runs, it is also possible to ensure that the parameters will converge to the global minimum rather than merely oscillate around the minimum.

Here, A_{ij} denotes the (i, j) entry of the matrix A. We then have

$$\nabla_A f(A) = \begin{bmatrix} \frac{3}{2} & 10A_{12} \\ A_{22} & A_{21} \end{bmatrix}.$$

1.2.2 Least squares revisited

Armed with the tools of matrix derivatives, let us now proceed to find in closed-form the value of θ that minimizes $J(\theta)$. We begin by re-writing J in matrix-vectorial notation.

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

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

Also, let $\vec{y}$ be the n-dimensional vector containing all the target values from the training set:

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

Now, since $h_\theta(x^{(i)}) = (x^{(i)})^T\theta$, we can easily verify that

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

Thus, using the fact that for a vector z, we have that $z^T z = \sum_i z_i^2$:

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

$\nabla_\theta J(\theta) = \nabla_\theta \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y})$
$= \frac{1}{2}\nabla_\theta (X\theta - \vec{y})^T(X\theta - \vec{y})$
$= \frac{1}{2}\nabla_\theta ((X\theta)^T - \vec{y}^T)(X\theta - \vec{y})$
$= \frac{1}{2}\nabla_\theta ((X\theta)^T X\theta - (X\theta)^T\vec{y} - \vec{y}^T(X\theta) + \vec{y}^T\vec{y}) = X^TX\theta - X^T\vec{y}$

$= \frac{1}{2}\nabla_\theta (\theta^T X^T X\theta - 2\vec{y}^T(X\theta))$
$= \frac{1}{2}(2X^TX\theta - 2\vec{y}^TX)$
$= \frac{1}{2}(2X^TX\theta - 2X^T\vec{y})$

Finally, to minimize J, let's find its derivatives with respect to θ. Hence,

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

In the third step, we used the fact that $a^Tb = b^Ta$, and in the fifth step used the facts $\nabla_x b^Tx = b$ and $\nabla_x x^TAx = 2Ax$ for symmetric matrix A (for more details, see Section 4.3 of "Linear Algebra Review and Reference"). To minimize J, we set its derivatives to zero, and obtain the **normal equations**:

$$X^TX\theta = X^T\vec{y}$$

Thus, the value of θ that minimizes $J(\theta)$ is given in closed form by the equation

$$\theta = (X^TX)^{-1}X^T\vec{y}.$$[3]

1.3 Probabilistic interpretation

When faced with a regression problem, why might linear regression, and specifically why might the least-squares cost function J, be a reasonable choice? In this section, we will give a set of probabilistic assumptions, under which least-squares regression is derived as a very natural algorithm.

Let us assume that the target variables and the inputs are related via the equation

$$y^{(i)} = \theta^Tx^{(i)} + \epsilon^{(i)},$$

[3]Note that in the above step, we are implicitly assuming that X^TX is an invertible matrix. 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, then X^TX will not be invertible. Even in such cases, it is possible to "fix" the situation with additional techniques, which we skip here for the sake of simplicty.