Machine Learning

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1 Introduction

Definition (Machine Learning - Tom Mitchell, 1998)**.** A computer program is said to *learn* from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.

2 Linear Regression

Notation (Training data)**.** We have a set of training examples, denoted by $x \in \mathbb{R}^n \times \mathbb{R}^m$ (m examples of n features). Concretely, $x^{(i)}$ denotes the features of the i^{th} training example, with $x_j^{(i)}$ being the value of feature j in the i^{th} training example.

Conventionally, we take an extra row of ones as the 0^{th} feature ($x_0 := 1$) and denote the corresponding $(m+1) \times n$ matrix X the *design matrix*.

The output variable is $y \in \mathbb{R}^m$.

Definition (Linear hypothesis)**.** Our hypothesis is

$$h_\theta(x) = \theta^T X$$

where $\theta \in \mathbb{R}^{n+1}$ is a vector of parameters to be estimated.

Definition (Squared Loss Cost Function)**.** The *cost function*

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

represents a measure of the fit of a particular choice of parameters θ.

We estimate θ as the value minimising $J(\theta)$.

2.1 Gradient Descent

Gradient descent involves following the gradient of this cost function to find its minimum. In practice, taking an initial estimate θ_0 and *learning rate* α we iteratively compute

$$\theta := \theta - \alpha \boldsymbol{\nabla} J$$

that is

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

for $j \in \{0, \dots, n+1\}$.

For linear regression,

$$\begin{aligned} \frac{\partial}{\partial \theta_j} J(\theta) &= \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^i) - y^i \right) x_j^{(i)} \\ &= \frac{1}{m} X(\theta^T X - y) \end{aligned}$$

We declare convergence when $J(\theta)$ decreases by less than ϵ in a single iteration.

The learning rate α must be chosen carefully. Too large and convergence may not occur, too small and convergence will be slow.

2.1.1 Feature scaling

We can speed up gradient descent via *feature scaling* and *mean normalization*. Intuitively, this involves scaling each feature so that the steps taken along the gradient are roughly uniform across the dimensions of the feature space. Concretely, we set

$$x = \frac{x - \mu}{\sigma}$$

where μ is the (row-wise) mean of x and σ is the (row-wise) standard deviation of x.

2.2 Analytic solution

The minimum of the cost function can also be found analytically (solve the system of equations $\boldsymbol{\nabla} J = 0$ to obtain the exact solution

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

in the cast where $(X^T X)$ is invertible. Even in the singular case, we can take a numerical solution with the pseudo-inverse, e.g. via the Octave function `pinv`. The singular case can occur when there are redundant (linearly dependent) features, or too many features $(m \leq n)$.

3 Logistic Regression - Classification

We now restrict $y \in \{0, 1\}^m$ so that we now have the problem of *classifying* an observation x.

Definition (Classification hypothesis)**.** Our hypothesis is

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

where $g(z)$ is the *sigmoid* function, so that $0 \leq h_\theta(x) \leq 1$. We interpret

$$\begin{aligned} h_\theta(x) &= \mathbb{P}_\theta(y = 1 \mid x) \\ &= \mathbb{P}(y = 1 \mid x, \theta) \end{aligned}$$

and 'predict' that $y = 1$ if $h_\theta(x) \geq 0.5$, i.e. if $\theta^T x \geq 0$. The surface $h_\theta(x) = 0.5$ is known as the *decision boundary.*

The squared loss cost function is not convex in the case of logistic regression, we instead use the logistic cost function.

Definition (Logistic Cost function)**.** The *logistic* cost function is

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

where

$$\begin{aligned} \mathrm{Cost}(h_\theta(x), y) &= \begin{cases} -\log(h_\theta(x)) & \text{for } y = 1 \\ -(1 - \log(h_\theta(x))) & \text{for } y = 0 \end{cases} \\ &= -y \log(h_\theta(x)) - (1 - y)(1 - \log(h_\theta(x))) \end{aligned}$$

This form of cost function can be derived from *maximum likelihood estimation* for the binomial distribution.

Gradient descent applies in the same way, and moreover we again find that

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^i) - y^i \right) x_j^{(i)}$$

though of course with the new hypothesis function.

3.0.1 Advanced optimization

There exist other, more complex algorithms to minimum the cost function, such as

(i) Conjugate gradient

(ii) BFGS

(iii) L-BFGS

which don't involve picking a learning rate and are often faster.

3.1 Multiclass classification

For the case of classifying $y \in \{1, \ldots, k\}$ we can apply the principle of *one-vs-all* to train k classifiers $h_\theta^{(i)}$ each of which is predicting the probability $\mathbb{P}_\theta(y = i \mid x)$ (against all other classes). The final prediction is then taken as the class i maximising $h_\theta^{(i)}$.

3.2 Addressing overfitting

With too many features, the learned hypothesis may fit the training set very well ($J(\theta) \approx 0$ but fail to generalize to new examples. This is known as *overfitting*.

This can be addressed by reducing the number of features (manually or alorithmically), or via regularization.

3.2.1 Regularization

The idea is too keep all features, but reduce the magnitude of the parameters θ_j. This works well when there are lots of features, each contributing a bit to predicting y.

To achieve this, we *penalize* the parameters inside the cost function.

For *linear regression*, we have

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(h_\theta(x^i) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\theta_j^2\right]$$

N.B. we conventionally do not penalize θ_0, so it is excluded from the sum.

The analytic solution is then

$$\theta = \left(X^TX + \lambda\begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1\end{bmatrix}\right)^{-1} X^Ty$$

which does not suffer from the problem of non-invertibility.

For *logistic regression*, we have

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left[-y\log(h_\theta(x^{(i)})) - (1-y)(1-\log(h_\theta(x^{(i)})))\right] + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

As with the learning rate, λ must be appropriately chosen: too small and the regulation will have little effect, but too large will lead to *underfitting*!

4 Neural Networks

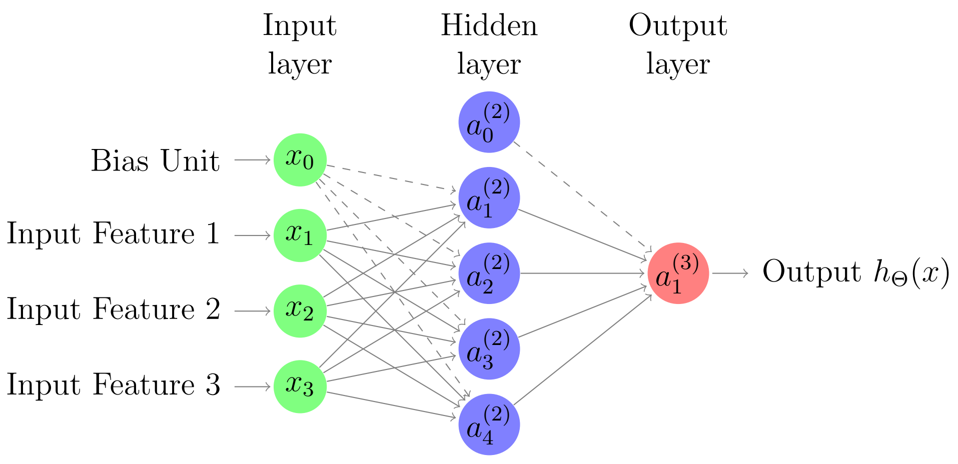
The neuron model mimics the biological neuron: depending on some *activation function* of the inputs (via *dendrites*), the unit outputs (via *axon*) some value (*signal*). The *neural network* simply connects such units in a sequence of layers, where the output of the unit in one layer is input for each unit in the next layer.

The activation function is the sigmoid logistic function $g(z) = \frac{1}{1+e^{-z}}$. Thus, each layer is a series of logistic regression models trained on the previous layer (to which we also add a *bias unit* of constant value 1).

The first layer is the actual *input* to the model, the last layer the *output*, while the intermediate layers are known as *hidden layers*. See Figure 1[1].

[1]adapted from http://www.texample.net/tikz/examples/neural-network/

Figure 1: Representation of Neural Network



4.1 Forward propagation

Forward propagation describes the method by which, given a trained neural network, we can compute predictions.

Consider a neural network with L layers, with s_j units in layer j.

Let $x_1, \dots, x_{s_0}$ be the training data, to which we add $x_0 := 1$. Set $a^{(1)} := x$.

Let $\Theta^{(j)}$ be the parameters (weights) of the mapping between layers j and $(j+1)$, so that the i^{th} row of $\Theta^{(j)}$ is the logistic regression parameters for the i^{th} unit in layer $(j+1)$. Thus $\Theta^{(j)}$ is of dimension $s_{j+1} \times (s_j + 1)$.

The *activations* of the units in layer j is given by the s_j dimensional vector $a^{(j)}$ where

$$\begin{aligned} z^{(j)} &= \Theta^{(j-1)} a^{(j-1)} \\ a^{(j)} &= g(z^{(j)}) \end{aligned}$$

and at each layer we also add the bias unit $a_0^{(j)} := 0$. The output is $h_\Theta(x) = a^{(L)}$ (which may be multi-dimensional).

4.2 Multiclass classification

Given labels $\{1, \dots, K\}$, we model label k as the unit coordinate vector for dimension k, i.e. a vector with 1 in dimension k, and 0 in all other dimensions.

For example, to represent $K = 3$ classes, we would use

$$1 \to \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, 2 \to \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ and } 3 \to \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

4.3 Examples of neural networks

As illustration of how neural networks can represent more advanced models than simple linear or logistic regression, we consider (approximate) representations of well-known binary operations.

Example (AND)**.** With $x_1, x_2 \in \{0, 1\}$ and $y = x_1 \wedge x_2$.

We use a neural network with no hidden layer, and one output unit (i.e. simple logistic regression!). Take $\Theta^{(1)} = \begin{pmatrix} -30 & 20 & 20 \end{pmatrix}$.

Figure 2: XNOR Neural Network

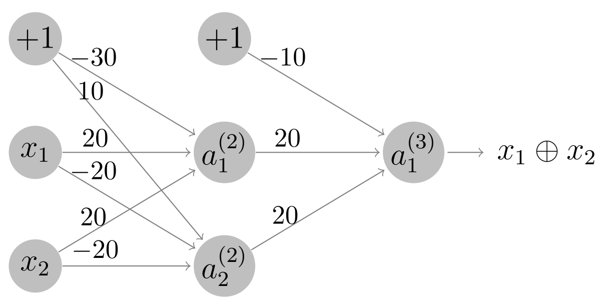


Table 1: XNOR neural network

x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
0	0	0	0	1
0	1	0	0	0
1	0	0	0	0
1	1	0	1	1

Example (OR)**.** With notation above, but to represent $y = x_1 \vee x_2$, we can take $\Theta^{(1)} = \begin{pmatrix} -10 & 20 & 20 \end{pmatrix}$.

Example (NOT)**.** With $x_1 \in \{0,1\}$ and $y = \neg x_1$, we can take $\Theta^{(1)} = \begin{pmatrix} 10 & -20 \end{pmatrix}$.

Example (XNOR)**.** We can represent $y = \neg(x_1 \oplus x_2)$, by combining the above examples into a neural networks with one hidden layer, using

$$\Theta^{(1)} = \begin{pmatrix} -30 & 20 & 20 \\ 10 & -20 & -20 \end{pmatrix}$$

and

$$\Theta^{(2)} = \begin{pmatrix} -10 & 20 & 20 \end{pmatrix}$$

which is taking the hidden layer activations as $a_1^{(2)} = x_1 \wedge x_2$ and $a_2^{(2)} = (\neg x_1) \wedge (\neg x_2)$, and the output is $y = h_\Theta(x) = a_1^{(3)} = a_1^{(2)} \vee a_2^{(2)}$. See Figure 2 and Table 1.

4.4 Backpropagation

Definition (Cost function for Neural Network)**.** Suppose we have m training examples $x^{(i)}, \ldots, x^{(m)}$, and K classes (so we represent the observed outputs as $y_i \in \{0,1\}^K$, as described in §4.2). Then the cost function is given by

$$\begin{aligned} J(\Theta) = &-\frac{1}{m}\left(\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log h_\Theta(x^{(i)})_k + (1 - y_k^{(i)}) \log\left(1 - h_\Theta(x^{(i)})_k\right)\right) \\ &+ \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}} (\Theta_{i,j}^{(l)})^2 \end{aligned}$$

where $h_\Theta(x^{(i)})$ is the prediction as obtained by forward-propagation (described in §4.1) for training example i, and λ is the *regularization parameter* (as in §3.2.1).

The method of *backpropagation* describes a way to compute the gradients $\frac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}}$ so that we can apply an optimization algorithm (such as gradient-descent) to minimize $J(\Theta)$.

Intuitively, we run a forward pass (§4.1) to compute the activations throughout the network, then for each node j in layer l we compute an *error term* $\delta_j^{(l)}$ that measures how much that node was 'responsible' for errors in the output. For the output layer, this can simply be the distance between $h(x)$ and y, while for the hidden layers we can take a weighted (by Θ) averaged of the errors in the following layer.

Definition (Backpropagation Algorithm)**.** For a given training example $x^{(t)}$, we compute the gradient as follows:

(i) Set the input layer $a^{(1)} := x^{(t)}$.

(ii) Perform forward propagation to compute the activations $(z^{(j)}, a^{(j)})$ for layers $2, \ldots, L$.

(iii) For the output layer L, compute $\delta^{(L)} = a^{(L)} - y$, where y is as in §4.2.

(iv) For layers $l = L-1, \ldots, 2$, compute $\delta^{(l)} = (\Theta^{(l)})^T \delta^{(l+1)} \odot g'(z^{(l)})$, where $g'(z^{(l)}) = a^{(l)} \odot (1 - a^{(l)})$. [2]

(v) Accumulate $\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$.

Finally, we have

$$\frac{\partial J(\Theta)}{\partial \Theta_{i,j}^{(l)}} = \begin{cases} \frac{1}{m}\left(\Delta_{i,j}^{(l)} + \lambda \Theta_{i,j}^{(l)}\right) & \text{for } j \neq 0 \\ \frac{1}{m}\Delta_{i,j}^{(l)} & \text{for } j = 0 \end{cases}$$

4.4.1 Gradient checking

It can be helpful in debugging to check the gradient computed in backpropagation against a numerical approximation, for example using the symmetric difference quotient $\frac{f(x+h)-f(x-h)}{2h}$ in each dimension of Θ, and comparing to the gradient from backpropagation which should be similar.

4.4.2 Random initialization

The initial parameters must be randomly initialized because if otherwise we started at $\Theta = 0$ uniformly then by symmetry the parameters in each layer would remain equal on every iteration.

5 Tuning and evaluating

5.1 Cross-validation

A common approach is to split the available data into 3 sets: training, (cross-)validation, and test data (often at a roughly 60-20-20 ratio). When a model has further parameters (other than θ) to be chosen, such as the dimension of a polynomial model or the regularization parameter λ, then for a specific choice of such parameters we can train the model on the *training data*. We can do this for a range of possible parameters, then choose which has the lower error (e.g. squared loss) on the *cross-validation* data. Finally, we can evaluate the overall choice of model by computing the error on the *test data*.

[2] Here I am using the notation $\odot$ to mean element-wise multiplication (i.e. $.*$ in Matlab).

Table 2: Type I and Type II Errors

		Actual	
		1	0
Predicted	1	true positive	false positive
	0	false negative	true negative

5.2 Bias-Variance Tradeoff

(i) High *bias* refers to a false assumption in the model (e.g. due to too *low* a degree polynomial) and causes *underfitting*. It manifests as high and similiar training and cross-validation error. We may try

   (a) adding further features;

   (b) decreasing λ.

(ii) High *variance* refers to an oversensitivity to small changes in the training data (e.g. due to too *high* a degree polynomial) and causes *overfitting*. It manifests as low training error but high cross-validation error. We may try

   (a) using a smaller set of features;

   (b) getting more training examples;

   (c) increasing λ.

Of course, λ may be chosen as in §5.1 by trying a range of values on the training data and choosing that which performs best on the cross-validation data (note that the regularization parameter should not be used in evaluating the cross-validation error).

Generally, it's best to start with a simple model, implement it quickly, and investigate the error to diagnose whether it may be suffering from high bias or variance.

5.3 Precision and recall

For a binary classification problem, we have a tradeoff between precision and recall (a.k.a. sensitivity), where

$$\begin{aligned} \text{precision} &= \frac{\text{true positives}}{\text{predicted positives}} &= \frac{\text{true positives}}{\text{true positives+false positives}} \\ \text{recall} &= \frac{\text{true positives}}{\text{actual positives}} &= \frac{\text{true positives}}{\text{true positives+false negatives}} \end{aligned}$$

and true/false positives/negatives are defined as in Table 2.

For example in the case of medical diagnosis, we might want to only diagnose if truly confident so as to avoid putting a patient through unnecessary stress (high precision), whereas we might also want to avoid missing dangerous cases (high recall).

5.3.1 F_1 score

The harmonic mean of precision (P) and recall (R) can be a useful comparison,

$$F_1 = 2\frac{PR}{P+R}$$

which has its best value at 1 and worst at 0.

6 Support Vector Machines

The Support Vector Machine (SVM) has a cost function that is similar to that of logistic regression (in §3), with $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \text{Cost}(\theta^T x^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$ except that now

$$\begin{aligned}\text{Cost}(z, y) &= \begin{cases} \max(0, 1-z) & \text{for } y = 1 \\ \max(0, 1+z) & \text{for } y = 0 \end{cases} \\ &= \max(0, 1 + (1-2y)z)\end{aligned}$$

Note that there is zero cost for $z \geq 1$ when $y = 1$ or $z \leq -1$ when $y = 0$, compared to logistic regression in which for $y = 1$ the cost was strictly positive, but asymptotically vanishing for $z \gg 0$ (and similarly for $y = 0$, $z \ll 0$). Again, we predict $h_\theta(x) = 1$ iff $\theta^T x \geq 0$.

Conventionally, we use a different scaling, and so take

$$J(\theta) = C\sum_{i=1}^{m} \text{Cost}(\theta^T x^{(i)}, y^{(i)}) + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2 \tag{1}$$

where C is now playing the opposite role to λ.

6.1 Large Margin Classification

The SVM is known as a *large margin classifier* meaning that in the linearly separable case (and for large C) the decision boundary divides the two classes whilst maximizing the distance to the nearest data point in each class - i.e. maximizing the margin. The parameter C determines the tradeoff between maximizing the margin and ensuring the training data are correctly classified. Smaller values of C make the SVM less susceptible to outliers (and therefore not strictly a large margin classifier).

6.1.1 Intuition

Consider $x \in \mathbb{R}^n$. The two parallel hyperplanes defining the margin (of which the decision boundary is in the middle) can be described by

$$\begin{aligned}\theta \cdot x - b &= 1 \\ \theta \cdot x - b &= -1\end{aligned}$$

where θ is the normal vector to the hyperplane (and $b = -\theta_0$), so the condition that points lie on the correct side of the margin is

$$\begin{cases} \theta \cdot x - b \geq 1 & \text{for } y = 1 \\ \theta \cdot x - b \leq -1 & \text{for } y = 0. \end{cases}$$

The distance between the hyperplanes is $\frac{2}{\|\theta\|}$, so is maximized by minimizing $\|\theta\|$. Note that $\text{Cost}(\theta \cdot x, y)$ is zero if x satisfies these conditions and assigns a cost proportional to the distance from the margin if not. Thus we recover the optimization objective (1).

6.2 Generalizations

The standard SVM only provides a linear decision boundary. However, we can map to a transformed (and higher dimensional) feature space, such that we learn a non-linear classifier in the input space.

6.2.1 Kernels

A common technique involves choosing 'landmark' points $l^{(1)}, l^{(2)}, l^{(3)}, \ldots$, which we may take to be $x^{(1)}, \ldots, x^{(m)}$. For each input feature $x \in \mathbb{R}^n$ we then have a transformed feature $f \in \mathbb{R}^m$ given by

$$\begin{aligned} f_i &= k(x, l^{(i)}) \\ &= \exp\left(-\frac{1}{2\sigma^2}\left\|x - l^{(i)}\right\|^2\right) \end{aligned}$$

which represents the 'similarity' between the point and each landmark. The function k is known as the Gaussian kernel. The linear SVM can then be trained on this new feature space, and we predict $h_\theta(x) = 1$ if $\theta^T f \geq 0$.

The parameter σ^2 can tune the transformation: larger σ^2 make the features vary more smoothly so leads to higher bias and lower variance.

Other kernels may also be used, such as the polynomial kernel $k(x, y) = (x^T y + c)^d$. In practice, a linear kernel (or logistic regression) should perform fine for large n, while for intermediate-sized m (say between 10 and 10,000) and small n the Gaussian kernel can be effective.

7 Clustering

The *clustering* problem is an *unsupervised* learning problem: given an *unlabelled* training set $\{x^{(1)}, \ldots, x^{(m)}\}$ with $x^{(i)} \in \mathbb{R}^n$, the task is to assign each point one of K clusters, where 'similar' examples should be assigned to the same cluster.

7.1 K-means

In K-means, each cluster is defined by a *centroid* μ_j (for $1 \leq j \leq K$), and a point $x^{(i)}$ is assigned to the cluster $c^{(i)}$ (for $1 \leq i \leq m$) associated with the nearest centroid. The idea is to minimize the average distance between each point and it's associated centroid, thus the optimization objective is

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K) = \frac{1}{m}\sum_{i=1}^{m}\left\|x^{(i)} - \mu_{c^{(i)}}\right\|^2$$

7.1.1 Algorithm

Given an initial set of centroid $\mu_1, \ldots, \mu_K$, the K-means algorithm repeatedly alternates between two steps:

Assignment Assign each example to the nearest centroid. That is, for each $1 \leq i \leq m$, set $c^{(i)}$ to be j that minimizes $\left\|x^{(i)} - \mu_j\right\|$.

Update Change each cluster centroid to be the mean of all points assigned to it. That is, for each $1 \leq j \leq K$, if $C_k = \{i : c^{(i)} = j\}$ is the set of examples in cluster j, then set $\mu_j = \frac{1}{|C_k|} \sum_{i \in C_k} x^{(i)}$.

and converges when the assignments no longer change.

7.1.2 Choosing input parameters

The initial centroids are usually taken to be a random choice of K training examples. Note that the algorithm is not guaranteed to converge to the true optimum, so best practice is to repeatedly try with different random initializations and choose the clusters minimizing the cost.

The number of clusters may be chosen using information from the problem domain if possible, e.g. you may know that you want to group customers into 3 groups by clothes size. Otherwise, the ‘elbow method’ may be used: choose the number of clusters such that adding another doesn’t significantly improve the model. This manifests itself as a sudden leveling-off if you plot cost J against K, reminiscent of an elbow shape.

8 Dimensionality Reduction

The technique of *dimensionality reduction* can be employed both for *data compression* (to speed up learning algorithms) and to aid *visualization* (by reducing to 2 or 3 dimensions). Note that dimensionality reduction is not always needed, and is not an appropriate solution to overfitting (regularization should be used instead).

8.1 Principal Component Analysis

PCA describes a technique for reducing points in $\mathbb{R}^n$ to points in $\mathbb{R}^k$ by projecting onto the space spanned by k vectors $\{u^{(1)}, \ldots, u^{(k)}\}$ such that the *projection error* is minimized. The projection error is the squared distance between a point and its ‘estimate’. For example, in the case of reducing $\mathbb{R}^2$ to $\mathbb{R}$ it is the perpendicular distance between the point x and the line u (as opposite to the vertical distance, as in linear regression).

8.1.1 Singular Value Decomposition

SVD decomposes the $m \times n$ matrix X into

$$X = U \Sigma V^T$$

where

- U is an $m \times n$ orthogonal matrix with linearly independent columns.
- Σ is a positive $n \times n$ diagonal matrix with $\sigma_1 \geq \ldots \geq \sigma_n$.
- V^T is a $n \times n$ orthogonal matrix.

That is, we represent the point x_i as the linear combination $\sum_{j=1}^{n} u_{ij} \sigma_j \bar{v}_j$.

For PCA, we simply cut off the SVD at dimension k, so $x_i \approx \sum_{j=1}^{k} u_{ij} \sigma_j \bar{v}_j$. The lower-dimensional representation is obtained from the truncated matrix U_k via $z_i = U_k^T x_i$.

The 'reconstructed' point is given by $U_k z_i$ with the projection error being the squared distance between this and the original x_i. Note that the diagonal entries in Σ represent the variance, so we are cutting off the dimensions with low variance.

8.1.2 Preprocessing

Feature scaling and mean normalization should be applied before carrying out PCA.

8.1.3 Choosing k

Typically, we choose k to be the smallest value such that

$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{\text{approx}}^{(i)}\|}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|} \leq p$$

where the numerator is the *average squared projection error*, the denominator is the *total variation* in the data, and we typically interpret the condition by saying that (1-p) (e.g. 99%) of the variance is retained (or explained). Using SVD, this is equivalent to choosing the minimum k such that

$$\frac{\sum_{i=1}^{k}\sigma_i}{\sum_{i=1}^{m}\sigma_i} \geq 1 - p$$