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The Canonical Distortion Measure for Vector Quantization and Function Approximation*

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Abstract. To measure the quality of a set of vector quantization points a means of measuring the distance between a random point and its quantization is required. Common metrics such as the Hamming and Euclidean metrics, while mathematically simple, are inappropriate for comparing natural signals such as speech or images. In this paper it is shown how an environment of functions on an input space X induces a canonical distortion measure (CDM) on X. The depiction "canonical" is justified because it is shown that optimizing the reconstruction error of X with respect to the CDM gives rise to optimal piecewise constant approximations of the functions in the environment. The CDM is calculated in closed form for several different function classes. An algorithm for training neural networks to implement the CDM is presented along with some encouraging experimental results.

Keywords: Canonical Distortion, Learning Distance Measures, Vector Quantization

1. Introduction

Consider the problems "What are appropriate distortion measures for images of handwritten characters, or images of faces, or representations of speech signals?" Simple measures such as squared Euclidean distance, while widely used in vector quantisation applications[7], do not correlate well with our own subjective notion of distance in these problems. For example, an image of an "A" and a slightly larger image of an "A" look subjectively very similar to a human observer, although their squared Euclidean separation (measured on a pixel by pixel basis) is very large. The same can be said for two images of my face viewed from slightly different angles. Finding distortion measures that more accurately correlate with our subjective experience is of great practical utility in vector-quantisation and machine learning. Quantisation with a poor distortion measure will cause the encoder to make inefficient use of the available codebook vectors. Also, learning using nearest neighbour techniques or by generating a piecewise constant approximation to the target function will be more effective if an appropriate measure of the distortion between input vectors is available.

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From a purely philosophical perspective there is no a priori natural distortion measure for a particular space X of images or signals. To generate a distortion measure some extra structure must be added to the problem. In this paper it is argued that the required extra structure is given in the form of an environment of functions \mathcal{F} on X. For example, consider each possible face classifier as a function on the space of images X. The classifier for "jon", f_{jon} , behaves as follows: $f_{jon}(x) = 1$ if x is an image of my face and $f_{\text{jon}}(x) = 0$ if x is not an image of my face. Note that f_{ion} is constant across images of the same face: it gives constant value "1" to images of my face and constant value "0" to images of anyone else's face. Similarly, there exists classifiers in the environment that correspond to "mary" (f_{mary}) , "joe" (f_{ioe}) and so on. All these classifiers possess the same property: they are constant across images of similar looking faces. Thus, information about the appropriate distortion measure to use for faces is somehow stored in the environment of face classifiers. Similar considerations suggest that it is the class of character classifiers that generate the natural distortion measure for characters, it is the class of spoken words that generate the natural distortion measure for speech signals, it is the class of smooth functions that generate the natural distortion measure for regression problems, and so on. A more formal justification for this assertion will be given in section 2.2 where an explicit formula is presented for the distortion measure generated by a function class. Such a distortion measure is termed the Canonical Distortion Measure or CDM for the function class. Loosely speaking, the canonical distortion between two inputs x and x' is defined to be the difference between f(x)and f(x'), averaged over all functions f in the environment.

In section 4 an optimality property of the CDM is proved, namely that it generates optimal quantization points and Voronoi regions for generating piecewise constant approximations of the functions in the environment. In section 3 the CDM is explicitly calculated for several simple environments. In particular it is shown that the squared Euclidean distance function is the CDM for a *linear environment*. This leads to the interesting observation that the squared Euclidean distance is optimal for approximating linear classes (and in fact *only* optimal for approximating linear classes).

In section 4.1 the optimal quantization points for a quadratic environment are calculated, and the relationship between the spacing of the points and the behaviour of the functions in the environment is discussed.

The relationship between the CDM and other approaches to learning distance metrics is discussed in section 5 (see also section 1.1 below), where we will see that the CDM provides a unifying conceptual framework for many seemingly disparate threads of research.

In section 6 it is shown how the CDM may be *learnt* by sampling both from the input space *and* the environment, and an (albeit toy) experiment is reported in which the CDM is learnt for a "robot arm" environment. The resulting CDM is then used to facilitate the learning of piecewise constant approximations to the functions in the environment. The same functions are also learnt without the help of the CDM and the results are compared. At least on this toy problem, learning

with the CDM gives far better generalisation from small training sets than learning without the CDM.

1.1. Related work

Other authors have investigated the possibility for using specially tailored distance functions in both machine learning and vector quantization contexts. The authors of [11] used a measure of distance that takes into account invariance with respect to affine transformations and thickness transformations of handwritten characters. They achieved a notable improvement in performance using this measure in a nearest neighbour classifier. Independently but simultaneously with some of the work in a previous incarnation of this paper [1], the authors of [12] proposed an "invariance measure" on images that has a close relationship to the CDM defined here, under certain restrictions on the functions in the environment. They also presented techniques for using the invariance measure to facilitate the learning of novel tasks. In work that is close to the spirit of the present paper, the authors of [9] considered vector quantization in a Bayes classifier environment. They modified the usual squared Euclidean reconstruction error ((2) in section 2.1 below, with $d = \|\cdot\|^2$) by adding a Bayes risk term, and presented results showing improved combined quantization and classification performance in several real-world problems. The relationship between all these approaches and the CDM is discussed further in section 5.

As an historical note, the idea of using a set of functions to generate a pseudometric was used at least twenty years ago as a technical tool in the theory of topology [4], although that application has little to do with the present paper.

2. The distortion measure and vector quantization

2.1. Vector quantization

As any real digital communication channel has only finite capacity, transmitting continuous data (e.g speech signals or images) requires first that such data be transformed into a discrete representation. Typically, given a probability space (X, Σ, P) (Σ is a σ -algebra of subsets of X and P is the probability distribution on X), one chooses a quantization or codebook $\{x_1, \ldots, x_k\} \subset X$, and instead of transmitting $x \in X$, the index of the "nearest" quantization point

$$q_d(x) := \operatorname{argmin}_{x_i} d(x_i, x) \tag{1}$$

is transmitted, where d is a distortion measure (not necessarily a metric) on X. The quantization points $\vec{x} = \{x_1, \dots, x_k\}$ are chosen so that the expected distortion between x and its quantization $q_d(x)$ is minimal, i.e \vec{x} are chosen to minimize the reconstruction error

$$E_d(\vec{x}) = \int_X d(x, q_d(x)) dP(x). \tag{2}$$

A common approach to minimizing (2) is Lloyd's algorithm which iteratively improves a set of quantization points based on a centroidal update (see [8, 5, 7]).

Some examples of distortion measures are the *Hamming metric*,

$$d(x, x') = 1 - \delta(x, x'),$$

where δ is the Kronecker delta function, and the squared Euclidean distortion measure for vector-valued X.

$$d(x, x') = ||x - x'||^2.$$

The use of these distortion measures has more to do with their convenient mathematical properties than their applicability to any particular problem domain. For example, suppose X is a space of images and it is images of characters that are being transmitted over the channel. An image of the character "A" and another translated image of the same character would be considered "close" in this context. although the squared Euclidean distance between the two images would be large, quite likely larger than the distance between an image of "A" and an image of "B" in the same location. Thus the squared Euclidean distortion measure does not capture well the idea of two images being "close". Another example is that of speech coding—there is a large squared Euclidean distance between a speech signal and a small translation of it in time, although both sound very similar to a human observer. A vector quantizer constructed using an inappropriate distortion measure will require a far larger set of quantization points to achieve satisfactory performance in environments where we are primarily interested in the *subjective* quality of the reconstruction. And in almost all applications of vector quantization it is the subjective quality of the reconstruction that is the most important: eventually the quality of the reconstructed speech signal or image is measured by how close it appears to be to the original for some observer.

In the next section we will see how the problem of choosing an appropriate distortion measure may be solved, at least *in principle*, by using the idea of the *environment* of a quantization process.

2.2. The Environment

What makes the translated image of an "A" close to the original, while an untranslated image of a "B" quite distant? And what makes two speech signals nearly identical even though they are miles apart from a Euclidean perspective? As discussed in the introduction, it is because there is an *environment* of functions (the character classifiers) that vary little across images of the same character, and similarly there is an environment of "speech classifiers" that vary little across utterances of the same sentences or words.

Note that the set of *possible* character classifiers is much larger than the set of particular classifiers for the English alphabet (English language). The particular

form of the letters we use is arbitrary (as evidenced by the existence of vastly different alphabets such as Hebrew or Kanji), the only thing that is required of a character is that different examples of it are recognisably the same object (to us). Thus the number of different character classifiers is potentially astronomical. A similar conclusion holds for speech: the set of spoken word classifiers is nearly infinite if one includes all possible words from all possible languages.

2.3. Formal definition of the Canonical Distortion Measure (CDM)

To formalize the idea that it is an environment of functions that determines the distortion measure on the input space, define the *environment* of any probability space (X, Σ, P) to be a pair (\mathcal{F}, Q) where \mathcal{F} is a set of functions mapping X into a space (Y, σ) , where $\sigma: Y \times Y \to R$ (σ may be a metric), and Q is a probability measure on \mathcal{F}^1 . An environment so defined induces the following natural distortion measure on X:

$$\rho(x, x') = \int_{\mathcal{F}} \sigma(f(x), f(x')) dQ(f), \tag{3}$$

for all $x, x' \in X$. In words, $\rho(x, x')$ is the average distance between f(x) and f(x') where f is a function chosen at random from the environment.

Note that if σ is a metric on Y then ρ is a pseudo-metric on X (recall that a pseudo-metric is the same as a metric except that $\rho(x, x') = 0$ does not necessarily imply x = x'). From now on ρ will be referred to as the *Canonical Distortion Measure* or *CDM* for the environment (\mathcal{F}, Q) .

In relation to the character transmission problem, \mathcal{F} would consist of all character like classifiers, Y would be the set [0,1] and we could take $\sigma(y,y')=(y-y')^2$ (here we are assuming that the functions $f \in \mathcal{F}$ are probabilistic classifiers, that is f(x) represents the probability that x belongs to the category represented by f). Given our limited capacity to learn characters, we could take the environmental probability measure Q to have support on at most 10,000 distinct elements of \mathcal{F} (so \mathcal{F} must contain more than just the 26 English letters). Then if x and x' are two images of the same character, $f(x) \approx f(x')$ for all f in the support of Q and so by (3), $\rho(x,x')\approx 0$, as required. If x and x' are images of different characters, the classifiers f_x and $f_{x'}$ corresponding to x and x' would have $f_x(x) \approx 1, f_x(x') \approx 0$ and $f_{x'}(x) \approx 0, f_{x'}(x') \approx 1$. Classifiers for characters that are subjectively similar to x(x') will behave in a similar way to $f_x(f_{x'})$, except that they will not assign such a high value to positive examples as f_x and $f_{x'}$ do. All other classifiers fwill have $f(x) \approx f(x') \approx 0$. Substituting this into (3) shows $\rho(x, x')$ will be larger if x and x' are images of different characters than if they are images of the same characters.

Note that ρ depends only upon the environment (\mathcal{F},Q) and not upon X or its probability measure P. Thus problems with the same X but different environments (for example character classification and face recognition—different environments for the space of images) will generate different canonical distortion measures. In

the next section we will show that ρ is the optimal distortion measure to use if piecewise constant approximation of the functions in the environment is the aim. Thus the fact that different environments generate different ρ 's shows that the optimal similarity measure between data points is highly dependent on what one is planning to do with the data.

The definition of ρ does not restrict us to considering only classifier environments, any kind of functions will do. For example, the environment might consist of all bounded linear functions on some compact subset of $X=R^n$, all threshold functions or all polynomials up to a certain degree. Noisy environments can also be modelled within this framework by making the functions $f \in \mathcal{F}$ distribution valued. For example, if the problem is to learn noisy concepts then these can be represented as a distribution P on X combined with a conditional distribution on $\{0,1\}$. Different concepts would have different conditional distributions, which we can represent as mappings $f: X \to Y$ where now Y is the set of all distributions on $\{0,1\}$. The distance measure σ is now a distance measure on probability distributions, such as Kullback-Liebler divergence or Hellinger distance. The CDM between two inputs x and x' would then equal the average distance between the distributions f(x) and f(x').

3. Examples calculatable in closed form

3.1. A linear environment

Suppose that $X=R^n$ and $\mathcal F$ consists of all linear maps from X into R. $\mathcal F$ is the vector space dual of X and so is itself isomorphic to R^n . With this in mind, take the measure Q on $\mathcal F$ to be Lebesgue measure on R^n , but restrict Q's support to the cube $[-\alpha,\alpha]^n$ for some $\alpha>0$, and renormalise so that $Q([-\alpha,\alpha]^n)=1$. Let $\sigma(y,y')=(y-y')^2$ for all $y,y'\in R$. ρ can then be reduced as follows:

$$\rho(x,x') = \int_{\mathcal{F}} \sigma(f(x),f(x')) dQ(f)$$

$$= \frac{1}{(2\alpha)^n} \int_{a \in [-\alpha,\alpha]^n} (a \cdot x - a \cdot x')^2 d^n a$$

$$= \frac{1}{(2\alpha)^n} \int_{-\alpha}^{\alpha} \dots \int_{-\alpha}^{\alpha} \left(\sum_{i=1}^n a_i x_i - \sum_{i=1}^n a_i x_i' \right)^2 da_1 \dots da_n$$

$$= \frac{4\alpha^2}{2} ||x - x'||^2.$$

Thus a linear environment induces the squared Euclidean distance on X. The reverse conclusion is also true, *i.e.* if one assumes that $\rho(x,x') = K\|x-x'\|^2$ for all x,x' then $\mathcal F$ must be a linear function class (almost everywhere). So based on the optimality result of the next section, using the squared Euclidean distortion is optimal if one wishes to approximate linear functions on the input space, but is

not optimal for any other environments. As it is very rare that one is interested in applying linear functions to images, or speech signals (for example face classifiers are not linear maps on image space, nor are word classifiers linear maps on speech signals), the use of squared Euclidean distortion in these environments is not the best thing to do.

Note that a uniform distribution over any *symmetric* region of weight space will yield a CDM that is proportional to Euclidean distance, while a general distribution will yield a CDM that is a quadratic form $\rho(x, x') = \langle x|A|x'\rangle$ where A is an $n \times n$ matrix.

3.2. A thresholded linear environment

Take the same example as above but this time threshold the output of each $f \in \mathcal{F}$ with the Heaviside step function, and take Q to have support only on the unit ball in \mathbb{R}^n , rather than the cube, $[-\alpha, \alpha]^n$ (this is done to make the calculations simple). After some algebra we find

$$\rho(x, x') = \frac{\theta}{\pi},$$

where θ is the angle between x and x'. Thus in an environment consisting of linear classifiers (*i.e.* thresholded linear functions) whose coefficients are distributed uniformly in the unit ball, the natural distortion measure on the input space is the angle between two input vectors.

3.3. A quadratic environment

Let X = Y = [-1, 1], $\sigma(y, y') = |y - y'|$ for all $y, y' \in Y$ and let $\mathcal{F} = \{f: x \mapsto ax^2\}$ with a uniformly distributed in the range [-1, 1]. With this environment,

$$\rho(x,y) = \int_{-1}^{1} |ax^{2} - ay^{2}| da$$
$$= |x - y||x + y|.$$

Note that $\rho(x,y)=0$ if x=y and if x=-y, so that x and -x are zero distance apart under ρ . This reflects the fact that f(x)=f(-x) for all $f\in\mathcal{F}$. Notice also that $\rho(x,y)$ is the ordinary Euclidean distance between x and y, scaled by |x+y|. Thus two points with fixed Euclidean distance become further and further apart under ρ as they are moved away from the origin. This reflects the fact that the quadratic functions in \mathcal{F} have larger variation in their range around large values of x than they do around small values of x. This can also be seen by calculating the ε -ball around a point x under ρ (i.e the set of points $x' \in X$ such that $\rho(x,x') \leq \varepsilon$). To first order in ε/x this is

$$\left[-x-\frac{\varepsilon}{2x},-x+\frac{\varepsilon}{2x}\right]\bigcup\left[x-\frac{\varepsilon}{2x},x+\frac{\varepsilon}{2x}\right].$$

Note that the Euclidean diameter of the ε -ball around x decreases inversely linearly with x's—Euclidean again—distance from the origin.

4. The optimality of the Canonical Distortion Measure

In this section it is shown that the CDM is the optimal distortion measure to use if the goal is to find piecewise constant approximations to the functions in the environment.

Piecewise constant approximations to $f \in \mathcal{F}$ are generated by specifying a quantization $\vec{x} = \{x_1, \dots, x_k\}$ $(x_i \in X)$ of X and a partition $\vec{X} = \{X_1, \dots, X_k\}$ $(X_i \subseteq X, X_i \cap X_j = \phi, X = \cup X_i)$ of X that is faithful to $\{x_1, \dots, x_k\}$ in the sense that $x_i \in X_i$ for $1 \le i \le k$. The piecewise constant approximation \hat{f} to any function f is then defined by $\hat{f}(x) = f(x_i)$ for all $x \in X_i$, $1 \le i \le k$.

If information about the function f is being transmitted from one person to another using the quantization \vec{x} and the partition \vec{X} then \hat{f} is the function that will be constructed by the person on the receiving end.

The most natural way to measure the deviation between f and \hat{f} in this context is with the pseudo-metric d_P ,

$$d_P(f,\hat{f}) := \int_{Y} \sigma(f(x),\hat{f}(x)) dP(x).$$

 $d_P(f, \hat{f})$ is the expected difference between f(x) and $\hat{f}(x)$ on a sample x drawn at random from X according to P. The reconstruction error of \mathcal{F} with respect to the pair $\vec{x} = \{x_1, \dots, x_k\}$ and $\vec{X} = \{X_1, \dots, X_k\}$ is defined to be the expected deviation between f and its approximation \hat{f} , measured according to the distribution Q on \mathcal{F} :

$$E_{\mathcal{F}}(\vec{x}, \vec{X}) := \int_{\mathcal{F}} d_P(f, \hat{f}) \, dQ(f). \tag{4}$$

The quantization \vec{x} and partition \vec{X} should be chosen so as to minimize $E_{\mathcal{F}}(\vec{x}, \vec{X})$. Given any quantization $\vec{x} = \{x_1, \dots, x_k\}$ and distortion measure ρ , define the partition $\vec{X}^{\rho} = \{X_1^{\rho}, \dots, X_k^{\rho}\}$ by

$$X_i^{\rho} := \{x \in X : \rho(x, x_i) \le \rho(x, x_i), \text{ for all } j \ne i\}$$

(break any ties by choosing the partition with the smallest index). Call this the partition of X induced by ρ and \vec{x} (it is the Voronoi partition). Define

$$E_{\mathcal{F}}^{\rho}(\vec{x}) := E_{\mathcal{F}}(\vec{x}, \vec{X}^{\rho}). \tag{5}$$

Lemma 1
$$E_{\mathcal{F}}^{\rho}(\vec{x}) = E_{\rho}(\vec{x}).$$
 (6)

Proof. Let $\vec{x} = \{x_1, \dots, x_k\}$ be any quantization of X and let $\vec{X}^{\rho} = \{X_1^{\rho}, \dots, X_k^{\rho}\}$ be the corresponding partition induced by ρ . Denote the approximation of $f \in \mathcal{F}$ with respect to this partition by \hat{f}_{ρ} . Then,

$$E_{\mathcal{F}}^{\rho}(\vec{x}) = \int_{\mathcal{F}} d_{P}(f, \hat{f}_{\rho}) dQ(f)$$

$$= \int_{\mathcal{F}} \int_{X} \sigma(f(x), \hat{f}_{\rho}(x)) dP(x) dQ(f)$$

$$= \int_{X} \int_{\mathcal{F}} \sigma(f(x), f(q_{\rho}(x))) dQ(f) dP(x)$$

$$= \int_{X} \rho(x, q_{\rho}(x)) dP(x)$$

$$= E_{\rho}(\vec{x})$$

Theorem 2 The reconstruction error $E_{\mathcal{F}}$ of \mathcal{F} is minimal with respect to a quantization $\vec{x} = \{x_1, \ldots, x_k\}$ minimizing the reconstruction error $E_{\rho}(\vec{x})$ of X, and the partition \vec{X}^{ρ} induced by the CDM ρ and \vec{x} .

Proof. Let $\vec{x} = \{x_1, \dots, x_k\}$ be any quantization of X and let $\vec{X}^{\rho} = \{X_1^{\rho}, \dots, X_k^{\rho}\}$ be the corresponding partition induced by ρ . Denote the approximation of $f \in \mathcal{F}$ with respect to this partition by \hat{f}_{ρ} . Let $\vec{X} = \{X_1, \dots, X_k\}$ be any other partition of X that is faithful to \vec{x} and let \hat{f} denote the approximation of f with respect to this second partition. Define $X_{ij} = X_i \cap X_j^{\rho}, 1 \leq i \leq k, 1 \leq j \leq k$. Note that the X_{ij} 's are also a partition of X. The reconstruction error of \mathcal{F} with respect to the partition \vec{X} satisfies:

$$E_{\mathcal{F}}(\vec{x}, \vec{X}) = \int_{\mathcal{F}} d_{P}(f, \hat{f}) dQ(f)$$

$$= \int_{\mathcal{F}} \int_{X} \sigma(f(x), \hat{f}(x)) dP(x) dQ(f)$$

$$= \sum_{i,j=1}^{k} \int_{X_{ij}} \int_{\mathcal{F}} \sigma(f(x), f(x_{i})) dQ(f) dP(x)$$

$$= \sum_{i,j=1}^{k} \int_{X_{ij}} \rho(x, x_{i}) dP(x)$$

$$\geq \sum_{i,j=1}^{k} \int_{X_{ij}} \rho(x, x_{j}) dP(x)$$

$$= \int_{\mathcal{F}} d_{P}(f, \hat{f}_{\rho}) dQ(f)$$

$$= E_{\mathcal{F}}^{\rho}(\vec{x}).$$

The theorem now follows from lemma 1.

Theorem 2 states that as far as generating piecewise constant approximations to the functions in the environment is concerned, there is *no better* partition of the input space than that induced by the CDM and its optimal quantization set.

4.1. Quadratic environment revisited

For the quadratic environment of example 3.3, the optimal quantization for k=6 is shown in figure 1 along with f and \hat{f}_{ρ} for $f(x)=x^2$. Note how the optimal quantization reduces the deviation between f and its approximation \hat{f}_{ρ} by spacing the points closer together for larger values of x.

To calculate the optimal quantization in this case, first note that by the symmetry of the environment, the quantization points $\{x_1, \ldots, x_6\}$ can all be assumed to be positive, and without loss of generality suppose that $x_1 \leq x_2 \leq \ldots \leq x_6$. Direct calculation of the reconstruction error $E_{\rho}(\vec{x})$ (2) shows that

$$x_i^2 = \frac{1}{4} \left(x_{i-1}^2 + x_{i+1}^2 \right) + \frac{1}{4\sqrt{2}} \sqrt{x_{i-1}^4 + 6x_{i-1}^2 x_{i+1}^2 + x_{i+1}^4}.$$

A similar procedure can be used to show that x_1 and x_6 must satisfy,

$$x_1 = \frac{x_2}{\sqrt{7}},$$

$$x_6 = \frac{4 + \sqrt{2 + 7x_5^2}}{7}.$$

Optimal quantization points can be found by solving these equations numerically.

5. Relationship between the CDM and other distance measures

5.1. Transformation invariant distance

The authors of [11] introduced a technique for comparing handwritten characters called $Transformation\ Distance$. They observed that images of characters are invariant under transformations such as rotation, dilation, shift, line thickening and so on. Denoting the set of all such transformations by G, and assuming that G can be parameterised by k real parameters, they noted that for each character x, the set

$$\mathcal{M}(x) := \{qx: q \in G\}$$

forms a k-dimensional manifold in the input space X. They defined the distance bewteen two images x and x' to be:

$$D(x, x') := \inf_{y \in \mathcal{M}(X), y' \in \mathcal{M}(x')} \|y - y'\|, \tag{7}$$

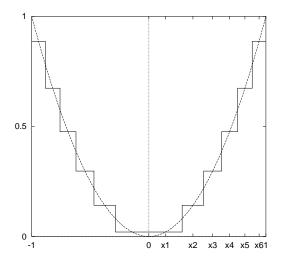


Figure 1. Optimal quantization points and the corresponding approximation to $f(x) = x^2$ for the quadratic environment of example 3.3. The six quantization points are (to three significant figures) $x_1 = 0.142$, $x_2 = 0.377$, $x_3 = 0.545$, $x_4 = 0.690$, $x_5 = 0.821$, $x_6 = 0.942$.

that is, D(x, x') is the smallest Euclidean distance between any transformed image of x and x' (and is called the *transformation distance between* x and x'). In order to simplify the computation, in [11] D(x, x') was approximated by a linearised version. However we will concentrate on the exact expression (7).

Relating the transformation distance to the CDM, note that invariance of characters under the action of G is equivalent to assuming that all character classifiers in the environment \mathcal{F} are invariant under the action of G. In other words, for all $f \in \mathcal{F}$, f(gx) = f(x) for all $g \in G$. Then clearly, if $x' \in \mathcal{M}(x)$, $\rho(x,x') = D(x,x') = 0$, so the CDM gives the same answer as the transformation distance in this case. However, if $x' \notin \mathcal{M}(x)$ then it is unlikely that D(x,x') and $\rho(x,x')$ will be the same, because D(x,x') (somewhat arbitrarily) measures the Euclidean distance between the manifolds $\mathcal{M}(x)$ and $\mathcal{M}(x')$, whereas $\rho(x,x')$ performs an average over the functions in the environment to compute the distance.

The transformation distance and the CDM share the important property that the distance between any pair of points in $\mathcal{M}(x)$ and $\mathcal{M}(x')$ respectively is always the same. This is trivial by the construction of D; to see it for the CDM let $x, x' \in \mathcal{M}(x)$ and $y, y' \in \mathcal{M}(y)$. Then $\rho(x, x') = \rho(y, y') = 0$ and combining this with the triangle inequality gives:

$$\rho(x,y) = \rho(x,y) + \rho(x,x') + \rho(y,y')
\geq \rho(x',y) + \rho(y,y')
\geq \rho(x',y').$$

Running the same argument with x and x' and y and y' interchanged shows that $\rho(x,y) = \rho(x',y')$ always.

5.2. The CDM and Edelman's Chorus of Prototypes

In [6], Edelman introduced a concept of representation he called the *Chorus of Prototypes*. The idea is to train a set of real-valued classifiers, f_1, \ldots, f_N , for a domain of *prototype* objects (so that $f_i(x) \in [0,1]$ is interpreted as the probability that x is an example of object i). All objects (not just the prototypes) are then represented by the vector of activations they induce at the output of the prototype classifiers. This vector of activations is a *Low Dimensional Representation* (LDR) of the input space. It is argued that the Euclidean distance between two representation vectors corresponds to the distal similarity of the objects.

Given that both the CDM and the Chorus of Prototypes represent similarity by making use of an environment of classifiers, it is natural to look for a connection between the two. There is a connection if one assumes that all functions in the environment can be implemented as linear maps composed with a fixed low dimensional representation. So let $h = (h_1, \ldots, h_k)$: $R^d \to R^k$ $(d \gg k)$ be the fixed LDR, and then each $f \in \mathcal{F}$ is of the form $\sum w_i h_i$ where the w_i depend on f. Suppose that k is minimal. Note that the f take values outside the range [0,1] and so cannot be interpreted as probabilities. However we can still interpret the output of f as a "degree of classification"—large positive values being high confidence and large negative values low confidence. In this case the environmental distribution Q is a distribution over the weights w. If Q is uniform over a symmetric region of weight space then by section 3.1, the CDM between two inputs x and x' will be proportional to the Euclidean distance between their transformed representations h(x) and h(x').

Now choose any f_1, \ldots, f_k such that their respective weight vectors w^1, \ldots, w^k are linearly independent (such a set of functions can always be found because we assumed k is minimal). (f_1, \ldots, f_k) will be the chorus of prototypes representation. Set

$$W = \begin{cases} w_1^1 & \dots & w_1^k \\ \vdots & \ddots & \vdots \\ w_k^1 & \dots & w_k^k \end{cases}$$
(8)

and note that W is nonsingular. For any input x, $(f_1(x), \ldots, f_k(x))$ (the representation of x by its similarity to the prototypes $i=1,\ldots,k$) is equal to Wh(x). Let $f=w\cdot h$ be any classifier in the environment. Set $w':=wW^{-1}$. Then $f=w'Wh=\sum w'_if_i(x)$. Thus any classifier in the environment is representable as a linear combination of prototype classifiers, as required for the chorus of prototypes idea.

5.3. Similarity measure of Thrun and Mitchell

The authors of [12] defined an "invariance function" $\sigma: X \times X \to \{0,1\}$ for a finite environment \mathcal{F} with the property that if there exists $f \in \mathcal{F}$ such that f(x) = 1 then f'(x) = 0 for all other $f' \in \mathcal{F}$:

$$\sigma(x, x') := \begin{cases} 1 & \text{if } \exists f \in \mathcal{F} \text{ with } f(x) = f(x') = 1 \\ 0 & \text{if } \exists f \in \mathcal{F} \text{ with } f(x) \neq f(x') \\ \text{undefined otherwise} \end{cases}$$

If we assume the environmental distribution Q is uniform on \mathcal{F} , a quick calculation shows that for all x, x' for which $\sigma(x, x')$ is defined,

$$\sigma(x, x') = 1 - \frac{|\mathcal{F}|}{2} \rho(x, x').$$

Thrun and Mitchell also showed how σ can be used to facilitate learning of novel tasks within their *lifelong learning framework*.

6. Learning the CDM with neural networks

For most environments encountered in practise (e.g speech recognition or image recognition), ρ will be unknown. In this section it is shown how ρ may be estimated or learnt using feed-forward neural networks. An experiment is presented in which the CDM ρ is learnt for a toy "robot arm" environment. The learnt CDM is then used to generate optimal Voronoi regions for the input space, and these are compared with the Voronoi regions of the true CDM (which can be calculated exactly for this environment). Piecewise-constant approximations to the functions in the environment are then learnt with respect to the Voronoi partition, and the results are compared with direct learning using feedforward nets. We conclude that learning piecewise-constant approximations using the CDM gives far better generalisation performance than the direct learning approach, at least on this toy problem. It should be emphasised that this problem is designed primarily to illustrate the ideas behind learning the CDM, and not as a practical test of the theory on real-world problems. The latter awaits more sophisticated experimentation.

6.1. Sampling the environment

To generate training sets for learning the CDM, both the distribution Q over the environment \mathcal{F} and the distribution P over the input space X must be sampled. So let $\{f_1, \ldots, f_M\}$ be M i.i.d. samples from \mathcal{F} according to Q and let $\{x_1, \ldots, x_N\}$ be N i.i.d. samples from X according to P. For any pair x_i, x_j an estimate of $\rho(x_i, x_j)$ is given by

$$\hat{\rho}(x_i, x_j) = \frac{1}{M} \sum_{i=1}^{M} \sigma(f_i(x_i), f_i(x_j)). \tag{9}$$

This generates N^2 training triples,

$$\{(x_1, x_1, \hat{\rho}(x_1, x_1)), (x_1, x_2, \hat{\rho}(x_1, x_3)), \dots, (x_N, x_N, \hat{\rho}(x_N, x_N))\},\$$

which can be used as data to train a neural network. That is, the neural network would have two sets of inputs—one set for x_i and one set for x_j —and a real-valued output $\rho^*(x_i, x_j)$ representing the network's estimate of $\hat{\rho}(x_i, x_j)$. The mean-squared error of the network on the training set is then

$$E = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[\rho^*(x_i, x_j) - \hat{\rho}(x_i, x_j) \right]^2.$$
 (10)

E is an estimate of the true distance between the network's ρ^* , and the true CDM ρ , where this is defined by:

$$d(\rho, \rho^*) := \int_{X^2} \left[\rho(x, x') - \rho^*(x, x') \right]^2 dP(x) dP(x'). \tag{11}$$

Note that the process of sampling from \mathcal{F} to generate f_1, \ldots, f_M is a form of multi-task learning (see *e.g.* [2, 3, 12, 10]) and that such sampling is a necessary condition for the empirical estimate of the CDM, ρ^* , to converge to the true CDM ρ .

6.2. "Robot arm" experiment

An artificial environment was created to test the effectiveness of training neural networks to learn the CDM. The environment was chosen to consist of a set of two link "robot arm" problems. That is, each function in the environment corresponded to a robot arm with two links of length r_1 and r_2 (see Figure 2. Note that the term "robot" is used fairly loosely here: the example doesn't have much to do with robotics). The function corresponding to r_1, r_2 is the map $f_{r_1, r_2} : [-\pi, \pi]^2 \to [0, (r_1 + r_2)^2]$ that computes the square of the distance of the end of the arm from the origin, given the angles of the links θ_1, θ_2 . Thus, $f_{r_1, r_2}(\theta_1, \theta_2) = r_1^2 + r_2^2 + 2r_1r_2\cos(\theta_1 - \theta_2)$. The link lengths r_1 and r_2 were chosen uniformly in the range [0, 1], so that $\mathcal{F} = \{f_{r_1, r_2} : (r_1, r_2) \in [0, 1]^2\}$. The goal was to train a neural network to correctly implement the CDM $\rho((\theta_1, \theta_2), (\theta'_1, \theta'_2))$. Note that in this case ρ can be calculated in closed form:

$$\rho((\theta_1, \theta_2), (\theta_1', \theta_2')) = \frac{4}{9} \left[\cos(\theta_1 - \theta_2) - \cos(\theta_1' - \theta_2') \right]^2. \tag{12}$$

The network architecture used was a single hidden layer neural network with tanh activation function on the hidden layer nodes and a linear output node. After some

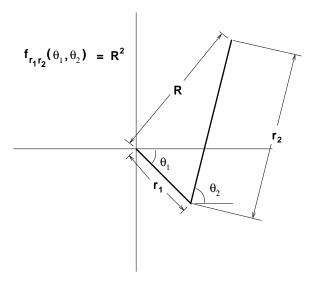


Figure 2. The robot arm environment is generated by all two link robot arms with link lengths $0 \le r_1 \le 1$ and $0 \le r_2 \le 1$. For each pair of angles (θ_1, θ_2) , $f_{r_1, r_2}(\theta_1, \theta_2)$ is the square of the distance of the end of the robot arm from the origin.

experimentation twenty hidden nodes was found to be sufficient. The network had four inputs, one each for $\theta_1, \theta_2, \theta_1'$ and θ_2' . The knowledge that ρ is symmetric was built into the network by taking the output of the network for inputs x_i and x_j to be

$$\frac{\rho^*(x_i, x_j) + \rho^*(x_j, x_i)}{2} \tag{13}$$

rather than just the "raw" network output $\rho^*(x_i, x_j)$. Note that (13) is automatically symmetric in x_i and x_j . With this choice of the estimate of ρ , the error measure (10) becomes

$$E = \frac{2}{N(N+1)} \sum_{i=1}^{N} \sum_{j=i}^{N} \left[\frac{\rho^*(x_i, x_j) + \rho^*(x_j, x_i)}{2} - \hat{\rho}(x_i, x_j) \right]^2.$$
 (14)

Back-propagation was used to compute the gradient of (14).

Training sets were generated by first sampling M times from the environment to generate f_1, \ldots, f_M , which in this case meant generating M pairs (r_1, r_2) uniformly at random in the square $[0, 1]^2$. Then the input space $[-\pi, \pi]^2$ was sampled uniformly at random N times to generate x_1, \ldots, x_N and the empirical estimate $\hat{\rho}(x_i, x_j)$ was constructed using (9) for each of the N(N+1)/2 pairs (x_i, x_j) for $1 \le i \le j \le N$. A separate cross-validation set was also generated using the

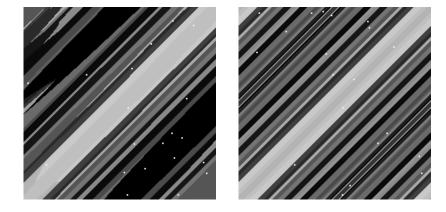


Figure 3. The picture on the left is the Voronoi diagram generated from 20 quantization points by a neural network approximation to the CDM (ρ^*) , trained on a sample size of M=100 functions and N=100 input points. The right-hand-side is the Voronoi diagram generated using the true CDM. All pixels with the same colour belong to the same Voronoi region. The white dots are the quantization points found by Lloyd's algorithm.

same values of M and N used for the training set. The network was trained using conjugate gradient descent—with the gradient computed from (14)—until the error on the cross-validation set failed to decrease for more than five iterations in a row. After the network had been trained, an initial quantization set q_1, \ldots, q_m of size $m \ll N$ was chosen uniformly at random from $\{x_1, \ldots, x_N\}$ and then the empirical Lloyd algorithm [8] was used to optimize the positions of the quantization points. The trained neural network—suitably symmetrised via (13)—was used as the distortion measure.

Several different experiments were performed with different values of M, N and m—the Voronoi regions for (M, N, m) = (100, 100, 20) are plotted in Figure 3, along with the optimal quantization set and corresponding Voronoi regions for the true CDM (12). Note that the regions generated by the neural net approximation are very similar to those generated by the true CDM. The reconstruction error of the input space was estimated from the training set $\{x_1, \ldots, x_N\}$ and also calculated (nearly) exactly by quantizing the input space into a 250×250 grid. These quantities are shown in the first two columns of table 1 for several different values of M, N and m. Note the good agreement between the estimate \hat{E}_{ρ^*} and the "true" value E_{ρ^*} in each case, and also that the reconstruction error is very small in all cases, improving as the training set size (M, N) for the CDM increases, and also as the number of quantization points m increases.

Recall that by lemma 1, $E_{\rho^*}(q_1,\ldots,q_m)$ equals the reconstruction error of the functions in the environment $(E_{\mathcal{F}}^{\rho^*}(q_1,\ldots,q_m))$. That is, if

- 1. a function f is picked at random (*i.e.* the link lengths r_1 and r_2 are picked at random),
- 2. the values $f(q_i)$ for each q_i in the optimal quantization set are generated and stored, and
- 3. the value of f at any novel input $x \in X$, chosen according to P, is estimated by $f(q_{\rho^*}(x))$,

then $E_{\rho^*}(q_1,\ldots,q_m)$ is the expected generalisation error: $E_X\left[f(x)-f(q_{\rho^*}(x))\right]^2$. Hence a small value of $E_{\rho^*}(q_1,\ldots,q_m)$ indicates that any function in the environment is likely to be learnable to high accuracy by this procedure². To demonstrate this, $E_{\mathcal{F}}^{\rho^*}(q_1,\ldots,q_m)$ was estimated by generating 100 new functions at random from the environment and learning them according to the above procedure. Each function's generalisation error was estimated using a fine grid on the input space, and then averaged across all 100 functions. The average generalisation error is plotted in the third column of table 1 for the various CDMs generated from different training set sizes and the different numbers of quantization points. Note the good agreement between the reconstruction error of the environment $(\hat{E}_{\mathcal{F}}^{\rho^*})$ and the reconstruction error of the input space E_{ρ^*} .

For comparison purposes the same 100 functions were learnt using a 10-hidden node neural network, without the assistance of the CDM. The average generalisation error across all 100 functions is displayed in Figure 4 along with the same quantity for the piecewise-constant approximations. The piecewise-constant approach based on the estimated CDM is clearly superior to the normal approach approach in this case.

Table 1. Empirical (\hat{E}_{ρ^*}) and true (E_{ρ^*}) reconstruction error of the input space using Voronoi regions and quantization points generated by the neural network approximation (ρ^*) to the CDM. The final column is the estimated reconstruction error of the functions in the environment. M is the number of functions sampled from the environment and N is the number of points sampled from the input space to train ρ^* . m is the number of quantization points.

(M,N)	m	$\hat{E}_{ ho^*}$	$E_{ ho^*}$	$\hat{E}_{\mathcal{F}}^{ ho^*}$
(100, 100)	5 20	$8.3 \times 10^{-3} \\ 6.5 \times 10^{-4}$	$1.0 \times 10^{-2} \\ 2.4 \times 10^{-3}$	$1.2 \times 10^{-2} \\ 6.9 \times 10^{-3}$
(200, 200)	5 20	$5.2 \times 10^{-3} \\ 6.0 \times 10^{-4}$	$5.0 \times 10^{-3} \\ 1.0 \times 10^{-3}$	$7.9 \times 10^{-3} \\ 1.8 \times 10^{-3}$

7. Conclusion

It has been shown that the existence of an *environment* of functions for a quantization process generates a *canonical distortion measure* (CDM) ρ on the input space. It has been proven that generating an optimal quantization set for the input

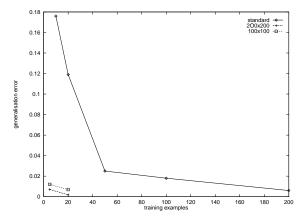


Figure 4. Average generalisation error as a function of training samples for the robot arm environment: standard approach vs. training using the estimated CDM. "Standard" means learning each function from scratch with a one-hidden layer, 10 hidden node neural net. " 100×100 " and " 200×200 " refer to the number of functions and input examples used to train the approximation to the CDM.

space using ρ as the distortion measure automatically produces Voronoi regions that are optimal for forming piecewise-constant approximations to the functions in the environment. The optimality theorem shows that the CDM contains *all* the information necessary for learning piecewise constant approximations to the functions in the environment. Hence learning the CDM is a process of *learning to learn*.

The CDM was calculated in closed form for several simple environments. A surprising result is that the squared Euclidean distortion measure is the CDM for a linear environment, and hence is optimal only if we are interested in approximating linear functions.

Techniques for estimating the CDM and training a neural network to implement it have been presented, and the results of several promising experiments on a toy environment have been reported. It remains to be seen whether these techniques work for more complex domains such as speech and character recognition.

One may be tempted to ask "Why bother going to all the trouble of learning the CDM first. Why not just learn the functions in the environment directly?" The answer to this question goes to the core of what distinguishes learning to learn from ordinary learning. Of course, if one is only interested in learning at most a handful of functions from the same environment then learning the CDM is overkill. Standard statistical learning techniques will be much more efficient. However, if one is interested in in learning a large number of functions from the environment, then learning the CDM will be a big advantage, because by theorem 2, the CDM contains all the information necessary for optimal learning of piecewise constant approximations to the functions in the environment.

In ordinary learning we are interested primarily in aquiring the information necessary to solve a particular learning problem, whereas in learning to learn we want to acquire the information necessary to solve a whole class of learning problems. As many real world problems are members of large classes of similar problems (speech, face and character recognition to name a few), tackling these problems from a learning to learn perspective should be a fruitful approach.

Notes

- 1. For Q to be well defined there needs to be a σ -algebra on \mathcal{F} . We leave that algebra unspecified in what follows, and simply assume that an appropriate one exists.
- 2. Note that this procedure is just 1 Nearest Neighbour, with ρ^* as the distance metric and the quantization points intelligently placed.

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