On a machine learning setup for discrete determinantal structures

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Abstract

Determinantal point processes are random subsets that exhibit a diversifying behaviour in the sense that the randomly selected points tend to be not similar in some way. This repellent structure first arrose in theortical physics and pure mathematics, but they have recently been used to model a variety of many real world scenarios in a machine learning setup. We aim to give an overview over the main ideas of this approach which is easily accessible even without prior knowledge in the area of machine learning and sometimes omit technical calculations in order to keep the focus on the concepts.

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Chapter II

Determinantal points processes: Basic notions and properties

II.1 Historical remarks

II.2 Definitions and properties

Let in the following $\mathcal{Y}$ be a finite set, which we call the *ground set* and $N := |\mathcal{Y}|$. A *point process* on $\mathcal{Y}$ is a random subset of $\mathcal{Y}$, i.e. a random variable with values in the powerset $2^{\mathcal{Y}}$. Usually we will identify this random variable with its law $\mathbb{P}$ and thus refer to probability measures $\mathbb{P}$ on $2^{\mathcal{Y}}$ as a point processes and not distinguish those objects. Let in the following $\mathbf{Y}$ be a random subset drawn according to $\mathbb{P}$, then we call $\mathbb{P}$ a *determinantal point process*, or in short a DPP, if we have

$$\mathbb{P}(A \subseteq \mathbf{Y}) = \det(K_A) \quad \text{for all } A \subseteq \mathcal{Y} \tag{2.1}$$

where K is a symmetric matrix indexed by the elements in $\mathcal{Y}$ and K_A denotes the restriction of the matrix K to indices in A. We call K the *marginal kernel* of the DPP and note immediately that K is necessarily non negative definite. Further it can be shown (cf. page 3 in [Borodin, 2009]) that also the complement of a DPP is a DPP with marginal kernel $I - K$ where I is the identity matrix, i.e.

$$\mathbb{P}(A \subseteq \mathbf{Y}^c) = \det(I_A - K_A)$$

and thus $I - K \geq 0$ and therefore $0 \leq K \leq I$. This actually turns out to be sufficient for K to define a DPP through (2.1) (cf. [Kulesza et al., 2012]). We call the elements of $\mathcal{Y}$ *items* and by choosing $A = \{i\}$ and $A = \{i, j\}$ for $i, j \in \mathcal{Y}$ and using (2.1) we obtain the probabilities of their occurrence

$$\begin{aligned} \mathbb{P}(i \in \mathbf{Y}) &= K_{ii} \quad \text{and} \\ \mathbb{P}(i, j \in \mathbf{Y}) &= K_{ii}K_{jj} - K_{ij}^2 = \mathbb{P}(i \in \mathbf{Y}) \cdot \mathbb{P}(j \in \mathbf{Y}) - K_{ij}^2, \end{aligned} \tag{2.2}$$

Thus the appearance of the two items i and j are always negatively correlated. In this light the fact that also $\mathbf{Y}^c$ exhibits negative correlations becomes less surprising, because since the set $\mathbf{Y}$ tends to spread out due to the repulsion in (2.2), the complement, which is nothing but the gaps that are left after eliminating the elements in $\mathbf{Y}$, tend to show a non clustering behaviour.

L-ensembles

Let us now introduce an important subclass of DPPs, namely the ones where not only the marginal probabilities can be expressed through a suitable kernel, but also the elementary probabilities. Because this will be convenient for us later on we will restrict ourselves to this case from now on. If we have even $K < I$, then we define the *elementary kernel*

$$L := K(I - K)^{-1}$$

which specifies the elementary probabilities since one can check

$$\mathbb{P}(A = \mathbf{Y}) = \frac{\det(L_A)}{\det(I + L)} \quad \text{for all } A \subseteq \mathcal{Y}. \tag{2.3}$$

Conversely for any $L \geq 0$ a DPP can be defined via (2.2) and the corresponding marginal kernel is given by

$$K = L(I + L)^{-1}.$$

We call DPPs which arise this way L *ensembles*. Note that L can be written as a Gram matrix

$$L = B^T B$$

where $B \in \mathbb{R}^{D \times N}$ whenever $D \geq \mathrm{Rk}(L)$. For example one could take the spectral decomposition $L = U^T C U$ of L and set $B := \sqrt{C} U$ and eventually drop some zero rows from $\sqrt{C}$. Let B_i denote the i-th column of B and write it as the product $q_i \cdot \phi_i$ where $q_i \geq 0$ and $\phi_i \in \mathbb{R}^D$ such that $\|\phi_i\| = 1$. This yields the representation

$$L_{ij} = q_i \phi_i^T \phi_j q_j =: q_i S_{ij} q_j$$

and we call q_i the *quality* of the item $i \in \mathcal{Y}$ and ϕ_i the *diversity feature vector* of i. Using this quality diversity decomposition we get

$$\mathbb{P}(A = \mathbf{Y}) \propto \det\big((B^T B)_A\big) = \left(\prod_{i \in A} q_i^2\right) \cdot \det(S_A) \quad \text{for all } A \subseteq \mathcal{Y} \tag{2.4}$$

which turns out to be a very helpful expression of the elementary probabilities.

An intuitive understanding of the quality diversity decomposition will play a central role later on if one wants to model real world phenomena as DPPs. To get this we can think of $q_i \geq 0$ as a measure of how important or high in quality the item is and the diversity feature vector $\phi_i \in \mathbb{R}^D$ can be thought of as some kind of state vector that consists of internal quantities that describe the item i in some way. Further we interpret the scalar product $\phi_i^T \phi_j \in [0, 1]$ as a measure of similarity between the items i and j and thus call S similarity matrix. Note that if i and j are perfectly similar or antisimilar, i.e. $\phi_i^T \phi_j = \pm 1$, then they can not occur at the same time, since

$$\mathbb{P}(i, j \in \mathbf{Y}) = \det \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix} = 0.$$

If we identify i with the vector $B_i = q_i \phi_i \in \mathbb{R}^D$, we can obtain a geometric interpretation of (2.4) since $\det((B^T B)_A)$ is the volume that is spanned by the columns $B_i, i \in A$, which is visualised in II.1. This volume increases if the lengths of the edges that correspond to the quality increase and decrease when the similarity feature vectors point into more similar directions.

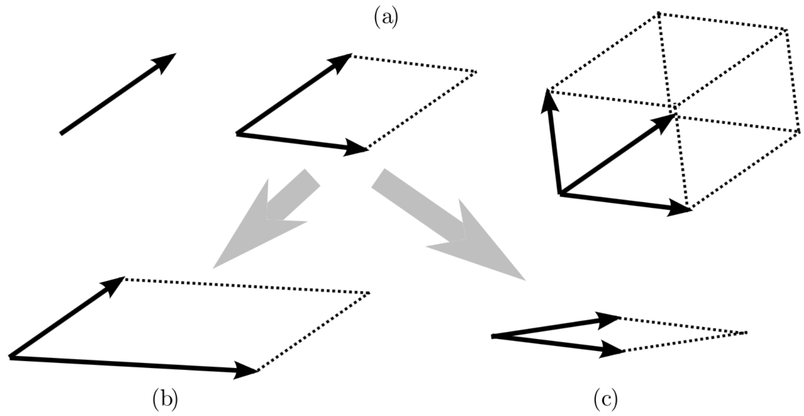

Figure II.1.: Taken from [Kulesza et al., 2012]; the first line (a) illustrates the volumes spanned by vectors, and in the second line it can be seen how this volume increases if the length – associated with the quality – increases (b) and decreases if they become more similar in direction which we interpret as two items becoming more similar (c)

One last property of DPPs that we shall mention is the fact that the negative correlations of the DPP posses a transient property in the sense, that if i and j and j and k are similar, then i and k are also similar. This is due to the fact

$$\left\|\phi_i - \phi_j\right\|^2 = \|\phi_i\|^2 + \left\|\phi_j\right\|^2 - 2\phi_i^T\phi_j = 2(1 - \phi_i^T\phi_j)$$

and thus

$$\sqrt{1 - \phi_i^T\phi_k} = \frac{1}{2}\|\phi_i - \phi_k\| \leq \frac{1}{2}\big(\|\phi_i - \phi_j\| + \|\phi_j - \phi_k\|\big) = \sqrt{1 - \phi_i^T\phi_j} + \sqrt{1 - \phi_j^T\phi_k}.$$

II.3 Related structures: conditional DPPs, structured DPPs and k-DPPs

Structured DPPs

We call a DPP *structured DPP* or short sDPP if the ground set is the cartesian product of some other set $\mathcal{M}$, which we will call the *set of parts*, i.e. if we have

$$\mathcal{Y} = \mathcal{M}^R = \left\{y_i = (y_i^r)_{r=1,\dots,R} \mid i = 1,\dots,N\right\}$$

where R is a natural number, $M = |\mathcal{M}|$ and $N = M^R$. The quality diversity decomposition of L take the form

$$L_{ij} = q(y_i)\phi(y_i)^T\phi(y_j)q(y_j)$$

and since $N = M^R$ is typically very big, it is impractical to define or store the quality and diversity features for every item $y_i \in \mathcal{Y}$. To deal with this problem we will assume that they admit factorisations and are thus a combination of only a few qualities and diversities.

More precisely we call $F \subseteq 2^{\{1,\dots,R\}}$ a *set of factorisations* and for a *factor* $\alpha \in F$, y_α denotes the subtupel of $y \in \mathcal{Y}$ that is indexed by α. Further we will work with the decompositions

$$\begin{aligned} q(y) &= \prod_{\alpha \in F} q_\alpha(y_\alpha) \\ \phi(y) &= \sum_{\alpha \in F} \phi_\alpha(y_\alpha) \end{aligned} \tag{2.5}$$

for a suitable set of factorisations F and qualities and diversities q_α and ϕ_α for $\alpha \in F$. Note that so far this is neither a restriction of generality – we could simply choose $F = \big\{\{1,\dots,R\}\big\}$ – nor a simplification – in that case we have the exact same number of qualities and diversities. However we are interested in the case where F consists only of small subsets of $\{1,\dots,R\}$. For example suppose that F is the set of all subsets with one or two elements, then we only have

$$R \cdot M + \binom{R}{2} \cdot M^2 = O(R^2 M^2)$$

quality and diversity features instead of

$$M^R = O(M^R).$$

This reduction of variables will make modelling, storing and estimating them feasible again in a lot of cases where naive approaches are foredoomed because of their shear size.

II.4 The magic properties of DPPs

II.5 The mode problem

Chapter III

Learning setups

III.1 What does learning mean?

III.2 Motivation for learning DPPs

III.3 Direct reconstruction of the kernel

In this section we want to see how we can learn, i.e. how we can estimate the marginal kernel from observations $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ that are distributed according to $\mathbb{P}$ and will sketch the procedure in [Urschel et al., 2017]. Let $\hat{\mathbb{P}}_n$ be the empirical distribution

$$\hat{\mathbb{P}}_n := \frac{1}{n} \sum_{i=1}^{n} \delta_{\mathbf{Y}_i}.$$

It is well known that due to the strong law of large numbers the empirical distributions weakly converge to $\mathbb{P}$ if the observations are independent. Therefore we can consistently estimate all principle minors of K, since

$$\hat{\mathbb{P}}_n(A \subseteq \mathbf{Y}) \xrightarrow{n \to \infty} \mathbb{P}(A \subseteq \mathbf{Y}) = \det(K_A) \quad \text{almost surely.}$$

Thus the question naturally arrises whether we can reconstruct the kernel K from the knowledge of all of its principle minors. This is known as the *principle minor assignment problem* and has been studied extensively (cf. [Griffin and Tsatsomeros, 2006] and [Urschel et al., 2017]) and an computationally efficient algorithm has been proposed for the problem in [Rising et al., 2015]. It is in fact possible to retain the matrix from its principle minors up to an equivalence relation which identifies matrices with each other, that have the same principle minors. Obviously this is sufficent for the task of learning a DPP, because those matrices are exactly those who give rise to the same point process. To see roughly how this reconstruction works we note that the diagonal is given by

$$K_{ii} = \det(K_{\{i\}})$$

and the absolute value of the off diagonal can be obtained through

$$K_{ij}^2 = K_{ii} K_{ii} - \det\left(K_{\{i,j\}}\right).$$

The reconstruction of the signs of the entries K_{ij} turns out to be the main problem, but this can be done analysing the cycles of the adjacency graph G_K corresponding to K. The adjacency graph has $\mathcal{Y}$ as its vertex set and the set of edges consists of the pairs $\{i, j\}$ such that $K_{ij} \neq 0$. The reconstruction now relies on the analysis of the cycles of this graph and it has been shown, that one only needs to know all the principle minors up to the order of the cycle sparsity of G_K (cf. [Urschel et al., 2017]). Following this method it is possible to compute estimators $\hat{K}_n$ of K in polynomial time and give a bound on the speed of convergence in some suitable metric.

In completely analogue fashion one can learn the elementary kernel L and those estimations can be used to sample from a DPP that was observed. This procedure might be sufficient in some scenarios, but this approach lacks the ability to extrapolate the knowledge one has of specific DPPs onto some new, unobserved DPPs which is exactly the point that would distinguish the procedure from classical statistics and would allow for far more interesting applications. To achieve this, we introduce the notion of conditional DPPs in the following section which are customised to describe families of DPPs with kernels that are in some way similar.

III.4 A learning approach to estimating the kernel

The approach described above is clearly of traditional statistical type and we want to touch on how the kernel estimation can be put into a machine learning task (cf. [Affandi et al., 2014]). For this we assume that we have a training set, i.e. a number of subsets $Y_1, \dots, Y_T \subseteq \mathcal{Y}$ drawn independently and according to the DPP $\mathbb{P}$. We aim to establish a quantity that gives an intuitive measure of how well a different DPP describes the training set and then we want to find the elementary kernel L for which the associated DPP $\mathbb{P}_L$ optimises this quantity. A widely used choice in the machine learning community for this is the so called *log likelihood function*

$$\log\left(\prod_{t=1}^{T} \mathbb{P}_L(Y_t)\right)$$

and we will work with its negative

$$\mathcal{L}(L) := -\log\left(\prod_{t=1}^{T} \mathbb{P}_L(Y_t)\right) = -\sum_{t=1}^{T} \log\big(\det(L_{Y_t})\big) + T\log\big(\det(L+I)\big)$$

where high values of $\mathcal{L}$ correspond to kernels L where at least one element Y_t of our training set is very unlikely. Thus it is natural to minimise the loss function $\mathcal{L}$ over all positive semidefinit $L \in \mathbb{R}^{N\times N}$. Note that we have $\mathcal{L}(L) = \infty$ if and only if an observation Y_t of our training set is impossible under the DPP $\mathbb{P}_L$, i.e. we do not consider those kernels in our estimation. We note that the loss function is smooth and the gradient of this can be explicitly expressed, at least on the domain $\{\mathcal{L} < \infty\}$. This is due to the fact that the determinants of the submatrices are polynomials in the entries of L and the composition of those with the smooth function $\log\colon (0,\infty) \to \mathbb{R}$ stays smooth. This property allows the use of gradient methods but they face the problem that the loss function is non convex and thus those algorithms will generally not converge to a global minimiser (cf. [Affandi et al., 2014]). Nevertheless it is worth investigating whether those local minima turn out to produce good results in real world scenarios.

Learning kernels of conditional DPPs

III.5 Learning the quality functions

III.6 Estimating the mixture coefficients of k-DPPs

Chapter IV

Toy examples and experiments

Chapter V

Summary and conclusion

Chapter A

Generated code

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