From Clustering to Cluster Explanations via Neural Networks

(SUPPLEMENTARY MATERIAL)

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This document contains supplementary material supporting the results and experiments from the main paper. Appendices A–C contain proofs and justifications for some of the non-trivial steps taken in Section 3 to neuralize the k-means models. Appendix D provides theoretical justification for the treatment of min-pooling layers in Section 4. Appendix E describes the modified training procedure used for producing the kernel k-means model of Section 5.

APPENDIX A
NEURALIZED SOFT CLUSTER ASSIGNMENTS

We prove Proposition 1 of the main paper, that expresses the logit of cluster assignment probabilities as a neural network type min-pooling over differences of outlier scores.

Proof. The soft cluster assignment model is given by

$$P(\omega_c \mid \boldsymbol{x}) = \frac{\exp(-\beta \cdot o_c(\boldsymbol{x}))}{\sum_k \exp(-\beta \cdot o_k(\boldsymbol{x}))}. \tag{1}$$

We consider the logit of the probability score

$$\mathrm{logit}(\omega_c \mid \boldsymbol{x}) = \log\Big(\frac{P(\omega_c \mid \boldsymbol{x})}{1 - P(\omega_c \mid \boldsymbol{x})}\Big) \tag{2}$$

which describes well the evidence for cluster membership. We would like to express this quantity as a neural network. Inserting (1) into (2) gives:

$$\begin{aligned}
\mathrm{logit}(\omega_c \mid \boldsymbol{x}) &= \log\left(\frac{\frac{\exp(-\beta\cdot o_c(\boldsymbol{x}))}{\sum_k \exp(-\beta\cdot o_k(\boldsymbol{x}))}}{1 - \frac{\exp(-\beta\cdot o_c(\boldsymbol{x}))}{\sum_k \exp(-\beta\cdot o_k(\boldsymbol{x}))}}\right)\\
&= \log \frac{\exp(-\beta \cdot o_c(\boldsymbol{x}))}{\sum_{k\neq c} \exp(-\beta \cdot o_k(\boldsymbol{x}))}\\
&= \log \frac{1}{\sum_{k\neq c} \exp(-\beta \cdot (o_k(\boldsymbol{x}) - o_c(\boldsymbol{x})))}\\
&= -\log \sum_{k\neq c} \exp(-\beta \cdot (o_k(\boldsymbol{x}) - o_c(\boldsymbol{x})))\\
&= \beta \cdot {\min_{k\neq c}}^{\beta} \{o_k(\boldsymbol{x}) - o_c(\boldsymbol{x})\}
\end{aligned}$$

where the underlying min-pooling structure of the cluster assignment logit now appears explicitly. □

APPENDIX B
CONNECTION TO POWER CLUSTER ASSIGNMENTS

This appendix proves Proposition 2 of the main paper stating for kernel k-means that the proposed soft-min cluster assignment over outlier scores defined as $o_c(\boldsymbol{x}) = -\gamma^{-1} \log \mathbb{i}_c(\boldsymbol{x})$ can also be expressed as a power-based softmax assignment via the measure of inlierness $\mathbb{i}_c(\boldsymbol{x})$.

Proof. This result follows directly from the property $a^b = \exp(b \cdot \log(a))$ for $a > 0$ and $b \in \mathbb{R}$:

$$\begin{aligned}
P(\omega_c \mid \boldsymbol{x}) &= \frac{\exp(-\beta \cdot o_c(\boldsymbol{x}))}{\sum_k \exp(-\beta \cdot o_k(\boldsymbol{x}))}\\
&= \frac{\exp(\frac{\beta}{\gamma} \log \mathbb{i}_c(\boldsymbol{x}))}{\sum_k \exp(\frac{\beta}{\gamma} \log \mathbb{i}_k(\boldsymbol{x}))}\\
&= \frac{\mathbb{i}_c(\boldsymbol{x})^{\beta/\gamma}}{\sum_k \mathbb{i}_k(\boldsymbol{x})^{\beta/\gamma}}
\end{aligned}$$

which is a power-based soft-assignment model. □

APPENDIX C
IMPROVED NEURALIZED KERNEL K-MEANS

In this appendix, we show the functional equivalence of the naive and improved variants of the neuralized kernel k-means model described in Section 3.3.

First, we show that the $\min^\beta \{\cdot\}$ operator is commutative w.r.t. additive scalars:

$$\begin{aligned}
{\min_j}^{\beta} \{a_j\} + c &= \Big[-\tfrac{1}{\beta} \log \sum_j \exp(-\beta \cdot a_j)\Big] + c\\
&= -\tfrac{1}{\beta} \log \sum_j \exp(-\beta \cdot (a_j + c))\\
&= {\min_j}^{\beta} \{a_j + c\}
\end{aligned}$$ □

This allows for a more high level point of view that holds for hard- as well as soft-min pools: a difference of minima equals a minimax of differences,

$$\min_j(a_j) - \min_i(b_i) = \min_j(\max_i(a_j - b_i)).$$

By exploiting this fact multiple times, we derive the following reformulation of the logit for kernel clustering:

$$\begin{aligned}
f_c &= \beta \cdot {\min_{k\neq c}}^{\beta} \{o_k - o_c\}\\
&= \beta \cdot {\min_{k\neq c}}^{\beta} \Big\{ {\min_{j\in\mathcal{C}_k}}^{\gamma} \{d_j\} - {\min_{i\in\mathcal{C}_c}}^{\gamma} \{d_i\} \Big\}\\
&= \beta \cdot {\min_{k\neq c}}^{\beta} \Big\{ {\min_{j\in\mathcal{C}_k}}^{\gamma} \Big\{ {\max_{i\in\mathcal{C}_c}}^{\gamma} \{d_j - d_i\} \Big\} \Big\}.
\end{aligned}$$

Finally, defining $a_{ij} \coloneqq d_j - d_i$ completes the derivation.

Appendix D
Redistribution in Min-Pooling Layers

This appendix proves Proposition 3 of the main paper. We show that the redistributed relevance in soft min-pooling layers is locally approximately linear in the input activations. For that, we show that p_j asymptotically approaches a (hard-min) indicator function.

Proof. We first rewrite the relevance function for input a_j of the pooling layer $\widehat{R}_k(\boldsymbol{a})$ as:

$$R_j = \underbrace{\frac{\exp(-\beta a_j)}{\sum_j \exp(-\beta a_j)}}_{p_j} \cdot \overbrace{p_k \cdot (a_j + \underbrace{\min_{j'}{}^{\beta}\{a_{j'} - a_j\}}_{\theta_j})}^{\widehat{R}_k}$$

We now show that the relevance R_j can be locally approximated as a linear function of a_j with $j = 1, \ldots, m$. For this, we identify two cases.

Case 1: When a_j is the smallest input by at least some margin Δ from the second smallest input, we can bound p_j by rewriting:

$$p_j = \frac{\exp(-\beta a_j)}{\sum_{j'} \exp(-\beta a_{j'})} = \frac{1}{1 + \sum_{j' \neq j} \exp(-\beta(\underbrace{a_{j'} - a_j}_{\geq \Delta}))}$$
$$\geq (1 + (m-1) \cdot e^{-\beta\Delta})^{-1}$$

such that p_j is bounded by $(1 + (m-1) \cdot e^{-\beta\Delta})^{-1} \leq p_j \leq 1$, which converges to 1 when $\beta \to \infty$ or $\Delta \to \infty$. Similarly, we can bound θ_j by rewriting:

$$\begin{aligned}
\theta_j &= \min_{j'}{}^{\beta}\{a_{j'} - a_j\} \\
&= -\beta^{-1} \log\Big[1 + \sum_{j' \neq j} \exp(-\beta(\underbrace{a_{j'} - a_j}_{\geq \Delta}))\Big] \\
&\geq -\beta^{-1} \log(1 + (m-1) \cdot e^{-\beta\Delta})
\end{aligned}$$

as $-\beta^{-1} \log(1 + (m-1) \cdot e^{-\beta\Delta}) \leq \theta_j \leq 0$ which converges to 0 when $\beta \to \infty$ or $\Delta \to \infty$. In this asymptotic case, the relevance R_j becomes the activation a_j itself and can thus be expressed in terms of quantities in the lower layers.

Case 2: When a_j fails to be the smallest input by at least some margin Δ, the term p_j can be bounded by $0 \leq p_j \leq (1 + e^{\beta\Delta})^{-1}$, which converges to 0 when $\beta \to \infty$. Then, the product $p_j\theta_j$ can also be bounded as $-p_j\beta^{-1} \log(1 + e^{\beta\Delta}) \leq p_j\theta_j \leq 0$, which converges to 0 when $\beta \to \infty$.

Therefore, both for all inputs, the linearity of the redistributed relevance holds when the stiffness parameter β grows large. □

Appendix E
Modified Training of Kernel K-Means

Here, we detail the training procedure for the kernel k-means model used in Section 5.2. Kernel k-means has an issue when the kernel bandwidth is small: the local density at point $\boldsymbol{x}_0$ is dominated by the Gaussian bump $\mathbb{K}(\boldsymbol{x}_0, \cdot)$ and the objective has local optima at almost every possible cluster assignment. To smooth the training procedure, we modify the standard expectation-maximization algorithm, by minimizing instead distance to the nearest centroid in feature space with bump $\mathbb{K}(\boldsymbol{x}_0, \cdot)$ being removed before computing the distances in feature space. The learning procedure can be summarized by the following steps [1]:

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1) Initialize a random assignment or some informed starting point, e.g. standard k-means or ground truth label assignments.
2) Compute the normalized leave-one-out centroids for every data point $\boldsymbol{x}_\ell$ and cluster $k = 1, \ldots, K$:
$$\boldsymbol{\mu}_k^{(-\ell)} = \alpha_k^{(-\ell)} \cdot \sum_{j \in \mathcal{C}_k \setminus \{\ell\}} \Phi(\boldsymbol{x}_j)$$
Normalization is performed via kernel expansion:
$$\alpha_k^{(-\ell)} = \big(\textstyle\sum_{j,j' \in \mathcal{C}_k \setminus \{\ell\}} \mathbb{K}(\boldsymbol{x}_j, \boldsymbol{x}_{j'})\big)^{-\frac{1}{2}}$$
3) Assign data point $\boldsymbol{x}_\ell$ to the cluster with smallest distance in feature space.
4) Reiterate from step 2 until convergence.

Note that the whole procedure can be performed with kernel expansions. The map Φ is never computed explicitly. The kernel matrix must be computed only once. The leave-one-out trick makes training more robust against bad local optima.

Once training is finished, final normalized centroids are computed from the full set of cluster members and the logit can be computed by the neural network equivalent from Section 3.

References

[1] X.-L. Meng and D. B. Rubin, "Maximum likelihood estimation via the ECM algorithm: A general framework," *Biometrika*, vol. 80, no. 2, pp. 267–278, 1993.