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# DAG-GNN: DAG Structure Learning with Graph Neural Networks (Supplementary Material)

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## 1. Proofs

*Proof of Theorem 1.* Let  $B = A \circ A$ . Clearly,  $B$  is nonnegative. The binomial expansion reads

$$(I + \alpha B)^m = I + \sum_{k=1}^m \binom{m}{k} \alpha^k B^k.$$

It is known that there is a cycle of length  $k$  if and only if  $\text{tr}(B^k) > 0$  when  $B \geq 0$ . Because if there is a cycle then there is a cycle of length at most  $m$ , we conclude that there is no cycle if and only if  $\text{tr}[(I + \alpha B)^m] = \text{tr}(I) = m$ .  $\square$

*Proof of Theorem 2.* Write

$$(1 + \alpha|\lambda|)^m = \left(1 + \frac{c|\lambda|}{m}\right)^m.$$

For given  $c$  and  $|\lambda|$ , the right-hand side of the equality is a function of  $m$ . This function monotonically increases for positive  $m$  and has a limit  $e^{c|\lambda|}$ . Hence, for any finite  $m > 0$ ,  $(1 + \alpha|\lambda|)^m \leq e^{c|\lambda|}$ .  $\square$

## 2. Structure Learning over KB Relations

We construct the data set from triples in FB15K-237 (Toutanova et al., 2015), which is a subset of FreeBase with approximately 15k entities and 237 relations. Each sample corresponds to an entity and each variable corresponds to a relation in this knowledge base. Each sample has on average 7.36 relations (i.e. 7.36 non-zero entries in each row).

Table 1 gives additional examples learned by our model with highest confidence scores. For each target relation on the right-hand side, we show the highest ranked relations within the same domain (i.e. the contents in the field before “/” such as “film” and “tvProgram”). On the left-hand side, we omit the relations that are common to the associated entity

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types, e.g. “profession” and “gender” to persons and “genre” to films, because almost all entities with these types will contain such a relation.

## References

Toutanova, K., Chen, D., Pantel, P., Poon, H., Choudhury, P., and Gamon, M. Representing text for joint embedding of text and knowledge bases. In *EMNLP*, 2015.

Table 1. (Continued from Table 3) Examples of extracted edges with high confidence. The dot · appearing in  $R_1.R_2$  means that the sample entity is connected to a virtual node (i.e. compound value types in FreeBase) via relation  $R_1$ , followed by a relation  $R_2$  to a real entity.

film/ProducedBy	⇒	film/Country
film/ProductionCompanies	⇒	film/Country
tvProgram/CountryOfOriginal	⇒	tvProgram/Language
tvProgram/RegularCast.regularTv/AppearanceActor	⇒	tvProgram/Language
person/Nationality	⇒	person/Languages
person/PlaceOfBirth	⇒	person/Languages
person/PlaceOfBirth	⇒	person/Nationality
person/PlaceLivedLocation	⇒	person/Nationality
organization/Headquarters.mailingAddress/Citytown	⇒	organization/PlaceFounded
organization/Headquarters.mailingAddress/StateProvince	⇒	organization/PlaceFounded