

The following is the supplementary Appendix for the paper; *Probabilistic Entity Representation Model for Reasoning over Knowledge Graphs*. All the references given in the following sections are made in context of the main paper.

A Derivation for Product of Multivariate Gaussians

The following sections provide the proof for the product of Gaussians for both the univariate case and multivariate case (used in Eqs. (6) and (10)).

A.1 Univariate Case

$$\begin{aligned}
\mathcal{N}(\mu, \sigma) &= \exp\left(\left(\frac{x - \mu}{\sigma}\right)^2\right) \\
P(\theta) &= P(\theta_1)P(\theta_2) = \exp\left(\left(\frac{x - \mu_1}{\sigma_1}\right)^2\right) \cdot \exp\left(\left(\frac{x - \mu_2}{\sigma_2}\right)^2\right) \\
\log P(\theta) &= \left(\frac{x - \mu_1}{\sigma_1}\right)^2 + \left(\frac{x - \mu_2}{\sigma_2}\right)^2 \\
&= \frac{(\sigma_2^2 + \sigma_1^2)x^2 - 2(\sigma_1^2\mu_2 + \sigma_2^2\mu_1)x + (\mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2)}{\sigma_1^2\sigma_2^2} \\
&= \frac{x^2 - 2\frac{(\sigma_1^2\mu_2 + \sigma_2^2\mu_1)}{\sigma_2^2 + \sigma_1^2}x + \frac{\mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2}{\sigma_2^2 + \sigma_1^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}} \\
&= \left(\frac{x - \frac{(\sigma_1^2\mu_2 + \sigma_2^2\mu_1)}{\sigma_2^2 + \sigma_1^2}}{\left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)^{-2}}\right)^2 + K, \text{ where } K = \frac{\mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2}{\sigma_1^2\sigma_2^2} - \left(\frac{\sigma_1^2\mu_2 + \sigma_2^2\mu_1}{\sigma_1^2\sigma_2^2}\right)^2 \\
P(\theta) &\propto \exp\left(\left(\frac{x - \frac{(\sigma_1^2\mu_2 + \sigma_2^2\mu_1)}{\sigma_2^2 + \sigma_1^2}}{\left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)^{-2}}\right)^2\right) \approx \mathcal{N}\left(\frac{(\sigma_1^2\mu_2 + \sigma_2^2\mu_1)}{\sigma_2^2 + \sigma_1^2}, \left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)^{-2}\right)
\end{aligned}$$

A.2 Multivariate Case

$$\begin{aligned}
\mathcal{N}(\mu, \Sigma) &= \exp\left((x - \mu)^T \Sigma^{-1} (x - \mu)\right) \\
P(\theta) &= P(\theta_1)P(\theta_2) = \exp\left((x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1)\right) \cdot \exp\left((x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2)\right) \\
\log(P(\theta)) &= (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \\
&= x^T \Sigma_1^{-1} x - \mu_1^T \Sigma_1^{-1} x - x^T \Sigma_1^{-1} \mu_1 - \mu_1^T \Sigma_1^{-1} \mu_1 + x^T \Sigma_2^{-1} x - \mu_2^T \Sigma_2^{-1} x - x^T \Sigma_2^{-1} \mu_2 - \mu_2^T \Sigma_2^{-1} \mu_2 \\
&= x^T (\Sigma_1^{-1} + \Sigma_2^{-1}) x - (\mu_1^T \Sigma_1^{-1} + \mu_2^T \Sigma_2^{-1}) x - x^T (\Sigma_1^{-1} \mu_1 + \Sigma_2^{-1} \mu_2) - (\mu_1^T \Sigma_1^{-1} \mu_1 + \mu_2^T \Sigma_2^{-1} \mu_2)
\end{aligned}$$

Let's assume $P(\theta) \propto \mathcal{N}(\mu_3, \Sigma_3)$, then,

$$\begin{aligned}
\log(P(\theta)) &= (x - \mu_3)^T \Sigma_3^{-1} (x - \mu_3) + K \\
&= x^T \Sigma_3^{-1} x - x^T \Sigma_3^{-1} \mu_3 - \mu_3^T \Sigma_3^{-1} x + \mu_3^T \Sigma_3^{-1} \mu_3 + K
\end{aligned}$$

Comparing coefficients,

$$\begin{aligned}
\Sigma_3^{-1} &= \Sigma_1^{-1} + \Sigma_2^{-1} \\
\Sigma_3^{-1} \mu_3 &= \Sigma_1^{-1} \mu_1 + \Sigma_2^{-1} \mu_2 \\
\Rightarrow \mu_3 &= \Sigma_3 (\Sigma_1^{-1} \mu_1 + \Sigma_2^{-1} \mu_2) \\
\mu_3 &= (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1} (\Sigma_1^{-1} \mu_1 + \Sigma_2^{-1} \mu_2)
\end{aligned}$$

Notice that we need Σ_3 while calculation μ_3 . However, to save computational memory, we only store the inverses of covariances, i.e., Σ_1^{-1} , Σ_2^{-1} and Σ_3^{-1} . So, to solve for μ_3 and avoid the computationally

expensive process of matrix inversion, we use the linear solver `torch.solve` on the equation $\Sigma_3^{-1}\mu_3 = \Sigma_1^{-1}\mu_1 + \Sigma_2^{-1}\mu_2$.

B Algorithm for KG Reasoning with PERM

Algorithm 1 provides an outline of PERM’s overall framework to learn representations of entities $e \in E$ and relations $r \in R$. The algorithm describes the training from FOE operations of translation (lines 4-7), intersection (lines 8-11), and union (lines 12-15).

Algorithm 1: PERM training algorithm

Input: Training data D_t, D_\cap, D_\cup , which are set of all (query (Q), result (V)) for translation, intersection, and union, respectively;

Output: Entity E and Relation R gaussian density functions;

- 1 Randomly initialize $e = \mathcal{N}(\mu_e, \Sigma_e) \in E$ and $r = \mathcal{N}(\mu_r, \Sigma_r) \in R$;
- 2 **for** number of epochs; until convergence **do**
- 3 $l = 0$; # Initialize loss
- 4 **for** $\{(e, r, V_t) \in D_t\}$ **do**
- 5 $q_t = \mathcal{N}(\mu_e + \mu_r, (\Sigma_e^{-1} + \Sigma_r^{-1})^{-1})$ from Eq. (5)
- 6 # Update loss for translation queries
- 7 $l = l + \sum_{v_t \in V_t} d_{\mathcal{N}}(v_t, q_t)$
- 8 **end**
- 9 **for** $\{(Q_\cap, V_\cap) \in D_\cap\}$ **do**
- 10 $q_\cap = \mathcal{N}(\mu_3, \Sigma_3)$, from Eq. (6)
- 11 # Update loss for intersection queries
- 12 $l = l + \sum_{v_\cap \in V_\cap} d_{\mathcal{N}}(v_\cap, q_\cap)$
- 13 **end**
- 14 **for** $\{(Q_\cup, V_\cup) \in D_\cup\}$ **do**
- 15 $q_\cup = \sum_{i=1}^n \phi_i \mathcal{N}(\mu_{e_i}, \Sigma_{e_i})$ from Eq. (7)
- 16 # Update loss for union queries
- 17 $l = l + \sum_{v_\cup \in V_\cup} \sum_{i=1}^n \phi_i d_{\mathcal{N}}(v_\cup, \mathcal{N}(\mu_{e_i}, \Sigma_{e_i}))$
- 18 **end**
- 19 # Update E and R with backpropagation
- 20 $E \leftarrow E - \Delta_E l$
- 21 $R \leftarrow R - \Delta_R l$
- 22 **end**
- 23 **return** E, R

C MRR metrics for Reasoning over KGs

Table 6 provides the Mean Reciprocal Rank (MRR) results for the reasoning over KGs experiment, given in section 5.

D Finer Evaluation of Ablation Study

Table 7 provides finer results of our ablation study.

Table 6: Performance comparison of PERM against the baselines to study the efficacy of the query representations. The columns present the different query structures and the overall average performance. The last two rows presents the Average Relative Improvement (%) of PERM compared to Q2B and CQD over all datasets across query types. Best results for each dataset are shown in bold.

Metrics		Mean Reciprocal Rank									
Dataset	Model	1t	2t	3t	2∩	3∩	2∪	∩t	t∩	∪t	Avg
FB15k-237	GQE	.346	.191	.144	.258	.361	.144	.087	.164	.149	.205
	BQE	.390	.109	.100	.228	.425	.124	.224	.126	.097	.203
	Q2B	.400	.225	.173	.275	.378	.198	.105	.180	.178	.235
	CQD	.439	.270	.206	.299	.381	.235	.271	.415	.112	.292
	PERM	.445	.268	.201	.306	.409	.253	.269	.353	.220	.303
NELL995	GQE	.311	.193	.175	.273	.399	.159	.078	.168	.130	.210
	BQE	.530	.130	.114	.376	.475	.122	.241	.143	.085	.246
	Q2B	.413	.227	.208	.288	.414	.266	.125	.193	.155	.254
	CQD	.442	.251	.226	.304	.441	.348	.124	.212	.104	.273
	PERM	.432	.244	.217	.296	.438	.332	.122	.178	.190	.272
DBPedia	GQE	.502	.005	N.A.	.749	.773	.320	.154	.597	0.00	.388
	BQE	.657	.006	N.A.	.964	.966	.306	.419	.527	0.00	.481
	Q2B	.619	.006	N.A.	.840	.863	.468	.212	.779	0.00	.473
	CQD	.648	.006	N.A.	.840	.863	.485	.206	.716	0.00	.471
	PERM	.706	.006	N.A.	.841	.862	.564	.219	.869	0.00	.508
DRKG	GQE	.313	.182	.132	.232	.360	.144	.097	.166	.163	.199
	BQE	.413	.118	.106	.298	.451	.147	.270	.154	.116	.230
	Q2B	.371	.225	.178	.283	.422	.205	.064	.122	.223	.233
	CQD	.413	.277	.213	.310	.427	.246	.174	.282	.143	.276
	PERM	.420	.276	.211	.325	.465	.271	.179	.249	.282	.298
PERM vs Q2B (%)		11.1	16.3	12.5	4.90	4.70	24.9	55.9	29.4	24.5	20.5
PERM vs CQD (%)		4.20	-1.2	-2.5	1.40	4.40	10.6	1.80	1.50	92.8	12.6

Table 7: Performance comparison of (final) PERM model against its variants to study the contributions of its components. The columns present the query structures and the overall average performance.

Metrics		HITS@3									
Dataset	Variants	1t	2t	3t	2n	3n	2u	nt	tn	ut	Avg
FB15k-237	1t	.516	.179	.119	.282	.360	.302	.071	.134	.133	.233
	translations	.516	.231	.167	.318	.413	.304	.096	.160	.185	.266
	single	.511	.282	.212	.359	.486	.296	.126	.207	.235	.302
	average	.499	.282	.209	.360	.482	.282	.119	.201	.234	.296
	MLP	.510	.285	.212	.363	.488	.293	.125	.208	.238	.302
	(final)	.520	.286	.216	.361	.490	.305	.128	.212	.239	.306
NELL995	1t	.576	.179	.134	.275	.373	.456	.072	.123	.111	.255
	translations	.576	.231	.188	.310	.428	.458	.097	.147	.155	.288
	single	.571	.282	.239	.350	.504	.446	.127	.190	.197	.323
	average	.558	.282	.235	.351	.500	.425	.120	.185	.196	.317
	MLP	.570	.285	.239	.354	.506	.442	.126	.191	.199	.324
	(final)	.581	.286	.243	.352	.508	.460	.129	.195	.200	.328
DBPedia	1t	.942	.004	N.A.	.781	.734	.775	.129	.600	0.00	.496
	translations	.942	.006	N.A.	.881	.843	.779	.174	.718	0.00	.543
	single	.934	.007	N.A.	1.00	1.00	.758	.228	.928	0.00	.607
	average	.912	.007	N.A.	.997	.984	.723	.216	.903	0.00	.593
	MLP	.932	.007	N.A.	.996	.992	.751	.227	.932	0.00	.605
	(final)	.950	.007	N.A.	1.00	1.00	.782	.232	.952	0.00	.615
DRKG	1t	.560	.202	.130	.302	.396	.373	.106	.172	.165	.267
	translations	.560	.260	.183	.341	.455	.374	.143	.206	.230	.306
	single	.555	.317	.232	.385	.536	.365	.187	.266	.293	.348
	average	.543	.317	.228	.386	.531	.347	.177	.259	.291	.342
	MLP	.554	.321	.232	.389	.538	.361	.186	.267	.296	.349
	(final)	.565	.322	.236	.387	.540	.376	.190	.273	.297	.354
Metrics		Mean Reciprocal Rank									
Dataset	Variants	1t	2t	3t	2n	3n	2u	nt	tn	ut	Avg
FB15k-237	PERM-1t	.410	.180	.122	.217	.274	.209	.085	.127	.145	.197
	translations	.410	.232	.171	.245	.314	.210	.115	.152	.202	.228
	single	.406	.283	.217	.277	.370	.204	.151	.197	.257	.262
	average	.396	.283	.214	.278	.367	.194	.143	.191	.256	.258
	MLP	.405	.286	.217	.280	.372	.202	.150	.198	.260	.263
	(final)	.445	.268	.201	.306	.409	.253	.269	.353	.220	.303
NELL995	1t	.432	.191	.160	.234	.275	.332	.094	.162	.125	.223
	translations	.428	.197	.168	.261	.369	.331	.092	.134	.147	.236
	single	.425	.241	.213	.294	.435	.322	.120	.173	.187	.268
	average	.415	.241	.210	.295	.431	.307	.113	.169	.186	.263
	MLP	.424	.243	.213	.298	.436	.319	.119	.174	.189	.268
	(final)	.432	.244	.217	.296	.438	.332	.122	.178	.190	.272
DBPedia	1t	.706	.005	N.A.	.665	.541	.564	.169	.791	0.00	.430
	translations	.700	.005	N.A.	.741	.727	.562	.164	.655	0.00	.444
	single	.694	.006	N.A.	.841	.862	.547	.215	.847	0.00	.502
	average	.678	.006	N.A.	.838	.848	.521	.204	.824	0.00	.490
	MLP	.693	.006	N.A.	.838	.855	.542	.214	.851	0.00	.500
	(final)	.706	.006	N.A.	.841	.862	.564	.219	.869	0.00	.452
DRKG	1t	.416	.173	.116	.254	.341	.269	.100	.157	.157	.220
	translations	.416	.223	.164	.286	.392	.270	.135	.188	.218	.255
	single	.413	.272	.207	.323	.462	.263	.176	.243	.278	.293
	average	.404	.272	.204	.324	.457	.250	.167	.236	.276	.288
	MLP	.412	.275	.207	.327	.463	.260	.175	.244	.281	.294
	(final)	.420	.276	.211	.325	.465	.271	.179	.249	.282	.298