Vector-valued Distance and Gyrocalculus on the Space of SPD Matrices

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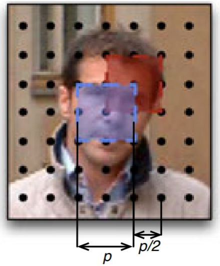
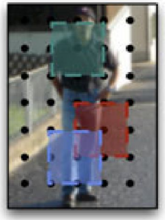
SPD Matrices FTW!

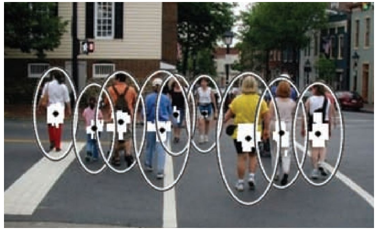
- SPDs have been used for:
  - Pedestrian detection
  - Action and face recognition
  - Image classification
  - Visual tracking
  - Medical image analysis

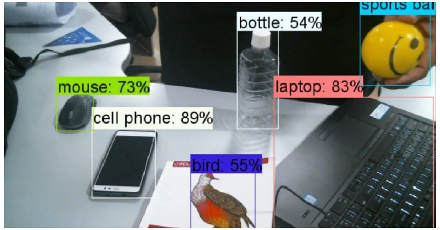
- They capture statistical notions
  - Gaussian distributions
  - Covariance

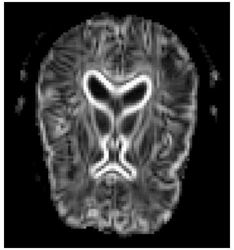
- Convenient trade-off between **structural richness** and **computational tractability**

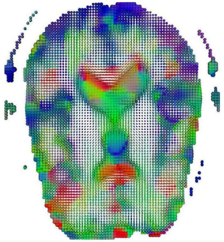


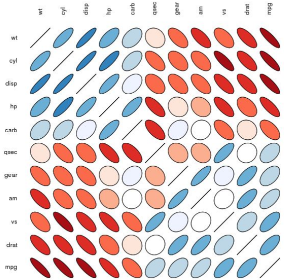


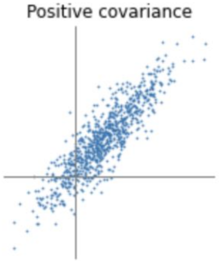


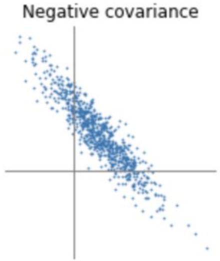


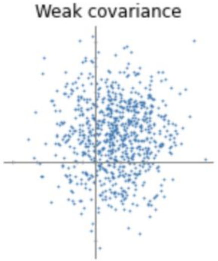










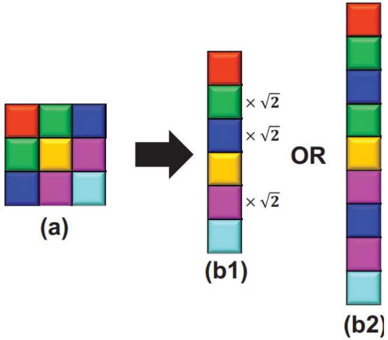


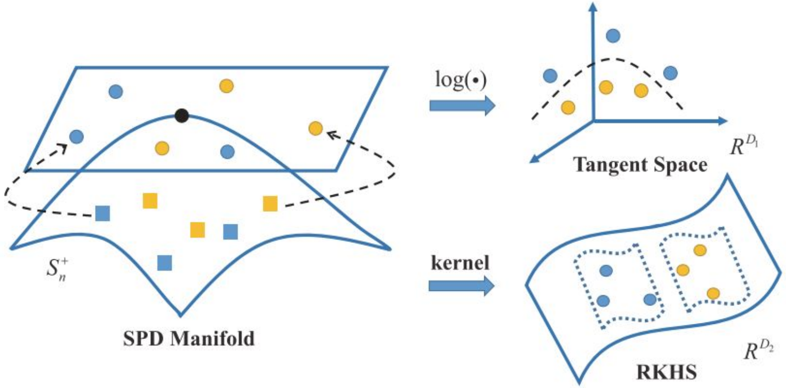
Previous Work

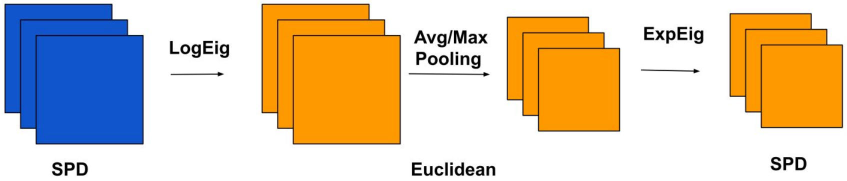
To operate with SPD matrices, previous work:

- Maps matrices to vectors
- Projects points into their tangent space
- Embedding the manifold into high-dimensional Hilbert spaces

These methods **distort the geometrical structure** of the manifold



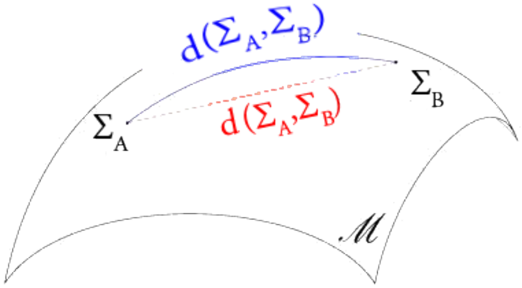




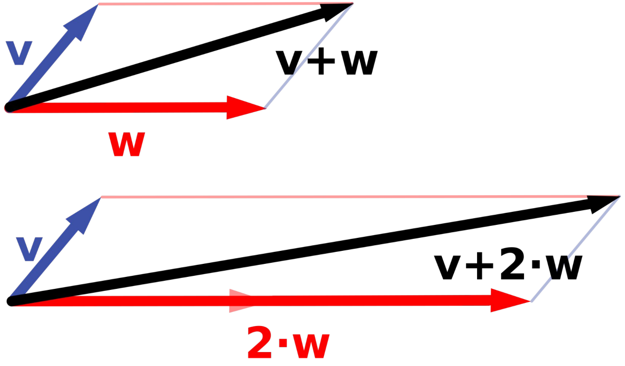
Previous Work

- Several distances proposed
  - Affine invariant metric
  - Stein metric
  - Bures–Wasserstein metric
  - Log-Euclidean Metric

  They do not fully exploit the representational power of SPD

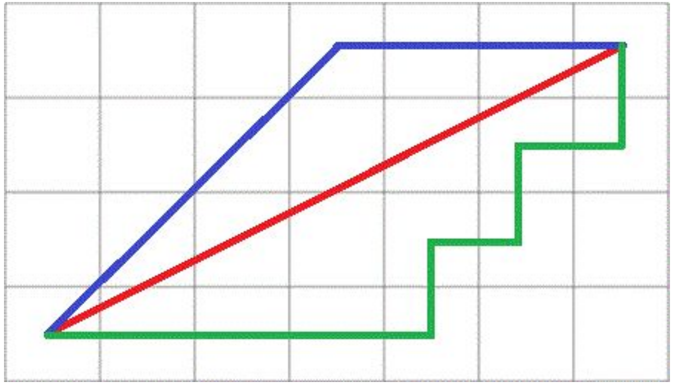


- Growing need to generalize basic operations into the SPD space
  - Hard to translate operations given the lack of closed-form expressions

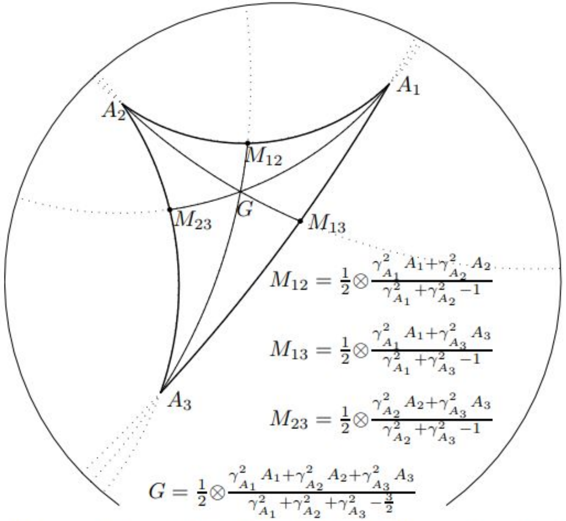


We Propose!

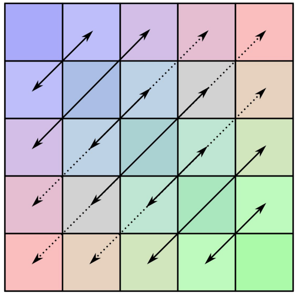
- Vector-valued distance function in SPD
  - Compute only one vector and derive multiple distances
  - Much more information than just the distance
    - Analysis and visualization tool



- Gyrocalculus on SPD
  - Arithmetic operations in the space
    - Addition
    - Scaling
    - Rotations
    - Reflections

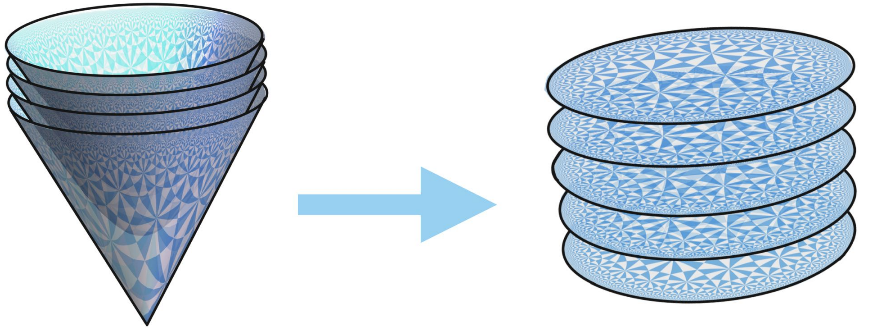


The Space SPD

$Z =$ 

- Points are positive definite real symmetric **n × n** matrices

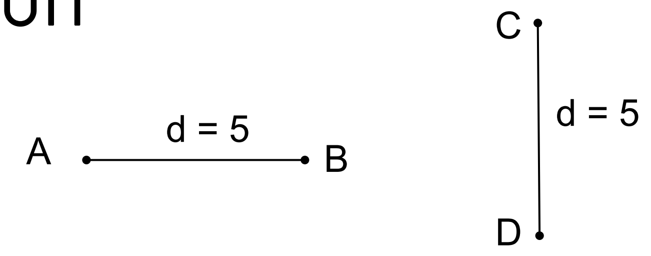
- SPD_n: Riemannian manifold of non-positive curvature of **n(n + 1)/2** dimensions
  - n-dimensional Euclidean subspaces
  - n−1 dimensional hyperbolic subspaces
  - $\lfloor \frac{n}{2} \rfloor$ hyperbolic planes



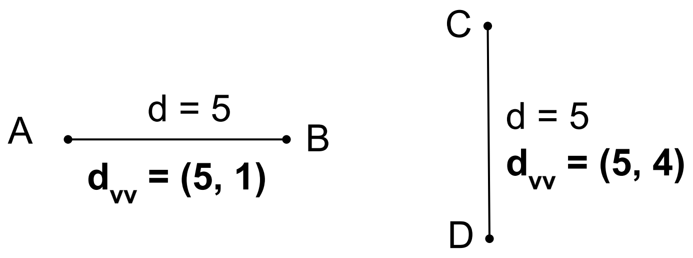
- They **combine hyperbolic and Euclidean geometry** thus they can accommodate:
  - Hierarchical structures -> hyperbolic subspaces
  - Flat structures -> Euclidean subspaces

Vector-valued Distance Function

- In Euclidean or hyperbolic spaces the only invariant of two points is their distance



- In the SPD_n space the invariant between two points is an **n**-dims distance vector



- To assign this vector we employ the vector-valued distance (VVD) function:

$$d_{vv}: \ \mathrm{SPD}_n \times \mathrm{SPD}_n \ \ \rightarrow \ \ \mathbb{R}^n$$

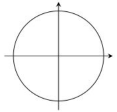
$$d_{vv}(P, Q) = \log(\lambda_1(P^{-1}Q), \ldots, \lambda_n(P^{-1}Q))$$

Advantages of the VVD

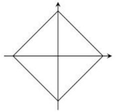
- By taking different norms on the VVD we can compute **several metrics**
  - Riemannian distance
  - Finsler distances
  - Generalize previous metrics

“One vector to rule them all”

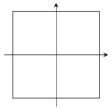
$$d^{R}(Z_1, Z_2) := \sqrt{\sum_{i=1}^{n} v_i^2}$$



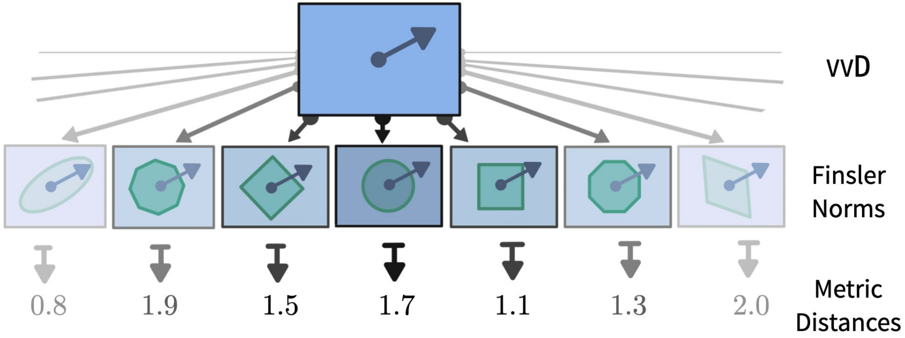
$$d^{F1}(Z_1, Z_2) := \sum_{i=1}^{n} v_i$$



$$d^{F\infty}(Z_1, Z_2) := \max\{v_i\}$$



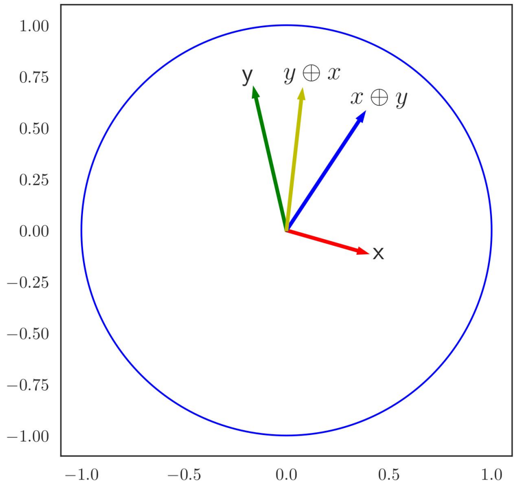
- VVD provides **much more information** than just the distance
  - Read the regularity of the geodesics joining two points
  - **Visualize and analyze** high-dimensional embeddings

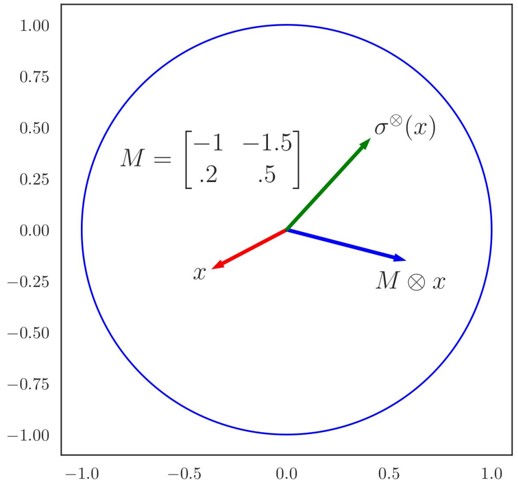


Gyrocalculus

- It is an algebraic formalisms to translate Euclidean operations to other spaces in a geometrically meaningful way

- Successful applications with Hyperbolic geometry [Ganea et al, 2018]
  - Addition
  - Matrix-vector multiplication
  - Pointwise non-linearities

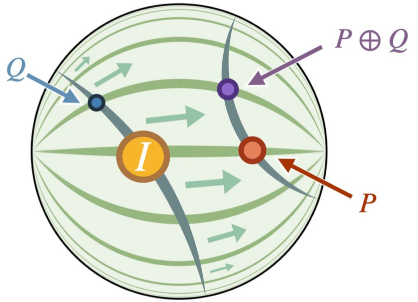




Gyrocalculus in SPD

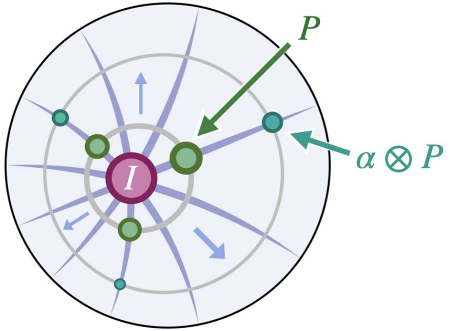
- Addition / subtraction

$$P \oplus Q = \sqrt{P} Q \sqrt{P}$$
$$\ominus P = P^{-1}$$



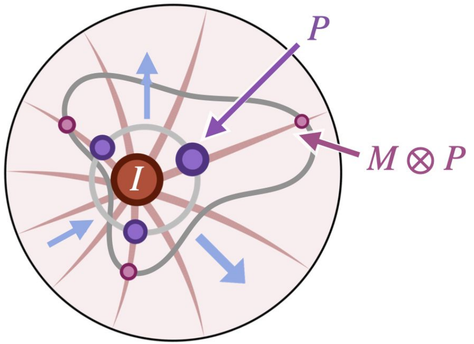
- Scalar multiplication

$$\alpha \otimes P = P^{\alpha} = \exp(\alpha \log(P))$$



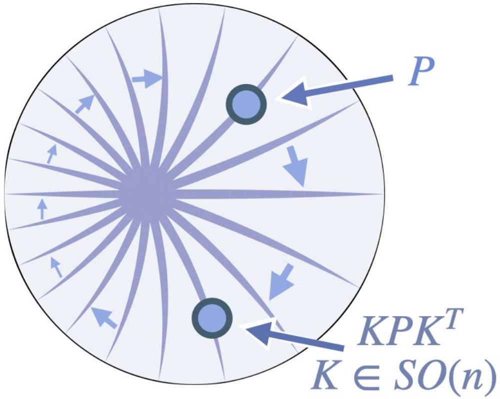
- Matrix scaling

$$A \otimes P = \exp(A \odot \log(P))$$



Isometries

- We also provide a way to learn rotations and reflections in SPD

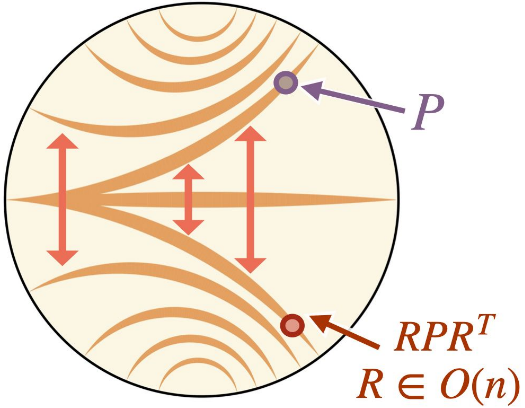


- Rotations

$$\mathrm{Rot}(\vec{\theta}) = \prod_{i<j} R^{+}_{ij}(\theta_{ij})$$

- Reflections

$$\mathrm{Refl}(\vec{\theta}) = \prod_{i<j} R^{-}_{ij}(\theta_{ij})$$



Knowledge Graph Completion

- Operations
  - Scaling

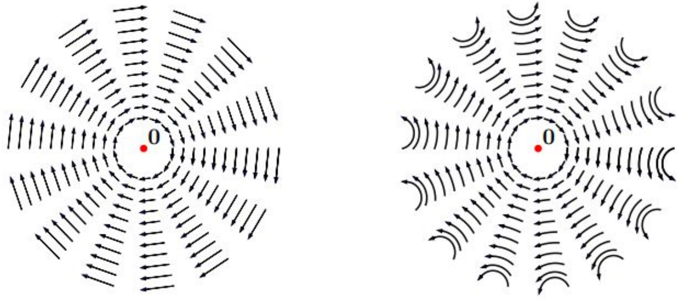
$$\phi(h,r,t) = -d((\mathbf{M}_r \otimes \mathbf{H}) \oplus \mathbf{R}, \mathbf{T})^2 + b_h + b_t$$

  - Rotations
  - Reflections

$$\phi(h,r,t) = -d((\mathbf{M}_r \circledcirc \mathbf{H}) \oplus \mathbf{R}, \mathbf{T})^2 + b_h + b_t$$

- Distances
  - Riemannian
  - Finsler One

- Baselines: scaling, rotations and reflections
  - Euclidean space
  - Hyperbolic spaces
  - Complex space



Results for Knowledge Graph Completion

		WN18RR				FB15k-237			
Operation	Model	MRR	HR@1	HR@3	HR@10	MRR	HR@1	HR@3	HR@10
Scaling	MuRE	47.5	43.6	48.7	55.4	33.6	24.5	37.0	52.1
	MuRP	48.1	**44.0**	49.5	56.6	33.5	24.3	36.7	51.8
	$\text{SPD}^{R}_{\text{Sca}}$	48.1	43.1	50.1	57.6	**34.5**	**25.1**	**38.0**	**53.5**
	$\text{SPD}^{F_1}_{\text{Sca}}$	**48.4**	42.6	**51.0**	**59.0**	32.9	23.6	36.3	51.5

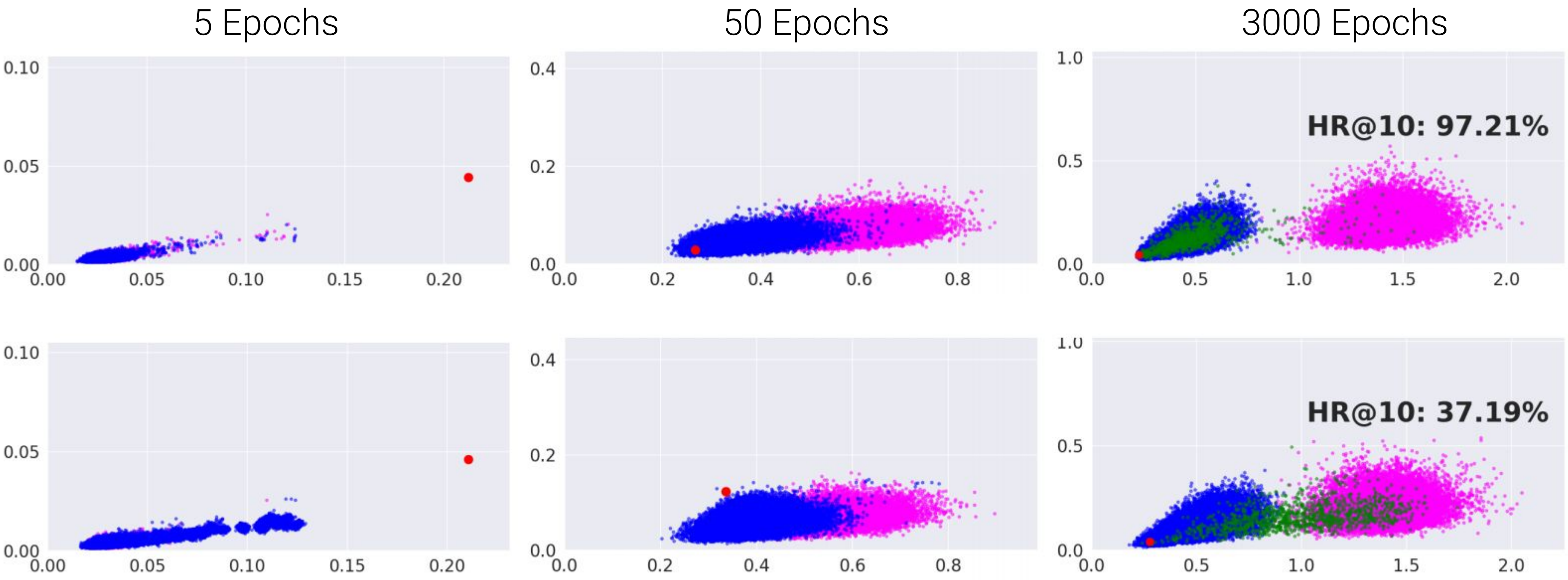
- SPD scaling **outperforms** Euclidean and hyperbolic models

Results for Knowledge Graph Completion

Operation	Model	WN18RR MRR	WN18RR HR@1	WN18RR HR@3	WN18RR HR@10	FB15k-237 MRR	FB15k-237 HR@1	FB15k-237 HR@3	FB15k-237 HR@10
Scaling	MuRE	47.5	43.6	48.7	55.4	33.6	24.5	37.0	52.1
	MuRP	48.1	**44.0**	49.5	56.6	33.5	24.3	36.7	51.8
	$\text{SPD}^{R}_{\text{Sca}}$	48.1	43.1	50.1	57.6	**34.5**	**25.1**	**38.0**	**53.5**
	$\text{SPD}^{F_1}_{\text{Sca}}$	**48.4**	42.6	**51.0**	**59.0**	32.9	23.6	36.3	51.5
Rotations	RotC	47.6	42.8	49.2	57.1	33.8	24.1	37.5	53.3
	RotE	49.4	44.6	51.2	58.5	**34.6**	**25.1**	**38.1**	**53.8**
	RotH	**49.6**	**44.9**	**51.4**	**58.6**	34.4	24.6	38.0	53.5
	$\text{SPD}^{R}_{\text{Rot}}$	46.2	39.7	49.6	57.8	32.9	23.6	36.3	51.6
	$\text{SPD}^{F_1}_{\text{Rot}}$	40.9	30.5	48.2	57.3	32.1	22.9	35.4	50.5
Reflections	RefE	47.3	43.0	48.5	56.1	**35.1**	**25.6**	**39.0**	**54.1**
	RefH	46.1	40.4	48.5	56.8	34.6	25.2	38.3	53.6
	$\text{SPD}^{R}_{\text{Ref}}$	48.3	44.0	49.7	56.7	32.5	23.4	35.6	51.0
	$\text{SPD}^{F_1}_{\text{Ref}}$	**48.7**	**44.3**	**50.1**	**57.4**	31.6	22.5	34.6	50.0

- Competitive results for rotations and reflections with **significantly less dimensions**
- In many cases **Finsler one metric** outperforms the Riemannian distance

Visualization of Embeddings

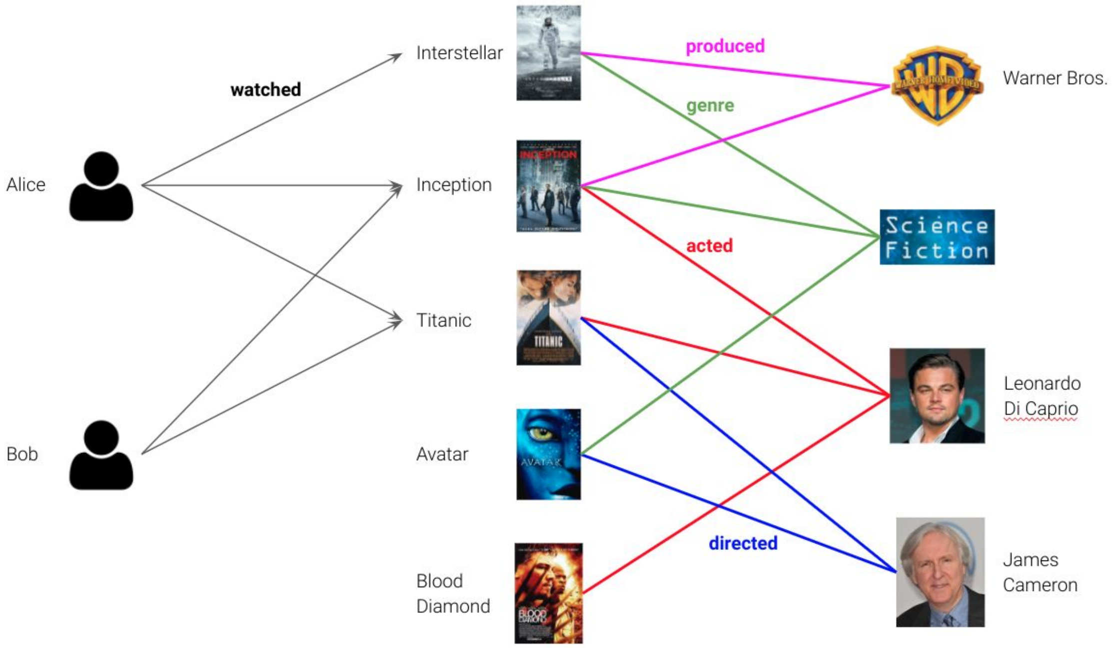


- **Train**, **negative** and **validation** triples for WN18RR relationships
- Position of **validation** triples directly correlates with performance

Knowledge Graph-based Recommender Systems

- Recommendation problem as a link prediction task over users and items enhanced with side information

- Same models than for Knowledge graph completion



Results for KG Recommender Systems

Model	Software		Luxury		Pantry		MindReader	
	MRR	H@10	MRR	H@10	MRR	H@10	MRR	H@10
TransE	28.5±0.1	47.2±0.5	35.6±0.1	52.3±0.1	16.6±0.0	35.3±0.1	19.1±0.4	37.6±0.1
RotC	28.5±0.3	45.4±1.4	33.0±0.1	49.8±0.2	14.5±0.0	31.3±0.2	25.3±0.3	50.3±0.6
MuRE	29.4±0.4	47.1±0.4	35.6±0.7	54.0±0.3	19.4±0.1	39.5±0.2	25.2±0.3	49.9±0.6
MuRP	29.6±0.3	47.9±0.3	**37.5±0.1**	**55.2±0.3**	19.4±0.1	39.8±0.2	25.3±0.3	49.3±0.2
$\mathrm{SPD}^{R}_{\mathrm{Sca}}$	29.4±0.4	48.1±0.8	**37.5±0.2**	55.1±0.2	19.5±0.0	39.6±0.3	25.4±0.1	49.8±0.3
$\mathrm{SPD}^{F_1}_{\mathrm{Sca}}$	28.8±0.1	46.9±0.5	37.3±0.3	54.1±0.9	19.0±0.1	38.8±0.2	**25.7±0.5**	49.5±0.1
$\mathrm{SPD}^{R}_{\mathrm{Rot}}$	**30.3±0.2**	48.6±0.9	37.2±0.1	54.8±0.4	**20.0±0.1**	**40.3±0.1**	25.3±0.0	**50.5±0.3**
$\mathrm{SPD}^{F_1}_{\mathrm{Rot}}$	30.1±0.1	**49.1±0.3**	36.9±0.1	54.5±0.6	19.2±0.0	39.3±0.1	**25.7±0.0**	49.5±0.2
$\mathrm{SPD}^{R}_{\mathrm{Ref}}$	29.6±0.2	48.0±0.5	37.3±0.2	55.0±0.2	19.3±0.0	39.7±0.3	25.3±0.0	49.1±0.1
$\mathrm{SPD}^{F_1}_{\mathrm{Ref}}$	29.3±0.1	47.5±0.6	36.8±0.0	54.8±0.1	18.6±0.2	38.3±0.3	24.8±0.2	47.9±1.8

- SPD models **tie or outperform baselines** in all cases
- **Rotations**, both in Riemannian and Finsler metrics, seem to be the most effective operator

Linear Layers on SPD

- Linear layer: feature transformation + bias addition
  - Scaling
  - Rotation
  - Reflection

$$y = Wx + b$$

$$y = W \otimes x \oplus b$$

- Experiments on Question Answering
  - Training word embeddings on SPD

- Model
  - Model question/answer as word embeddings summation followed by a linear transformation

$$\mathbf{Q} = T(\bigoplus_{i=1}^{n} t_i^q) \oplus B$$

  - Rank question-answer similarity

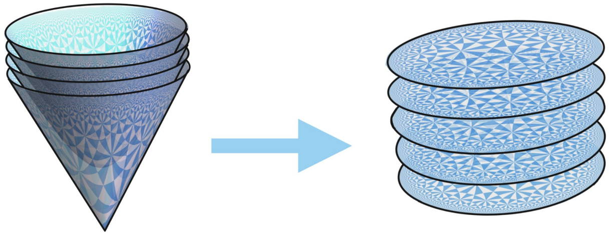
$$\text{sim}(q, a) = -w_f d(\mathbf{Q}, \mathbf{A}) + w_b$$

Results for Question Answering

Model	TrecQA		WikiQA	
	MRR	H@1	MRR	H@1
Euclidean	55.9±2.0	41.0±2.0	43.4±0.3	22.4±1.1
Hyperbolic	58.0±1.3	39.3±2.0	44.0±0.4	22.8±0.6
$\mathrm{SPD}^{R}_{\mathrm{Sca}}$	55.4±0.1	37.1±0.1	**45.5±0.5**	24.4±1.1
$\mathrm{SPD}^{F_1}_{\mathrm{Sca}}$	57.1±0.7	38.6±0.2	44.8±0.5	24.0±0.6
$\mathrm{SPD}^{R}_{\mathrm{Rot}}$	58.7±1.5	41.4±2.9	44.6±0.6	23.6±0.6
$\mathrm{SPD}^{F_1}_{\mathrm{Rot}}$	58.1±0.5	**43.6±1.0**	43.7±0.4	23.8±0.8
$\mathrm{SPD}^{R}_{\mathrm{Ref}}$	57.3±0.3	40.7±1.1	43.9±0.7	23.4±2.0
$\mathrm{SPD}^{F_1}_{\mathrm{Ref}}$	**59.6±0.5**	42.1±1.0	44.7±1.2	**25.0±2.5**

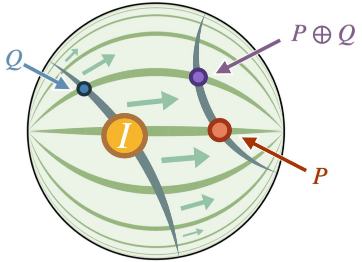
- SPD models **outperform baselines** in all cases
- **Embeddings in SPD manifolds** exploited for downstream tasks
- We showcase how to build **linear layers on SPD**

Summary

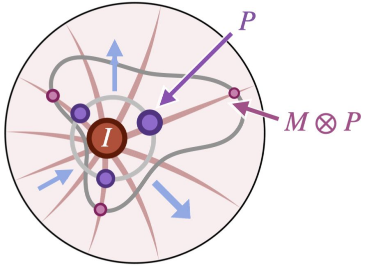


- Growing need to **generalize tools** for SPD manifolds

- Introduce the **vector-valued distance for SPD**
  - Riemannian, Finsler and more distances
  - Visualization and analysis tools



- **Gyrocalculus** on SPD
  - Arithmetic operations that respect the geometry of the space



- Experiments on three tasks and eight datasets
  - **Versatility** of the approach for different types of data
  - **Ease of integration** with downstream tasks
  - Reflect the **superior expressivity** of SPD