Mrep Averages and PCA via Lie Algebras

Tom Fletcher

October 21, 2002

Motivation

Motivation

- Given a set of *corresponding* Mrep models, how can we perform a PCA on those models?

Motivation

- Given a set of *corresponding* Mrep models, how can we perform a PCA on those models?
- Mrep parameters include angles and rotations, but PCA assumes a linear model.

Motivation

- Given a set of *corresponding* Mrep models, how can we perform a PCA on those models?
- Mrep parameters include angles and rotations, but PCA assumes a linear model.
- Thus we need a method to linearize Mrep models.

Groups

A *group* is a nonempty set G with a binary operation, $\cdot$, that has the following properties for all $a, b, c \in G$:

- **Closure:** $a \cdot b \in G$.
- **Associativity:** $(a \cdot b) \cdot c = a \cdot (b \cdot c)$.
- **Identity:** There exists an element $1 \in G$ such that $a \cdot 1 = 1 \cdot a = a$.
- **Inverses:** There exists an element $a^{-1} \in G$ such that $a \cdot a^{-1} = a^{-1} \cdot a = 1$.

Abelian Groups

- Notice we don't require the group product to be commutative. (xy may or may not equal yx)

- When the product is commutative, the group is called *abelian*.

- The group of rotations in 3D (which we are concerned with) is nonabelian.

Differentiable Manifolds

A topological space M is a *differentiable manifold* of dimension n if it can be covered by a collection of sets $\{U_\alpha\}_{\alpha \in A}$ such that

- M is Hausdorff with a countable basis.
- For each U_α there is a homeomorphism $\phi_\alpha : M \to \mathbb{R}^n$.
- If $U = U_\alpha \cap U_\beta$ is nonempty for any two indices $\alpha, \beta \in A$, then the restriction of $\phi_\alpha^{-1}\phi_\beta$ to $\phi_\alpha(U)$ is differentiable.

Lie Groups

A $Lie\ group$ is a group G is also a differentiable manifold, where the group operations are differentiable maps.

Lie Groups

A *Lie group* is a group G is also a differentiable manifold, where the group operations are differentiable maps.

That is,

$$\mu : (x, y) \mapsto xy : G \times G \to G, \quad \text{and}$$
$$\iota : x \mapsto x^{-1} : G \to G$$

are differentiable maps.

Lie Algebras

A *Lie algebra* is a vector space $\mathfrak{g}$ over $\mathbb{R}$, with a bilinear mapping $(X, Y) \mapsto [X, Y]$ called the *Lie bracket*. The Lie bracket also satisfies

$$[X, Y] = -[Y, X]$$

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0$$

The Exponential Map

The Exponential Map

- It turns out that the tangent space to the identity of a Lie group G is a Lie algebra $\mathfrak{g}$.

The Exponential Map

- It turns out that the tangent space to the identity of a Lie group G is a Lie algebra $\mathfrak{g}$.
- The exponential map, $\exp : \mathfrak{g} \rightarrow G$, provides a way to associate tangent vectors with elements of G.

The Exponential Map

- It turns out that the tangent space to the identity of a Lie group G is a Lie algebra $\mathfrak{g}$.
- The exponential map, $\exp : \mathfrak{g} \to G$, provides a way to associate tangent vectors with elements of G.
- The exponential map is a diffeomorphism from a neighborhood of 0 into a neighborhood of 1.

The Exponential Map

- It turns out that the tangent space to the identity of a Lie group G is a Lie algebra $\mathfrak{g}$.
- The exponential map, $\exp : \mathfrak{g} \rightarrow G$, provides a way to associate tangent vectors with elements of G.
- The exponential map is a diffeomorphism from a neighborhood of 0 into a neighborhood of 1.
- As you might guess it's inverse is called the log map.

Matrix Exponents

Matrix Exponents

- The exponent map for $\mathbf{L}(\mathbb{R}^n, \mathbb{R}^n)$ ($n \times n$ matrices) is

$$\exp(X) = \sum_{k=0}^{\infty} \frac{1}{k!} X^k.$$

Matrix Exponents

- The exponent map for $\mathbf{L}(\mathbb{R}^n, \mathbb{R}^n)$ ($n \times n$ matrices) is

$$\exp(X) = \sum_{k=0}^{\infty} \frac{1}{k!} X^k.$$

- This series converges.

$\mathbf{SO}(3)$

- For the group of 3D rotations, $\mathbf{SO}(3)$, the Lie algebra is $\mathfrak{so}(3)$, the antisymmetric 3×3 matrices.

- If $X \in \mathbf{SO}(3)$, then

$$\log(X) = \begin{pmatrix} 0 & -\mathbf{v}_z & \mathbf{v}_y \\ \mathbf{v}_z & 0 & -\mathbf{v}_x \\ -\mathbf{v}_y & \mathbf{v}_x & 0 \end{pmatrix},$$

  where $\mathbf{v}$ is the axis of rotation and $|\mathbf{v}|$ is the angle.

- The Lie bracket is the cross product of these axes.

Exponents with Rotations

- For $A_{\mathbf{v}} \in \mathfrak{so}(3)$ the exponent map simplifies to

$$\exp(A_{\mathbf{v}}) = I + \frac{\sin|\mathbf{v}|}{|\mathbf{v}|} A_{\mathbf{v}} + \frac{1-\cos|\mathbf{v}|}{|\mathbf{v}|^2} A_{\mathbf{v}}^2$$

- This is easier for a quaternion representation

$$\mathbf{q} = (\sin(\frac{|\mathbf{v}|}{2})\mathbf{v}, \cos(\frac{|\mathbf{v}|}{2})).$$

The “Correct” Way to Average Rotations

The "Correct" Way to Average Rotations

- The best way would be to minimize total geodesic distance on $\mathbf{SO}(3)$.

The “Correct” Way to Average Rotations

- The best way would be to minimize total geodesic distance on $\mathbf{SO}(3)$.

- That is, given rotations $R_1, R_2, ..., R_n$, the average rotation R minimizes
$$\sum_{k=1}^{n} ||Log(R_n^T R)||^2.$$

The "Correct" Way to Average Rotations

- The best way would be to minimize total geodesic distance on $\mathbf{SO}(3)$.

- That is, given rotations $R_1, R_2, ..., R_n$, the average rotation R minimizes
$$\sum_{k=1}^{n} ||Log(R_n^T R)||^2.$$

- This is not easy - requires optimization.

The Campbell-Baker-Hausdorff Formula

The Campbell-Baker-Hausdorff Formula

- Define Lie group multiplication in *logarithmic coordinates* by a mapping $\mu : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, such that

$$\exp(X)\exp(Y) = \exp(\mu(X, Y)).$$

The Campbell-Baker-Hausdorff Formula

- Define Lie group multiplication in *logarithmic coordinates* by a mapping $\mu : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, such that

$$\exp(X)\exp(Y) = \exp(\mu(X,Y)).$$

- The CBH formula is the Taylor series expansion for μ:

$$\mu(X,Y) = X + Y + \frac{1}{2}[X,Y] + O(|(X,Y)|^3).$$

Averaging Rotations in Logarithmic Coordinates

Averaging Rotations in Logarithmic Coordinates

- We can use the log map to linearize our rotations, and then just take averages as normal.

Averaging Rotations in Logarithmic Coordinates

- We can use the log map to linearize our rotations, and then just take averages as normal.
- The CBH Formula tells us that this is a first-order approximation to the optimal geodesic solution.

Averaging Rotations in Logarithmic Coordinates

- We can use the log map to linearize our rotations, and then just take averages as normal.
- The CBH Formula tells us that this is a first-order approximation to the optimal geodesic solution.
- Notice the error is proportional to the Lie bracket (cross product).

Averaging Rotations in Logarithmic Coordinates

- We can use the log map to linearize our rotations, and then just take averages as normal.
- The CBH Formula tells us that this is a first-order approximation to the optimal geodesic solution.
- Notice the error is proportional to the Lie bracket (cross product).
- Thus, rotations with similar axes of rotation have low error.

Mrep PCA

Mrep PCA

- Using the above Lie algebra technique, we can linearize the rotations in an mrep model.

Mrep PCA

- Using the above Lie algebra technique, we can linearize the rotations in an mrep model.
- But our parameters are still not commensurate (rotation axes vs. positions vs. object angles).

Mrep PCA

- Using the above Lie algebra technique, we can linearize the rotations in an mrep model.

- But our parameters are still not commensurate (rotation axes vs. positions vs. object angles).

- Two ways to fix this:

Mrep PCA

- Using the above Lie algebra technique, we can linearize the rotations in an mrep model.

- But our parameters are still not commensurate (rotation axes vs. positions vs. object angles).

- Two ways to fix this:

  ⋆ Use correlation matrix instead of covariance matrix.

Mrep PCA

- Using the above Lie algebra technique, we can linearize the rotations in an mrep model.

- But our parameters are still not commensurate (rotation axes vs. positions vs. object angles).

- Two ways to fix this:

  ⋆ Use correlation matrix instead of covariance matrix.
  ⋆ Multiply the rotation axis and object angle by the radius.

Mrep Data Vector

Mrep Data Vector

A single atom is an element $\mathbf{m} \in M$

$$\mathbf{m} = (\mathbf{x}, r, \mathbf{v}, \theta),$$

$$M = \mathbb{R}^3 \times \mathbb{R}^+ \times \mathfrak{so}(3) \times [0, \frac{\pi}{2}].$$

Mrep Data Vector

A single atom is an element $\mathbf{m} \in M$

$$\mathbf{m} = (\mathbf{x}, r, \mathbf{v}, \theta),$$

$$M = \mathbb{R}^3 \times \mathbb{R}^+ \times \mathfrak{so}(3) \times [0, \frac{\pi}{2}].$$

So, an $m \times n$ m-rep model is represented as an element of M^{mn}.

Mrep Data Vector

A single atom is an element $\mathbf{m} \in M$

$$\mathbf{m} = (\mathbf{x}, r, \mathbf{v}, \theta),$$

$$M = \mathbb{R}^3 \times \mathbb{R}^+ \times \mathfrak{so}(3) \times [0, \frac{\pi}{2}].$$

So, an $m \times n$ m-rep model is represented as an element of M^{mn}.

Notice that the deformations of an m-rep model form a Lie group!

Results

What Lies Ahead

What Lies Ahead

- Does linear PCA really fit mrep model populations?

What Lies Ahead

- Does linear PCA really fit mrep model populations?
- How does the approximation error in the rotations affect the analysis?

What Lies Ahead

- Does linear PCA really fit mrep model populations?
- How does the approximation error in the rotations affect the analysis?
- How does this method for rotation averaging stack up against other methods?

What Lies Ahead

- Does linear PCA really fit mrep model populations?
- How does the approximation error in the rotations affect the analysis?
- How does this method for rotation averaging stack up against other methods?