Local–Global Frames vs. Pure Change of Basis

Study Notes

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1 Question

Are the local–global coordinate transforms used in the AF2 structure module merely "change of basis" operations?

Short answer: *no*. The local $\to$ global maps in AF2 are not just change of basis in the strict linear-algebra sense, although the *rotational* part can be viewed as a change of orthonormal basis. The full local $\to$ global map is an *affine rigid transform*: rotation plus translation. That distinction matters.

2 What "Change of Basis" Means in Linear Algebra

In a pure change of basis:

- We fix a single vector space V with one origin.

- We choose two bases B and B' for V.

- Coordinates of the *same* vector v in these bases are related by an invertible matrix S:
$$[v]_{B'} = S^{-1}[v]_B, \qquad [v]_B = S[v]_{B'}.$$

- The underlying map on V is the identity: we are simply reexpressing the same geometric vector in different coordinates.

- The map is linear and sends 0 to 0.

Thus a pure basis change is:

- global (one basis for the entire space),

- linear,

- origin-preserving.

3 AF2's Local → Global Map

For residue i, the structure module maintains a frame

$$T_i = (R_i, t_i),$$

and defines the local → global map by

$$x_{\text{global}} = T_i \circ x_{\text{local}} = R_i x_{\text{local}} + t_i.$$

Key observations:

- There is a nonzero translation t_i: the origin of the local frame is at the Cα atom of residue i, which generally does not coincide with the global origin.

- As a map $\mathbb{R}^3 \to \mathbb{R}^3$, $x \mapsto R_i x + t_i$ is *not* linear:
  - $T_i(0) = t_i \neq 0$,
  - $T_i(x + y) \neq T_i(x) + T_i(y)$ unless $t_i = 0$.

- Each residue has its own frame, hence its own translation t_i. There is no single global basis change relating all local frames simultaneously.

Therefore T_i is an element of the Euclidean group SE(3): a rigid motion (rotation + translation), not merely a change of basis in a single vector space with fixed origin.

4 How Rotation R_i Relates to Change of Basis

If we ignore the translation and consider only the rotation

$$R_i : \mathbb{R}^3 \to \mathbb{R}^3,$$

then R_i can be viewed as a change of orthonormal basis between:

- the residue's local axes (basis vectors $e_1^{(i)}, e_2^{(i)}, e_3^{(i)}$),

- the global axes (standard basis).

In this interpretation:

- R_i encodes how the local basis sits inside the global basis.

- The relationships

$$x_{\text{global}} - t_i = R_i x_{\text{local}}, \qquad x_{\text{local}} = R_i^\top (x_{\text{global}} - t_i)$$

are exactly "change of basis + shift of origin".

So we may summarize:

- the rotational part R_i behaves like a change of basis between directions;

- the full frame T_i combines that change of basis with moving the origin to the Cα of residue i.

5   Active vs. Passive Viewpoints

There is also a conceptual difference between two viewpoints:

- **Passive (coordinate) viewpoint.** We keep the physical point fixed and reexpress it in another frame. This is what

$$x_{\text{local}} = T_i^{-1} \circ x_{\text{global}}$$

  is doing: expressing a global point in residue-i coordinates.

- **Active (transform) viewpoint.** We move the point cloud itself in space, for example by applying a global T_{global} to all frames T_i. This corresponds to physically rotating/translating the entire structure.

In Euclidean spaces these share the same matrices, but:

- change of basis in the strict linear-algebra sense is purely passive and linear (no translations),

- AF2's T_i is an *affine frame map*: it combines a passive change of axes with an origin shift tied to residue i.

6   Why This Matters for IPA and FAPE

Both IPA and FAPE rely on expressing points via the transforms

$$x_{\text{global}} = R_i x_{\text{local}} + t_i, \qquad x_{\text{local}} = R_i^\top (x_{\text{global}} - t_i),$$

which treat frames as rigid placements of local coordinate systems in global space.

Distances such as

$$\left\| T_i \circ \tilde{q}_i^{hp} - T_j \circ \tilde{k}_j^{hp} \right\|$$

are distances between concrete points in global space whose positions arise from both the rotations R_i, R_j and the translations t_i, t_j.

If the transforms were merely a single global change of basis, we would have:

- one linear map for all positions,

- no per-residue translations t_i,

- no notion of "where in the protein" a point is attached beyond direction.

The per-residue affine frames T_i give precisely the geometric structure (placement + orientation) needed for IPA and FAPE to make sense.

7   Conclusion

- The rotational part R_i is a change of orthonormal basis between local and global axes.

- The full local ↔ global maps

$$x \mapsto R_i x + t_i, \qquad x \mapsto R_i^\top (x - t_i)$$

are *affine rigid transforms* (elements of SE(3)), not pure basis changes:

  - they move the origin,
  - they are residue-specific,
  - they correspond to placing a small coordinate system at each residue in 3D space.

Thus, while the rotational component is closely related to change of basis, the full AF2 local–global frame transforms are more than that.

$$x \mapsto R_i x \qquad 4 \qquad x \mapsto R_i^\top (x - t_i)$$