Contact-assisted protein threading: an evolving new direction

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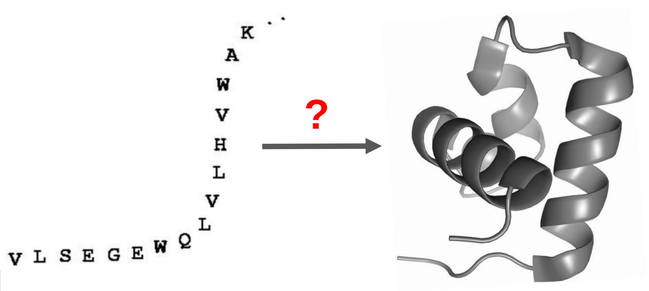
1. Background

What is the three-dimensional (3D) structure of the given sequence?



Sequence 3D Structure

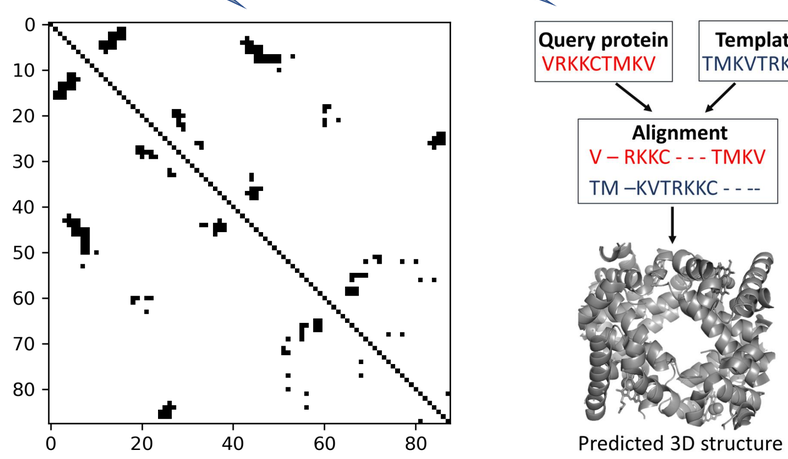
Contact Map is a symmetric, binary, square matrix where a pair of residue is in contact if the distance between a pair of residues < 8Å.

Protein threading is a powerful approach for predicting protein three-dimensional structure particularly when direct homologous relationships with known structures cannot be easily detected. However, **remote homology detection** via threading remains challenging.

Our **new contact-assisted threading method [Ref. (i)]:** Considering the recent advancements in contact prediction, we have developed a **new threading method** by **integrating contact** with various sequential and structural features to improve threading scoring function for better template selection.

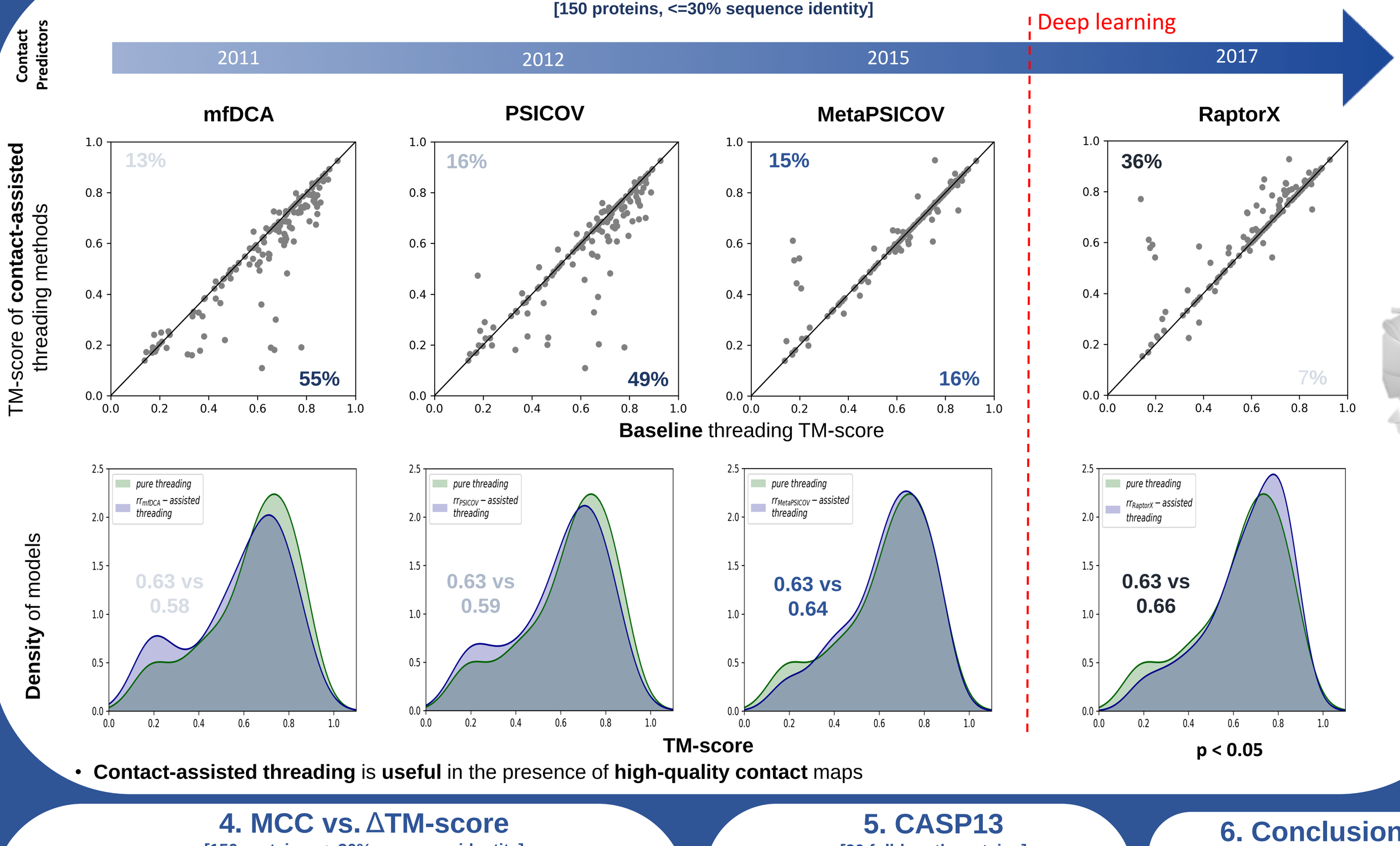
2. Research question

contact -assisted threading : when useful?



3. Evolution of contact-assisted threading

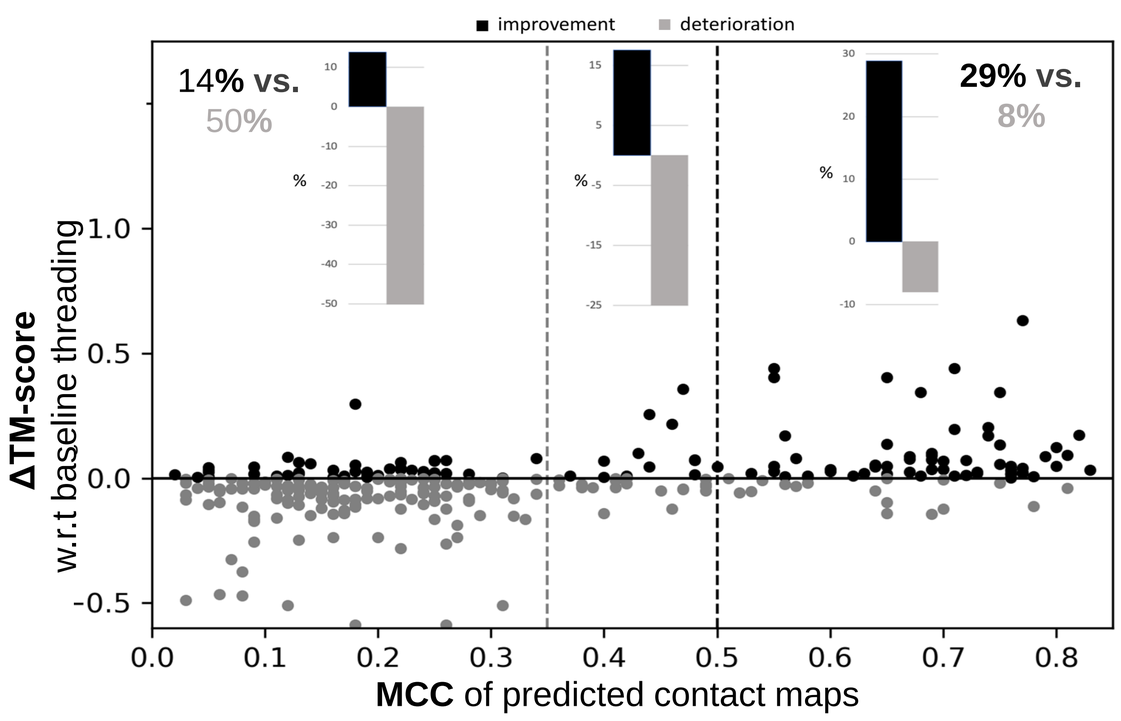
[150 proteins, <=30% sequence identity]



- **Contact-assisted threading** is **useful** in the presence of **high-quality contact** maps

4. MCC vs. ΔTM-score

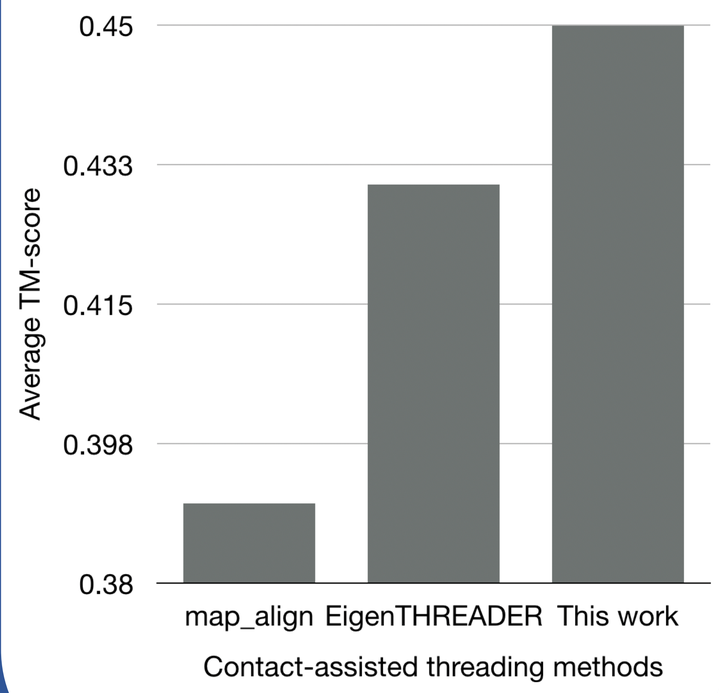
[150 proteins, <=30% sequence identity]



- **MCC >=0.5**: contact **boosts** threading in **~30%** cases
- **MCC<0.35** : contact **deteriorates** threading in **~50%** cases

5. CASP13

[20 full-length proteins]



6. Conclusions

- **Incorporating contact** is highly **effective** for improved protein threading particularly in the **presence** of **high-quality** contact maps.
- Contact prediction is likely to mature further – making **contact-assisted threading** method **an evolving new direction.**

7. References

i. **Bhattacharya S**, Bhattacharya D. **Does inclusion of residue-residue contact information boost protein threading?** Proteins Struct Funct Bioinforma. 87(7): 596-606 (2019). doi:10.1002/prot.25684.

ii. **Bhattacharya S**, Bhattacharya D. **Contact-assisted protein threading: when is it useful?** (Submitted)