Boosting alignment accuracy through adaptive local realignment

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*work performed at The University of Arizona

The University of Arizona | Computer Science UA Science

Motivation

Multiple sequence alignment is a fundamental problem in bioinformatics.

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- multiple sequence alignment is NP-Complete
- many popular aligners for multiple sequence alignment
- each aligner has many parameters whose values affect the alignment that is output

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[Kececioglu and Kim 2007]

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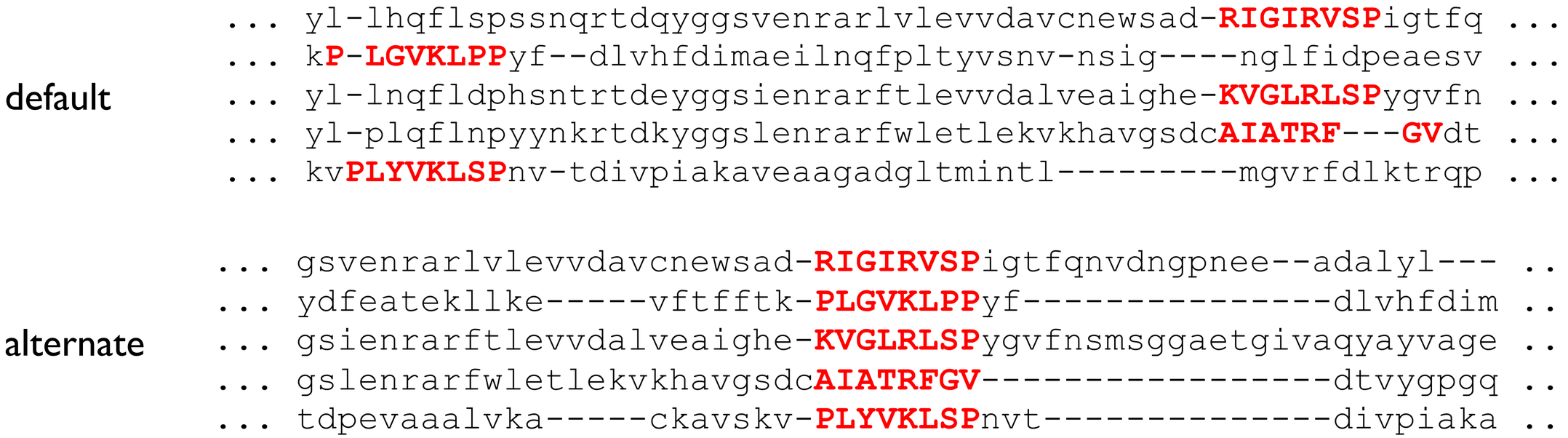
- The default has good *average accuracy* across all benchmarks.
- The optimal default choice can be found by inverse alignment.
- The default may be a poor choice for specific inputs.



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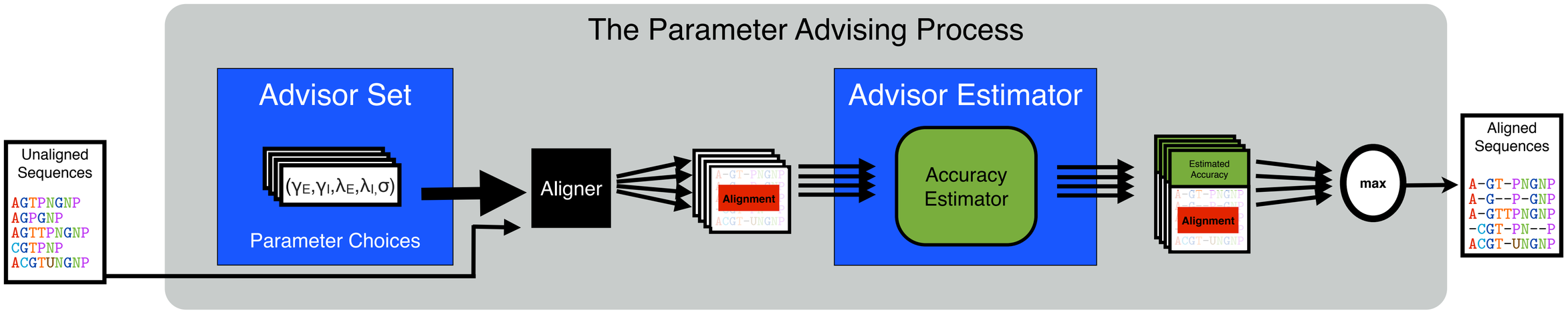
Can we find a parameter choice
that is best for *each region*
of a given input?

Parameter advising

Advising for unaligned input sequences



[RECOMB 2012]

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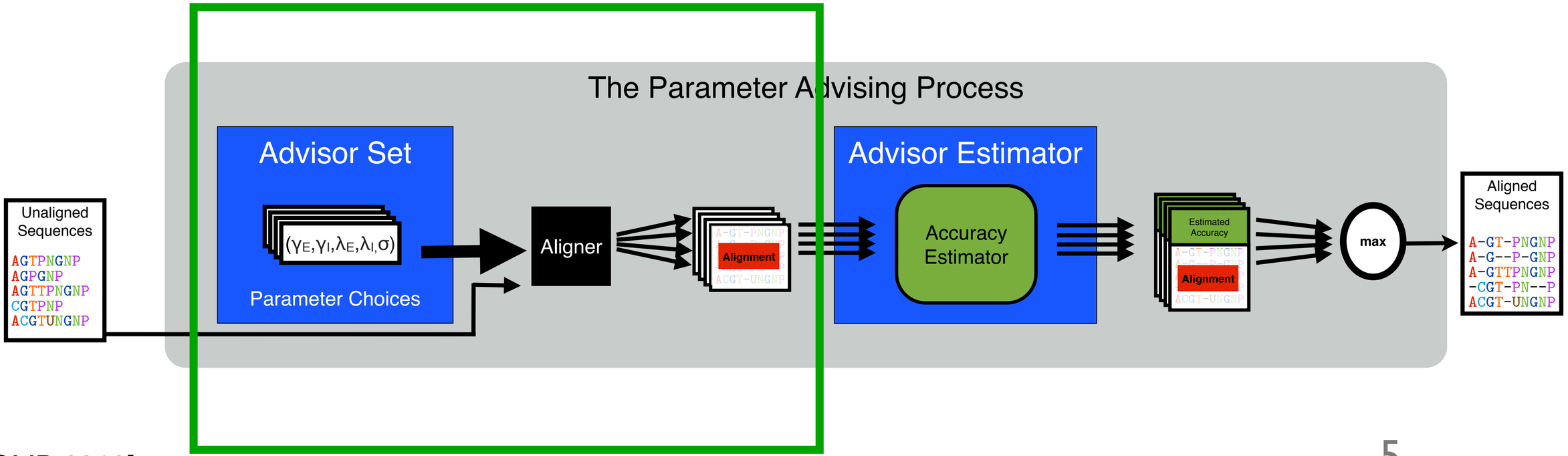

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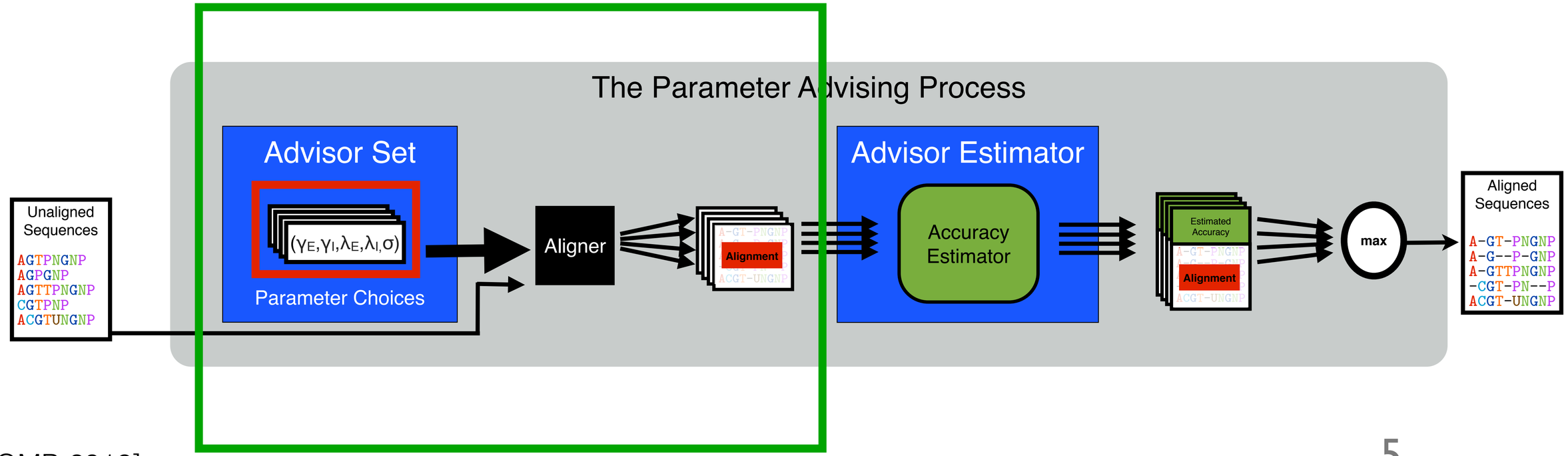

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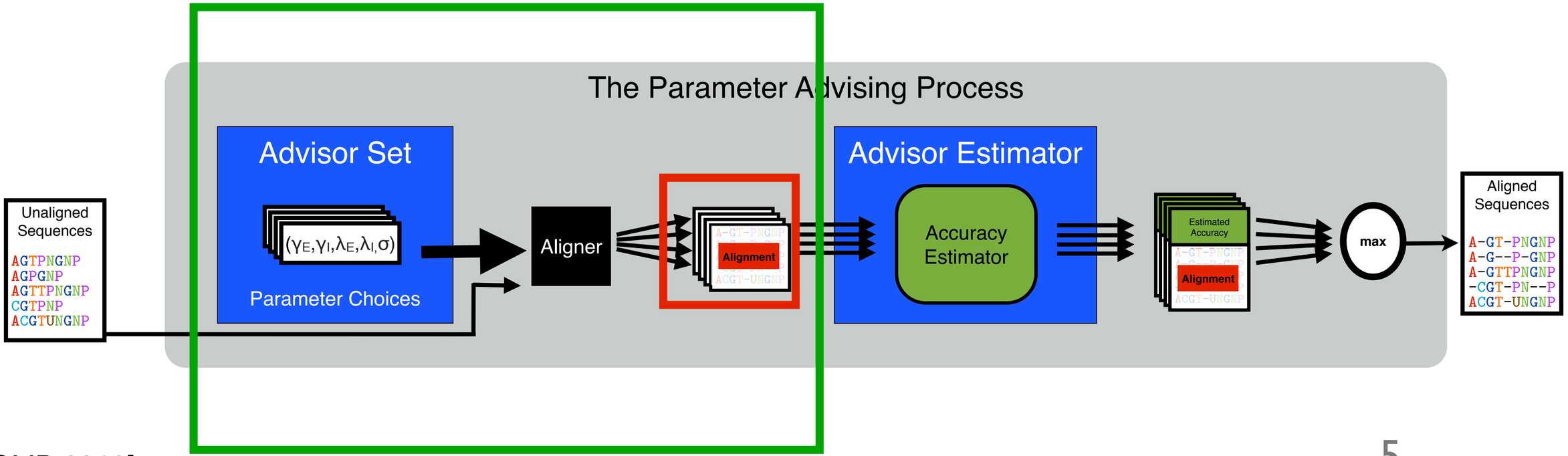

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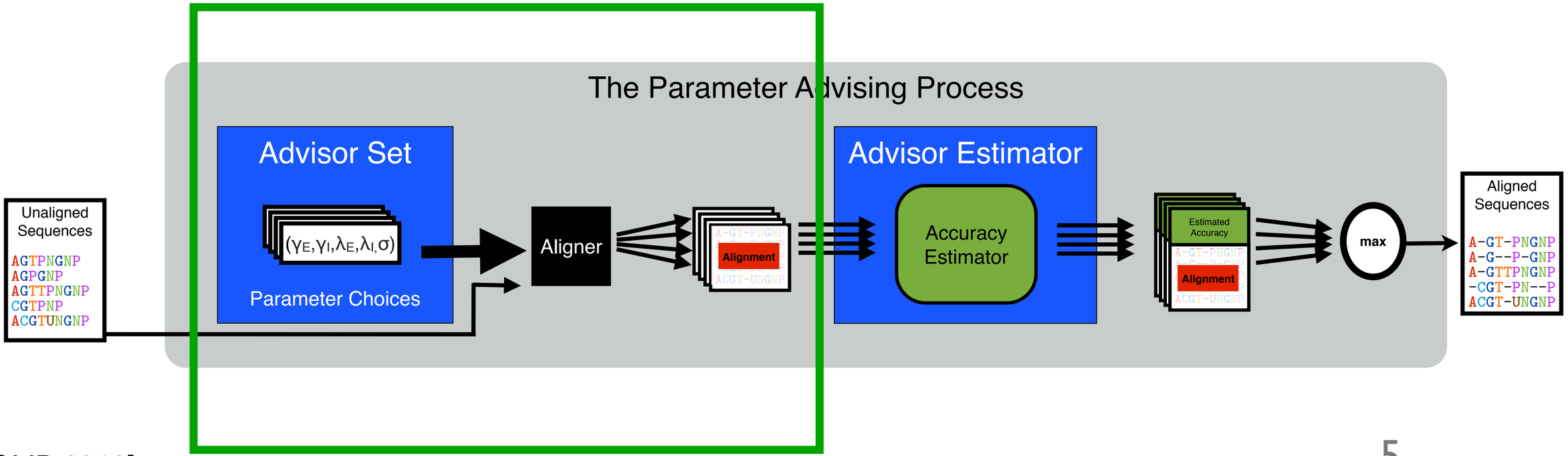

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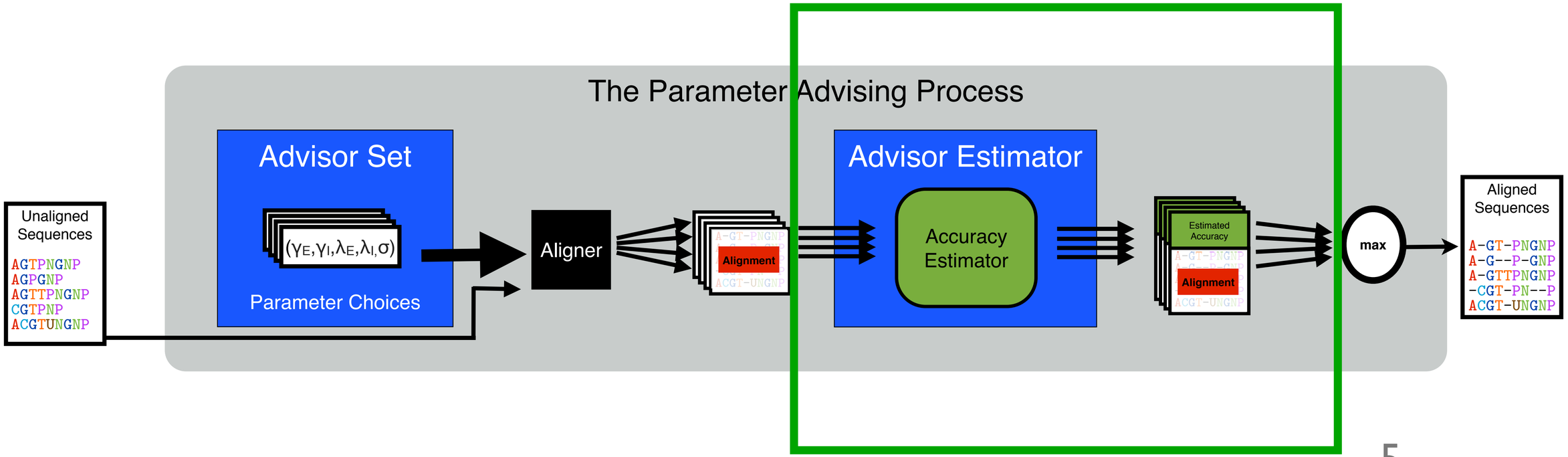

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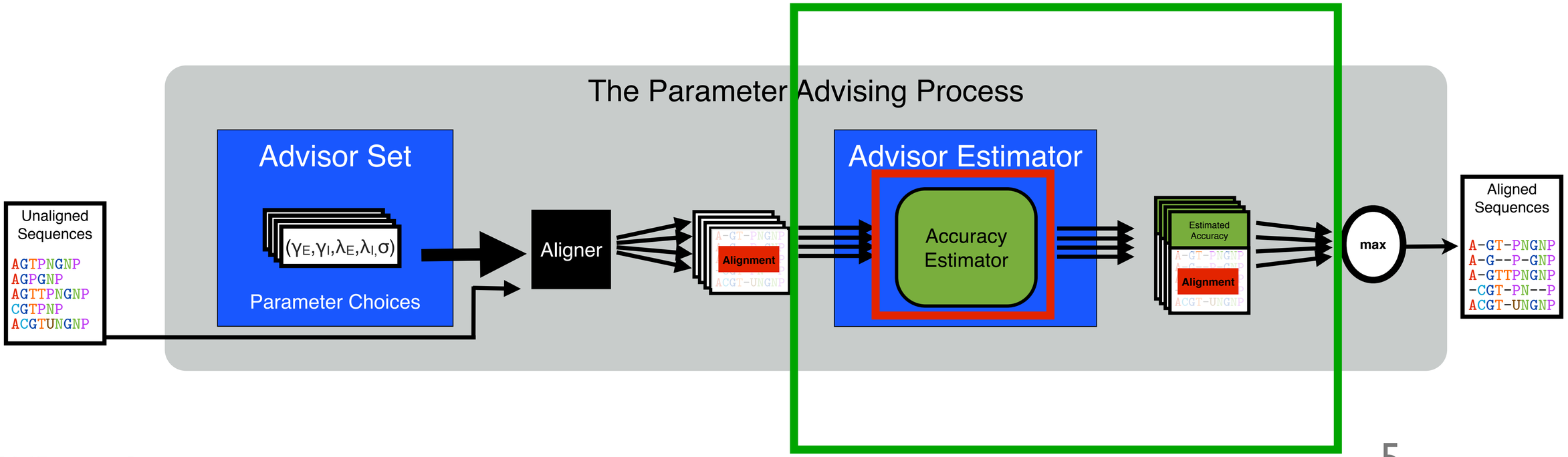

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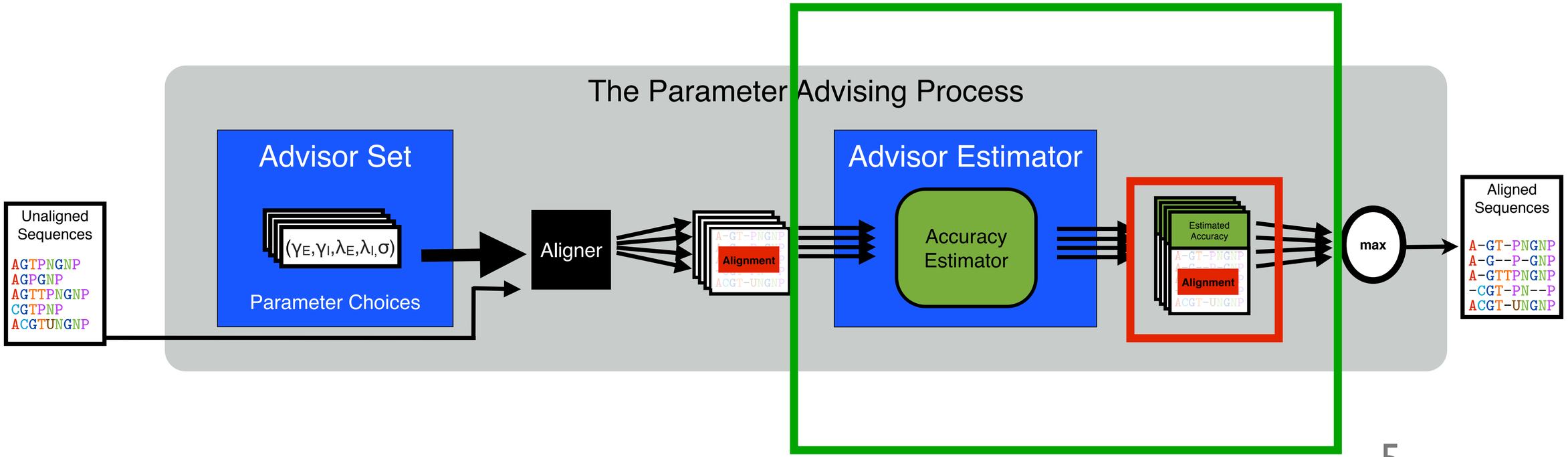

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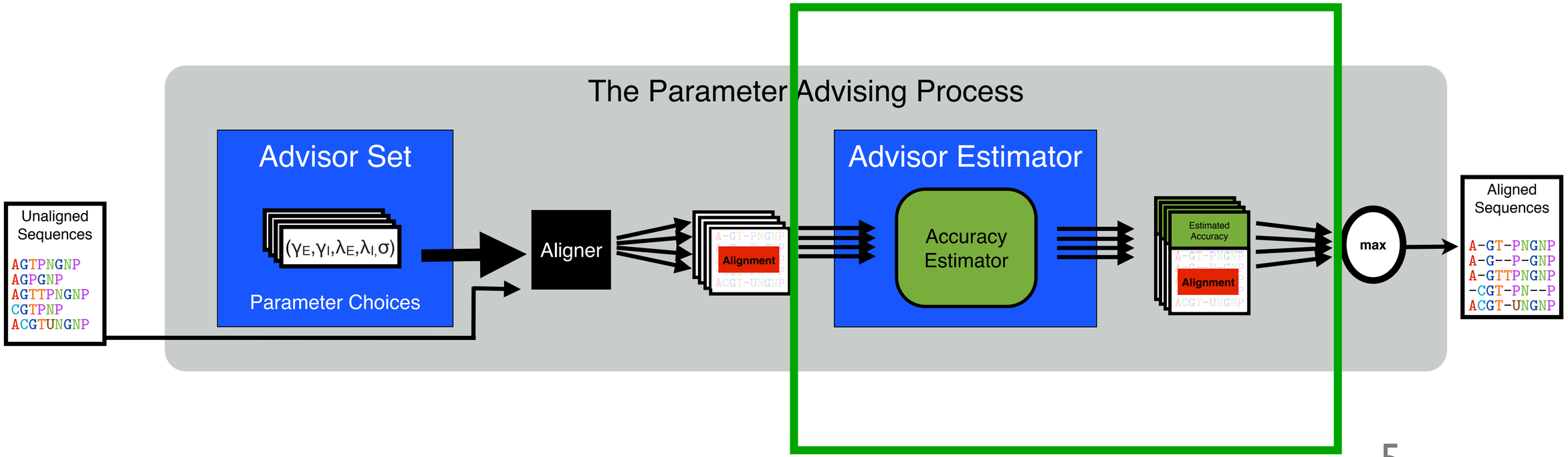

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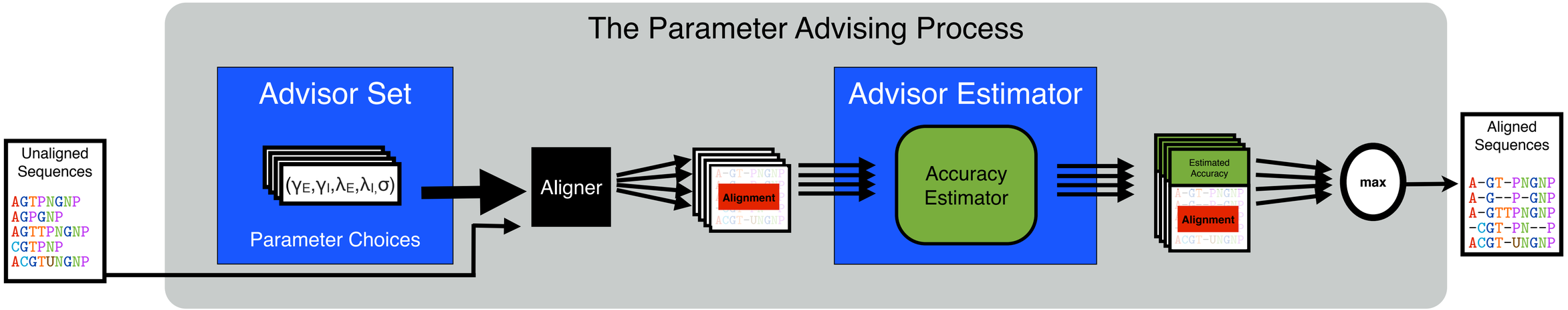
- selects the alignment with the highest estimated accuracy.



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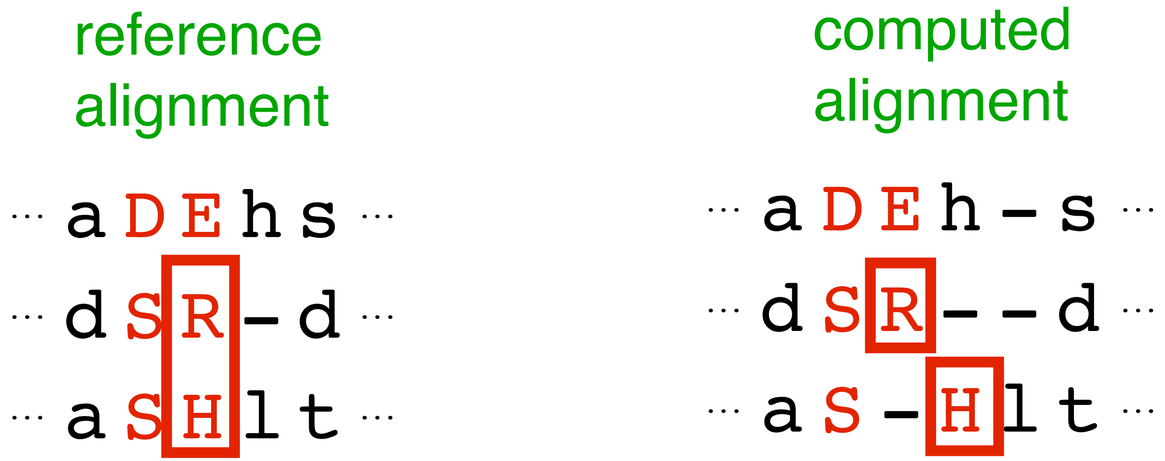

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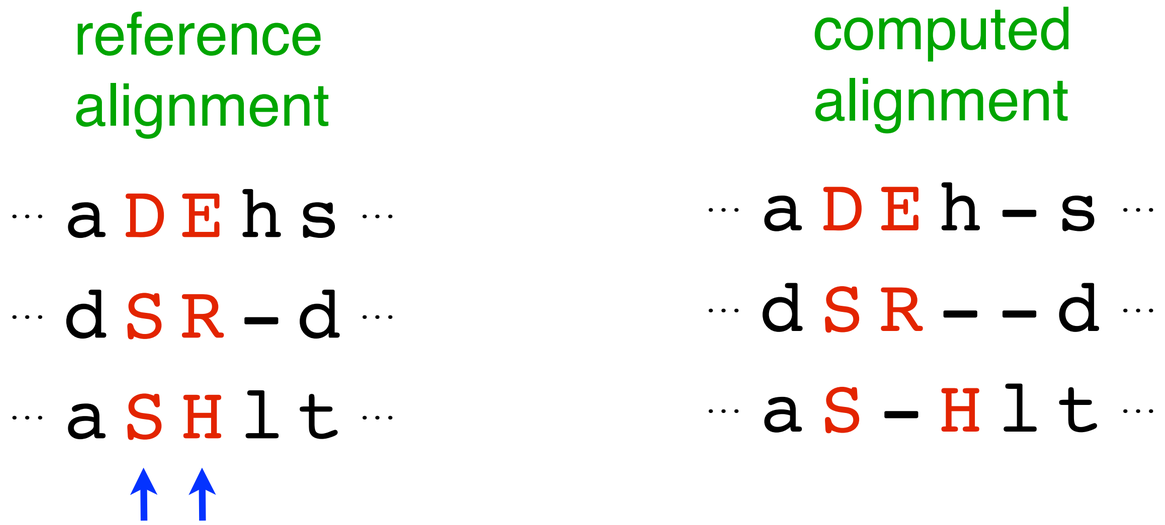

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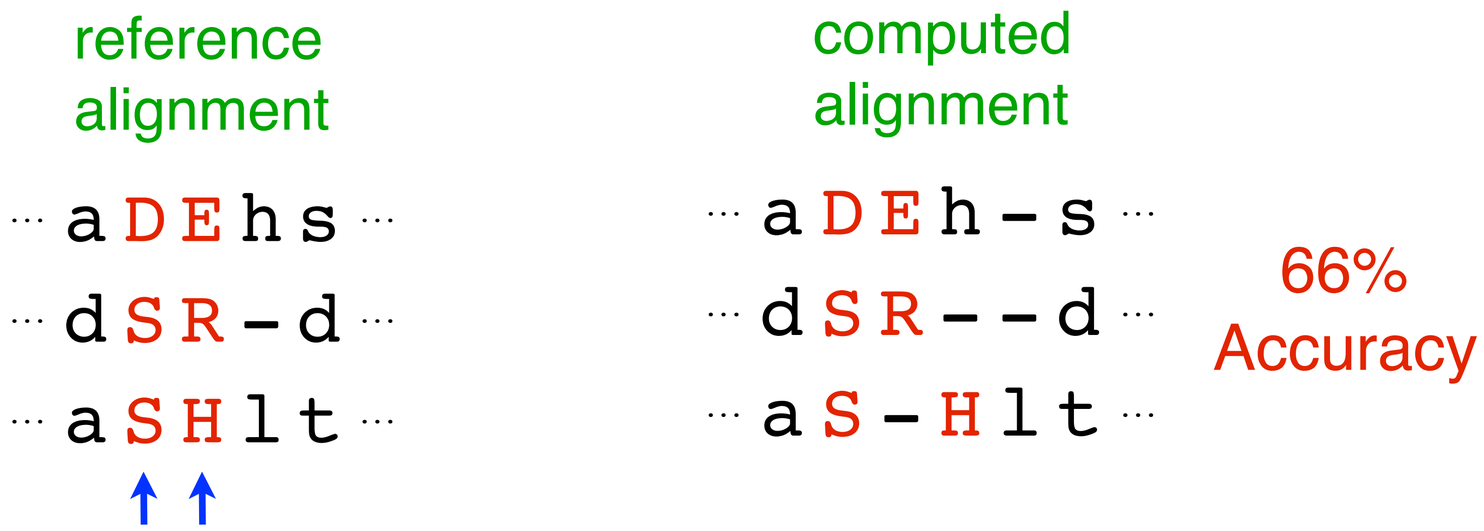

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- uses novel features that are efficient to evaluate,
- efficiently learns the polynomial coefficients from examples.

[RECOMB 2012]

Advisor sets

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[ACM-BCB 2014]

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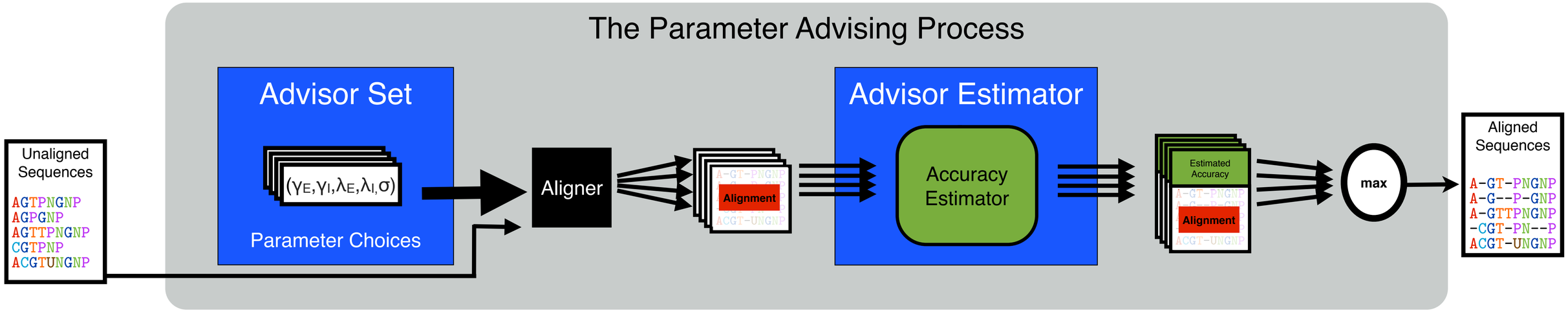
- can be found by integer linear programming,
- can work well with an actual advisor.

[ACM-BCB 2014]

Parameter advising

A parameter advisor has two components:

- an accuracy estimator, and
- a set of candidate parameter choices.



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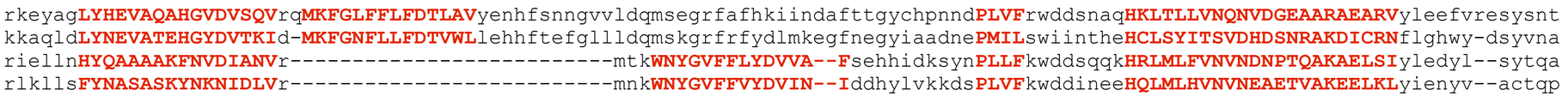
Adaptive local realignment



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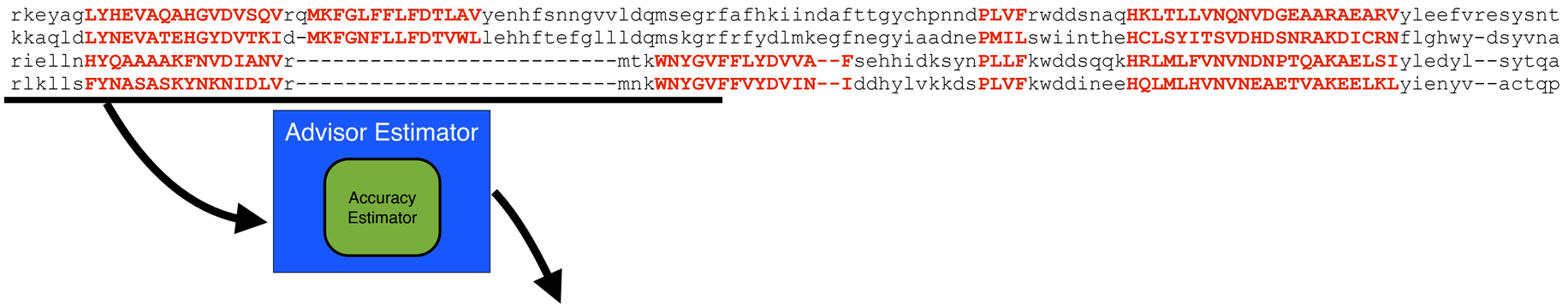

Adaptive local realignment

```
rkeyagLYHEVAQAHGVDVSQVrqMKFGLFFLFDTLAVyenhfsnngvvldqmsegrfafhkiindafttgychpnndPLVFrwddsnaqHKLTLLVNQNVDGEAARAEARVyleefvresysnt
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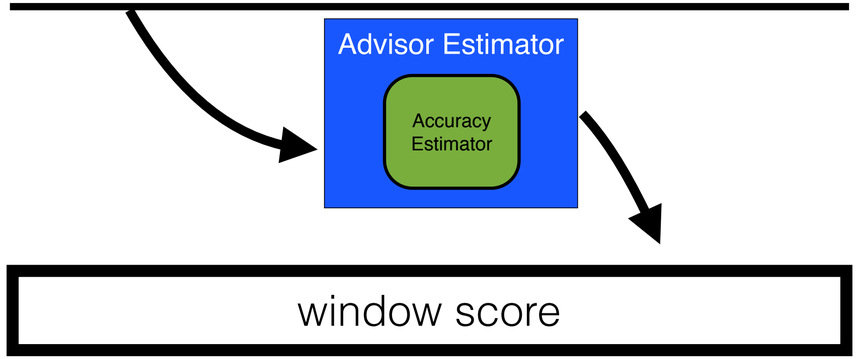

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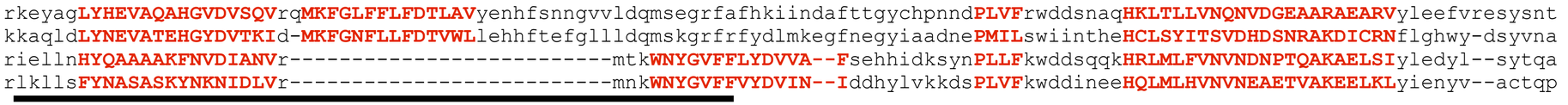

window score

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kkaqldLYNEVATEHGYDVTKId-MKFGNFLLFDTVWLlehhftefgllldqmskgrfrfydlmkegfnegyiaadnePMILswiintheHCLSYITSVDHDSNRAKDICRNflghwy-dsyvna
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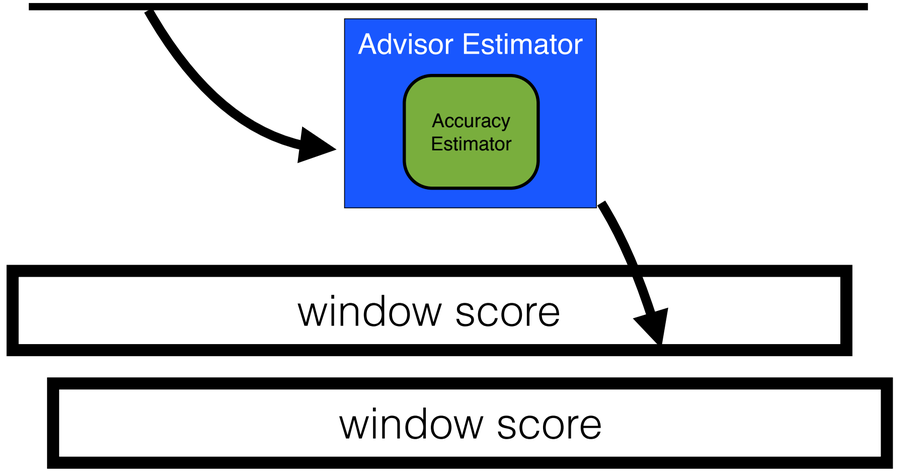

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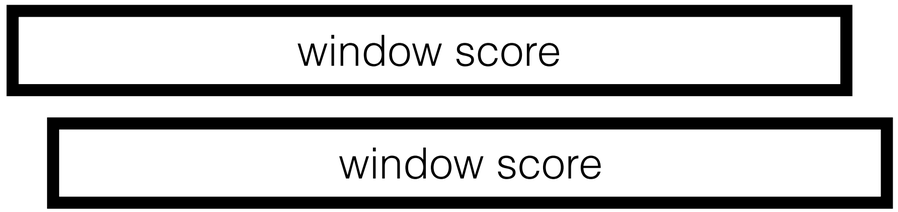

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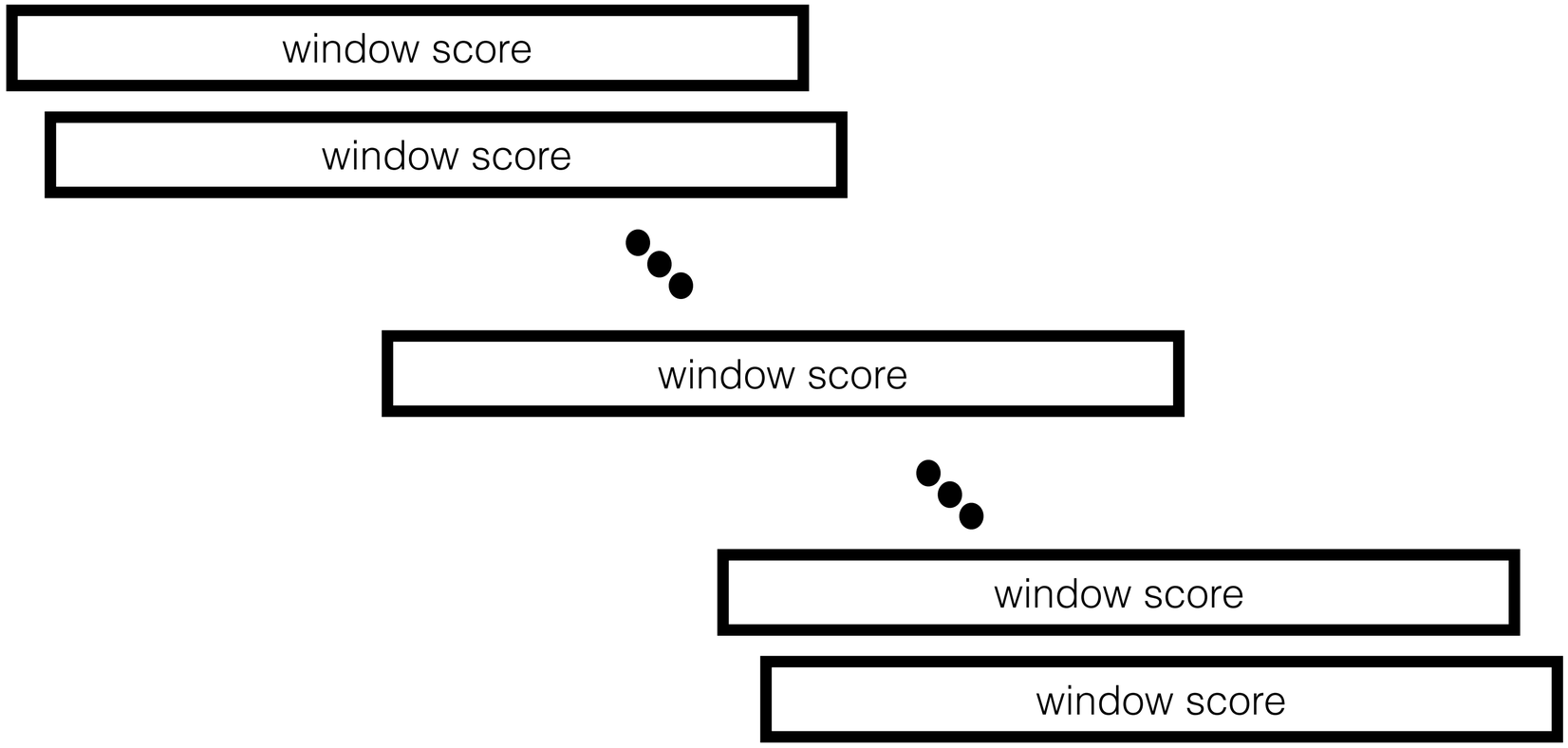

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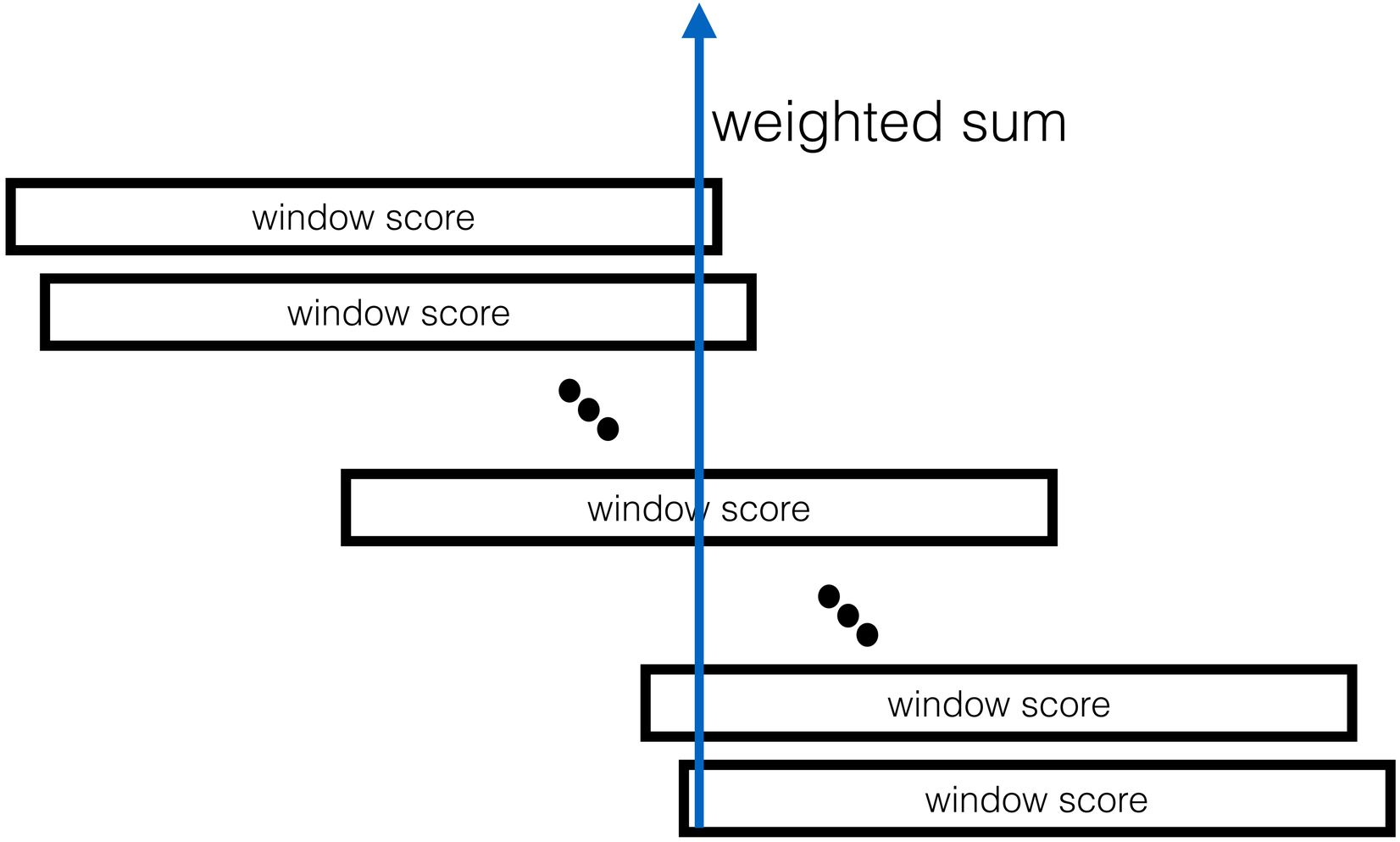

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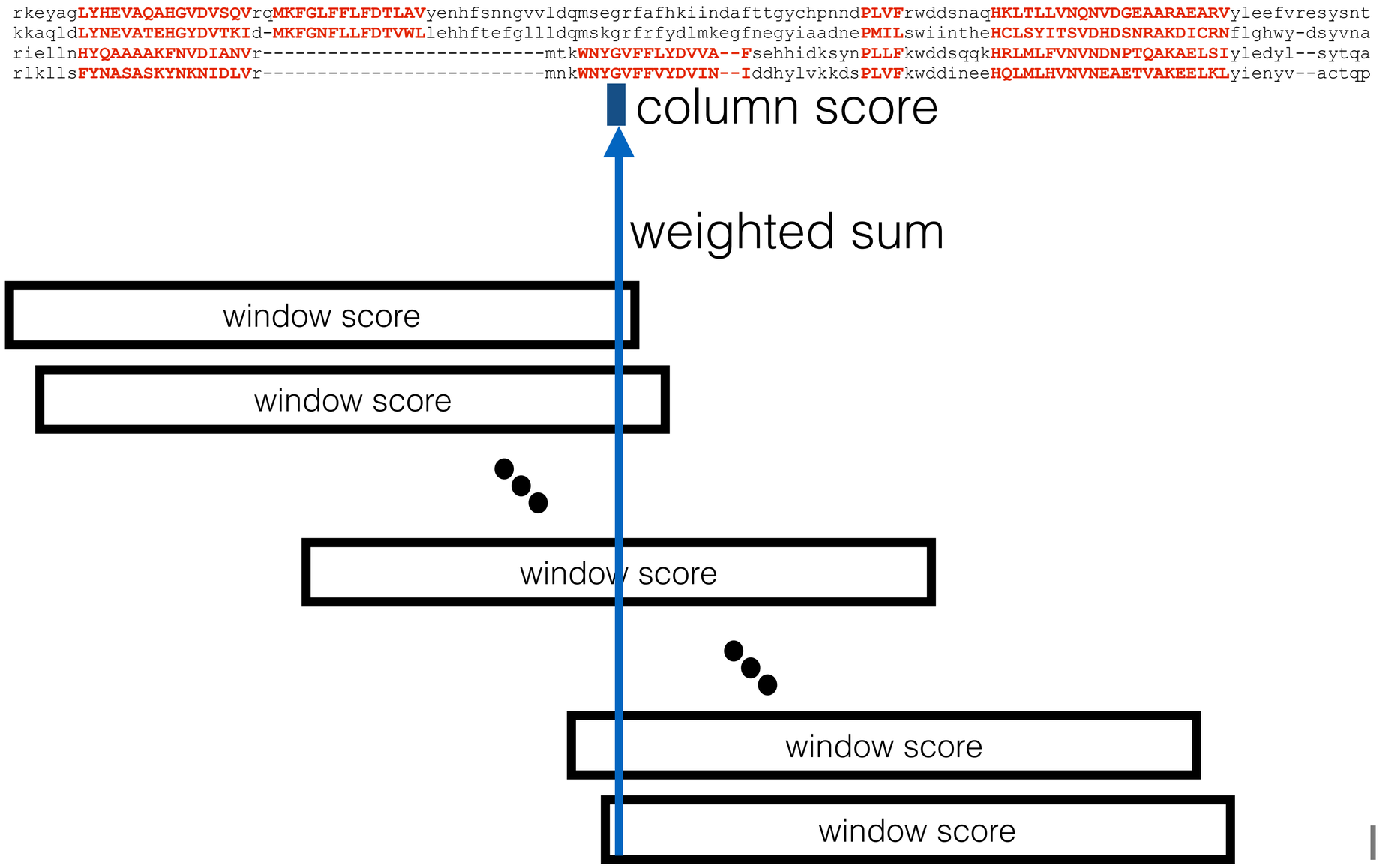

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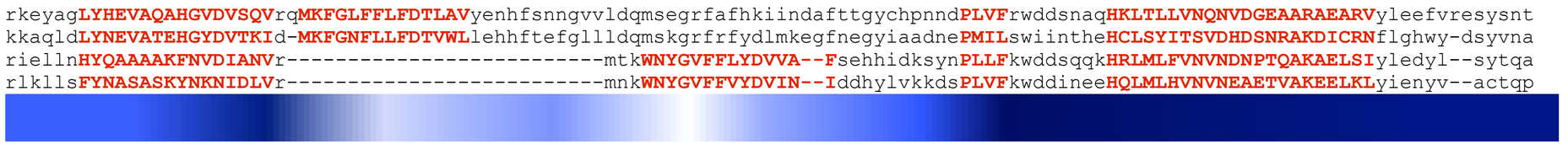

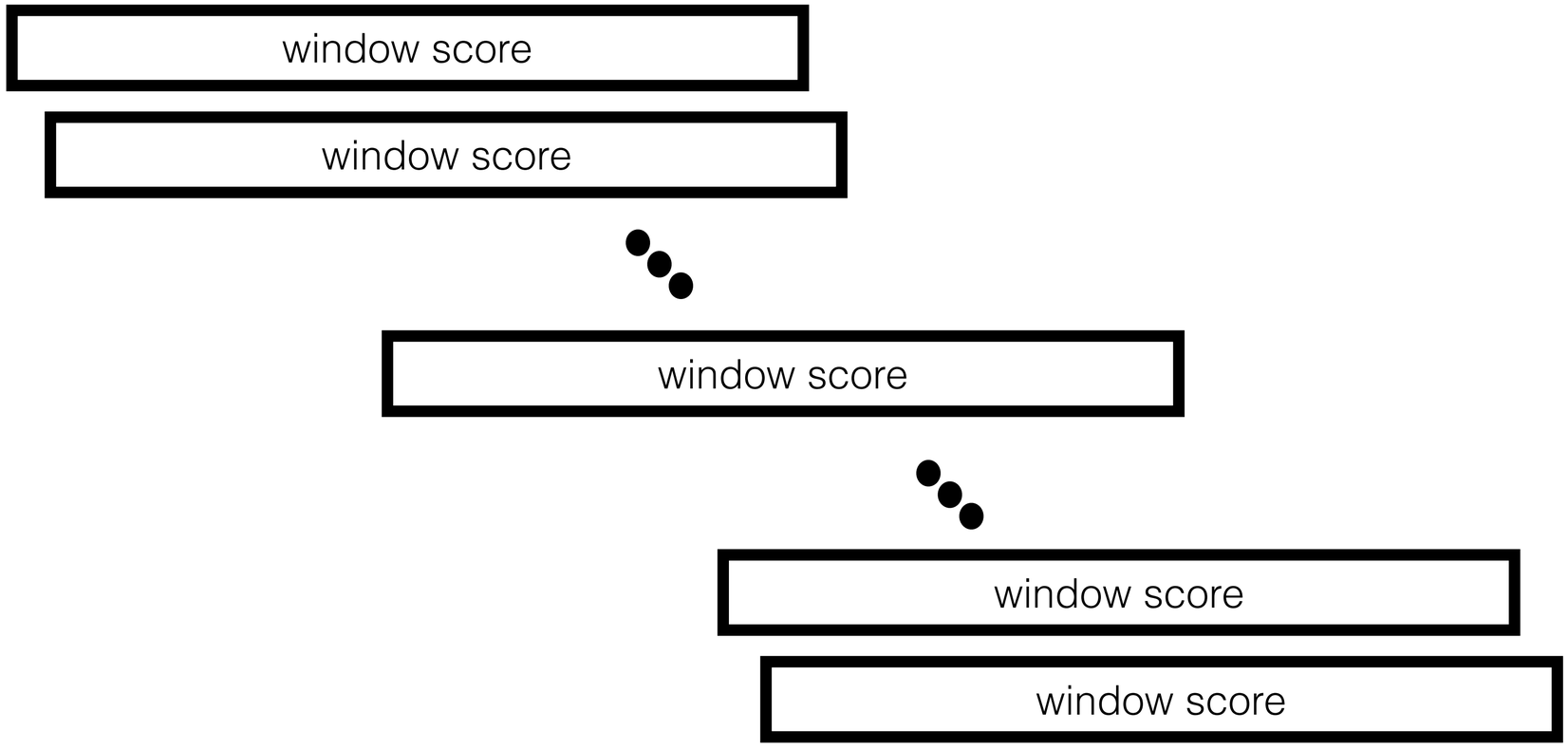

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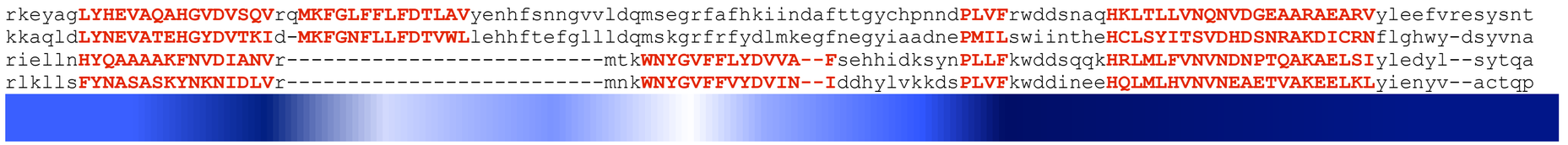

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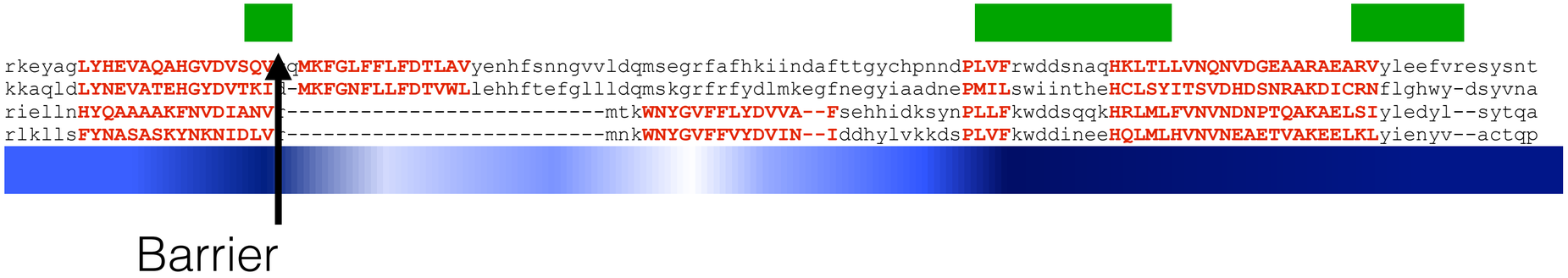

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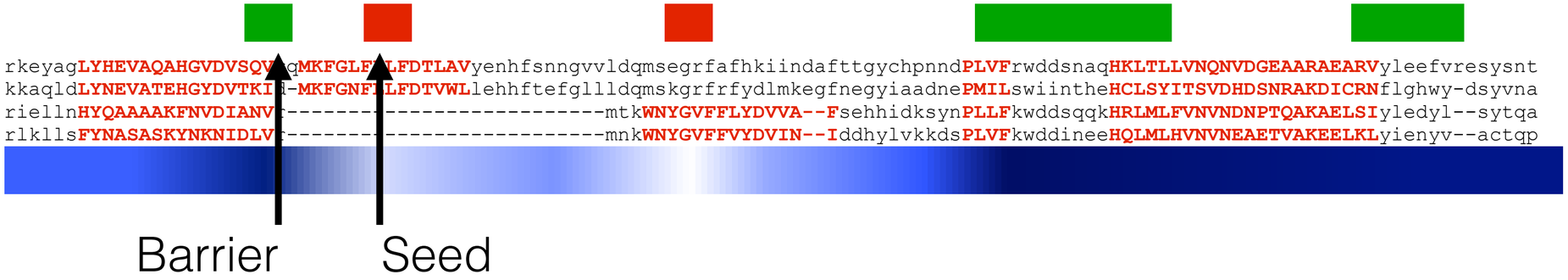

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rielln HYQAAAAKFNVDIANVr-------------------------mtkWNYGVFFLYDVVA--Fsehhidksyn PLLFkwddsqqkHRLMLFVNVNDNPTQAKAELSIyledyl--sytqa
rlklls FYNASASKYNKNIDLVr-------------------------mnkWNYGVFFVYDVIN--Iddhylvkkds PLVFkwddineeHQLMLHVNVNEAETVAKEELKLyienyv--actqp
```
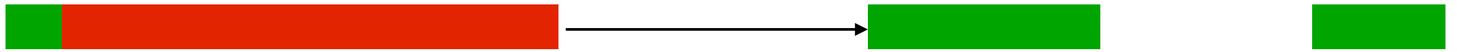

Adaptive local realignment



```
rkeyagLYHEVAQAHGVDVSQVrqMKFGLFFLFDTLAVyenhfsnngvvldqmsegrfafhkiindafttgychpnndPLVFrwddsnaqHKLTLLVNQNVDGEAARAEARVyleefvresysnt
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rielnnHYQAAAAKFNVDIANVr-------------------------mtkWNYGVFFLYDVVA--Fsehhidksyn PLLFkwddsqqkHRLMLFVNVNDNPTQAKAELSIyledyl--sytqa
rlkllsFYNASASKYNKNIDLVr-------------------------mnkWNYGVFFVYDVIN--Iddhylvkkds PLVFkwddineeHQLMLHVNVNEAETVAKEELKLyienyv--actqp
```

Adaptive local realignment

```
rkeyagLYHEVAQAHGVDVSQVrqMKFGLFFLFDTLAVyenhfsnngvvldqmsegrfafhkiindafttgychpnndPLVFrwddsnaqHKLTLLVNQNVDGEAARAEARVyleefvresysnt
kkaqldLYNEVATEHGYDVTKId-MKFGNFLLFDTVWLlehhftefgllldqmskgrfrfydlmkegfnegyiaadnePMILswiintheHCLSYITSVDHDSNRAKDICRNflghwy-dsyvna
rielln HYQAAAAKFNVDIANVr-------------------------mtkWNYGVFFLYDVVA--Fsehhidksyn PLLFkwddsqqkHRLMLFVNVNDNPTQAKAELSIyledyl--sytqa
rlklls FYNASASKYNKNIDLVr-------------------------mnkWNYGVFFVYDVIN--Iddhylvkkds PLVFkwddineeHQLMLHVNVNEAETVAKEELKLyienyv--actqp
```

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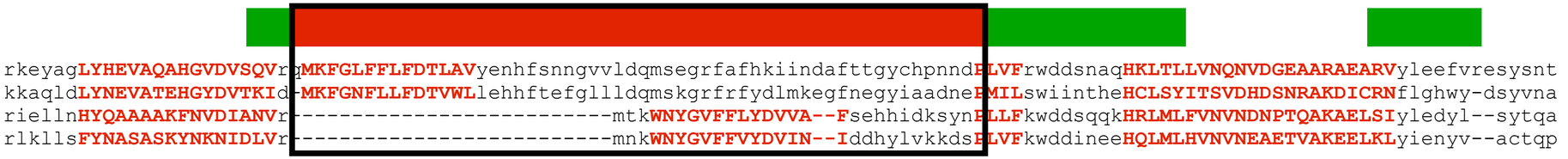

Adaptive local realignment

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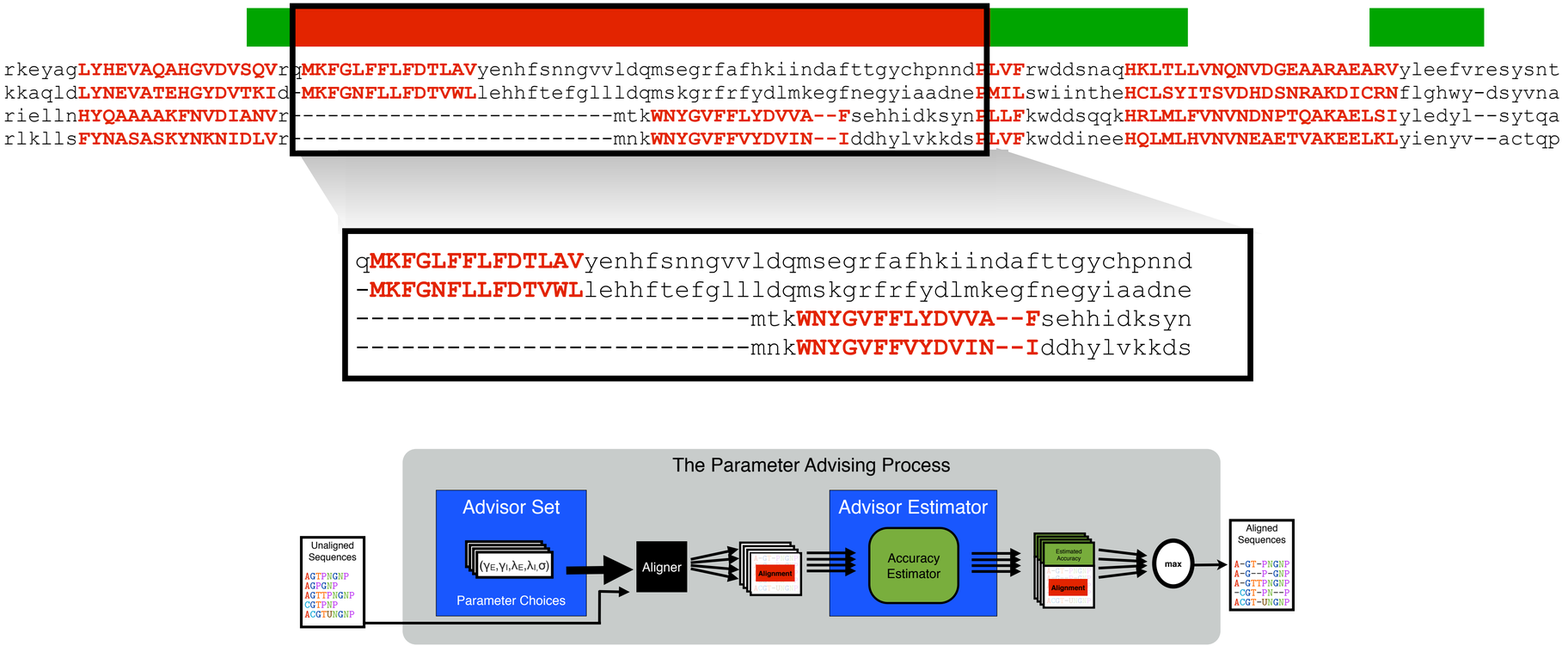

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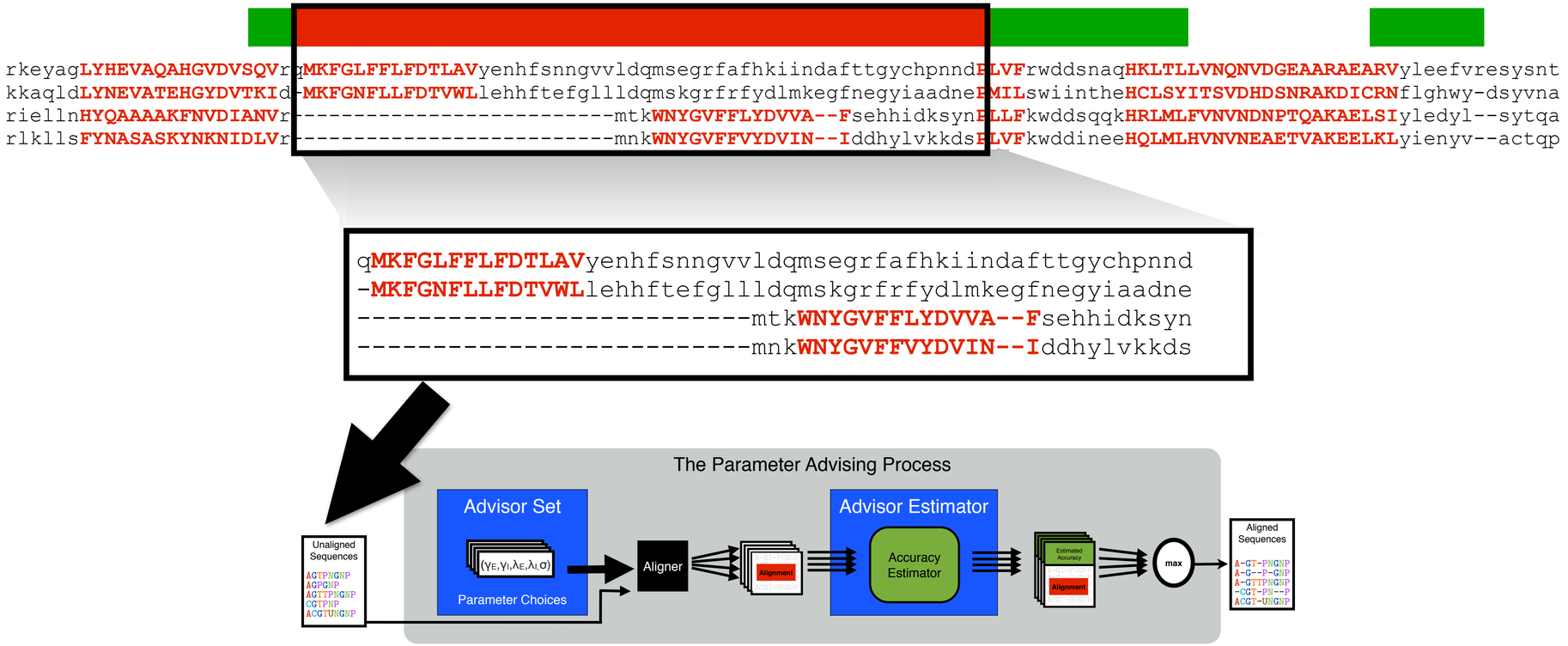
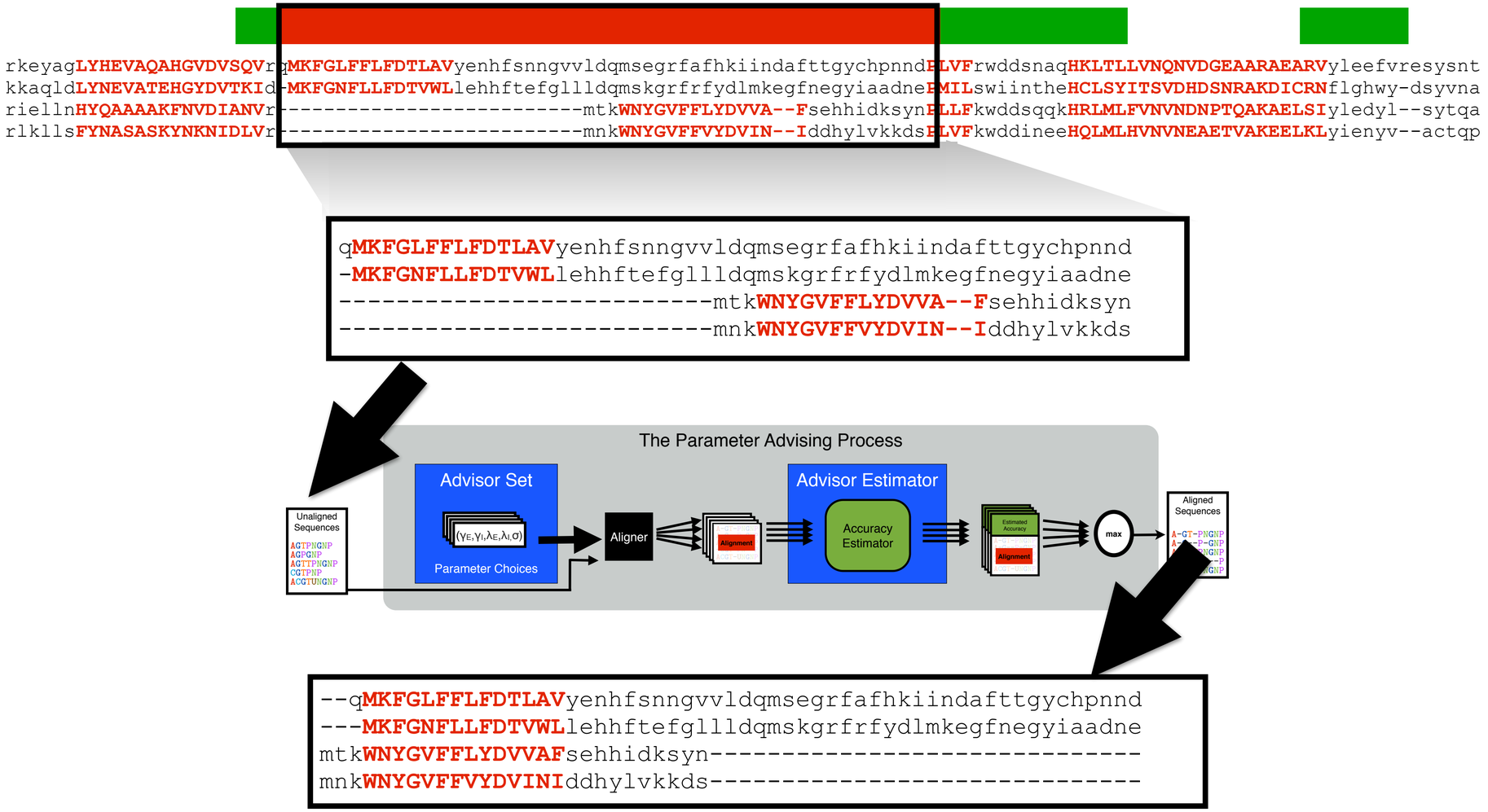


Adaptive local realignment



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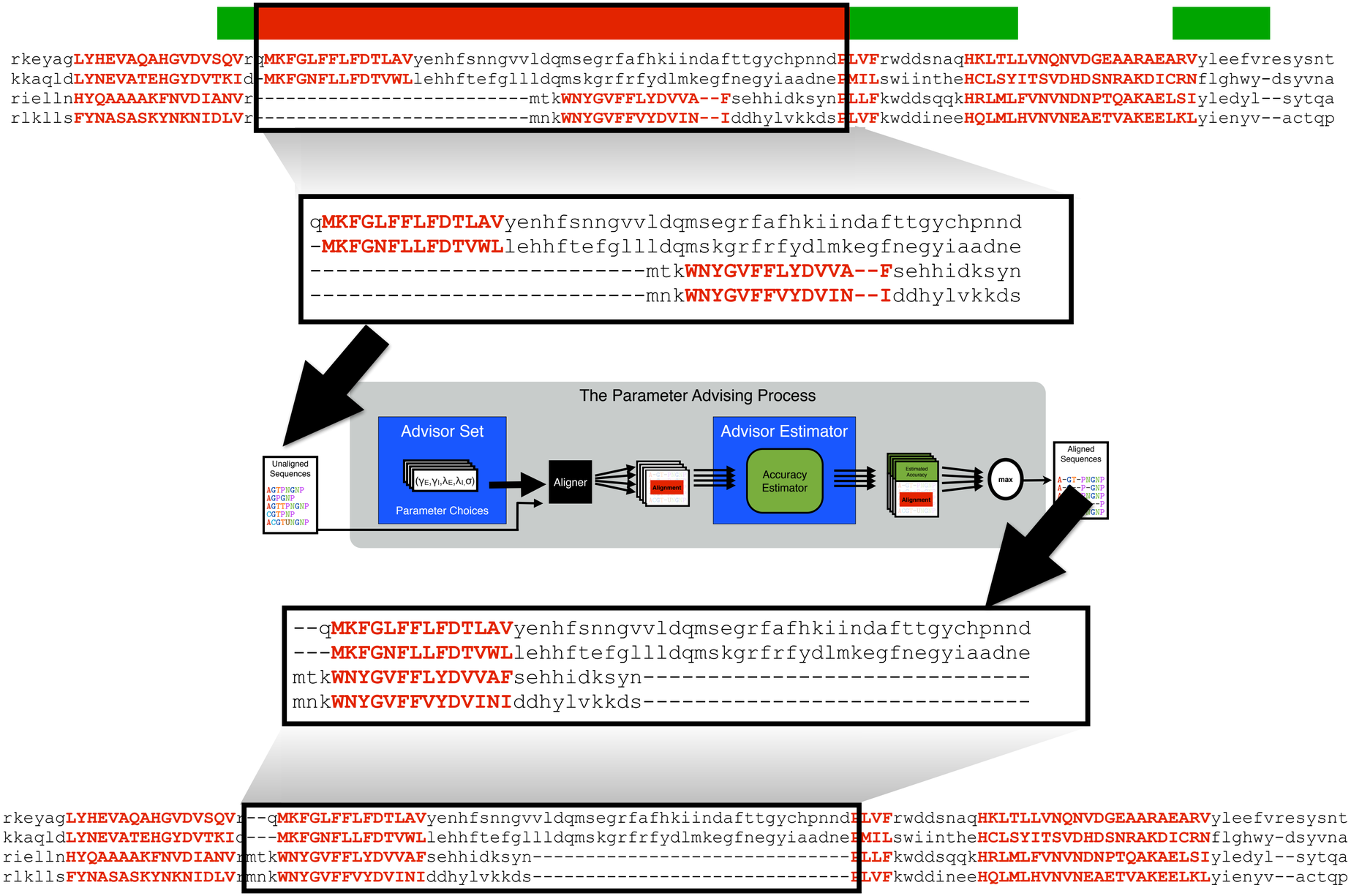


Adaptive local realignment

Accuracy
33%

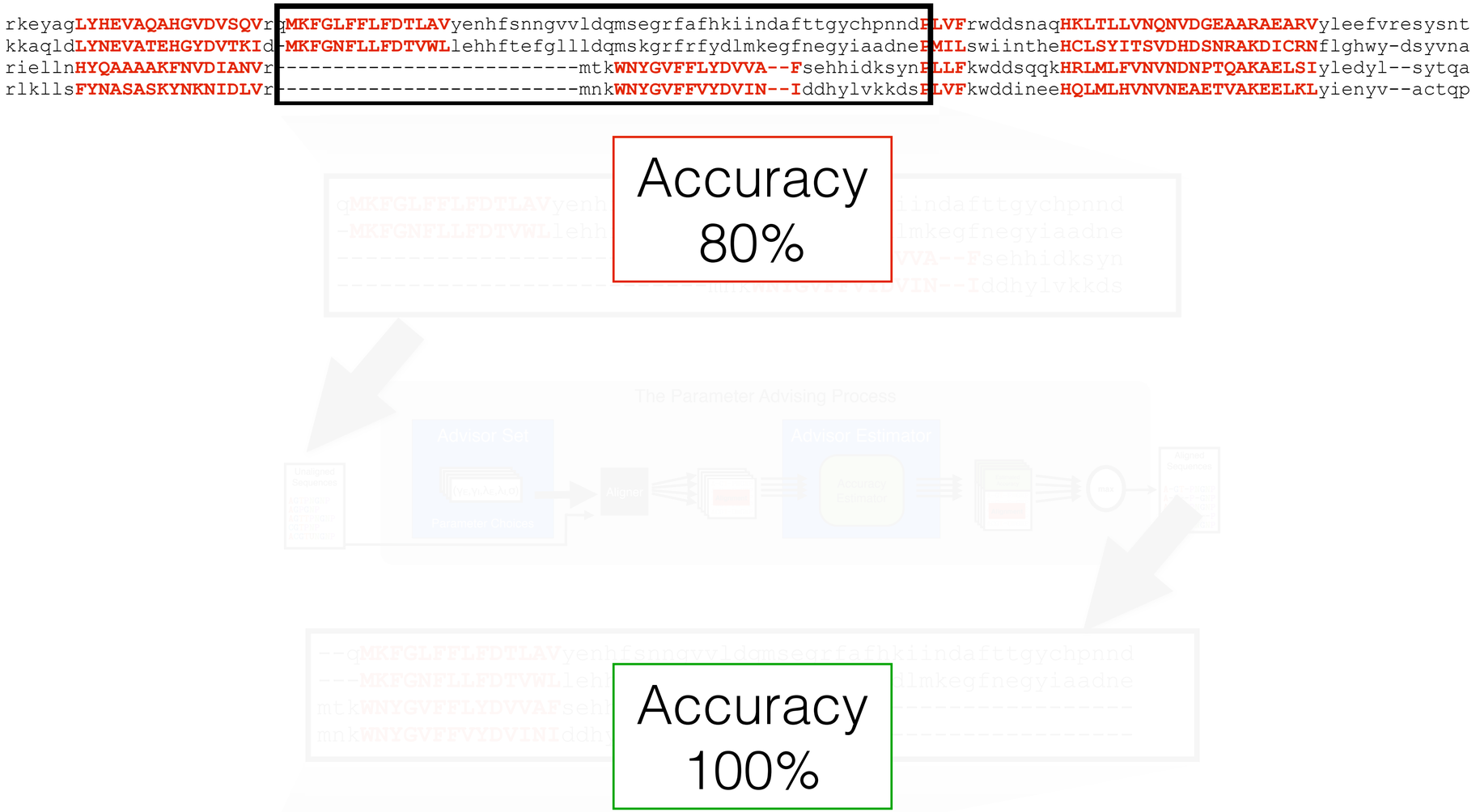
```
qMKFGLFFLFDTLAVyenhfsnngvvldqmsegrfafhkiindafttgychpnnd
-MKFGNFLLFDTVWLlehhftefglllqmskgrfrfydlmkegfnegyiaadne
-------------------------mtkWNYGVFFLYDVVA--Fsehhidksyn
-------------------------mnkWNYGVFFVYDVIN--Iddhylvkkds
```



```
--qMKFGLFFLFDTLAVyenhfsnngvvldqmsegrfafhkiindafttgychpnnd
---MKFGNFLLFDTVWLlehhftefglllqmskgrfrfydlmkegfnegyiaadne
mtkWNYGVFFLYDVVAFsehhidksyn------------------------------
mnkWNYGVFFVYDVINIddhylvkkds------------------------------
```

Accuracy
100%

Adaptive local realignment



Adaptive local realignment

Adaptive local realignment takes as input

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- an initial alignment,

Adaptive local realignment

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- an initial alignment,
- an advisor set,

Adaptive local realignment

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- an initial alignment,
- an advisor set,
- window sizes, and

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And outputs

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- window sizes, and
- column score thresholds.

And outputs

- a new alignment

Adaptive local realignment

Adaptive local realignment takes as input

- an initial alignment,
- an advisor set,
- window sizes, and
- column score thresholds.

And outputs

- a new alignment
- constructed by realigning regions of low estimated accuracy.

Experimental results

We evaluate the accuracy of adaptive local realignment

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- with the `Opal` aligner and `Facet` estimator,

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We evaluate the accuracy of adaptive local realignment

- with the `Opal` aligner and `Facet` estimator,
- on over 800 benchmarks from `BENCH` and `PALI`,
- using 12-fold cross-validation.

Experimental results

We correct for the bias in over-representation of easy-to-align benchmarks.

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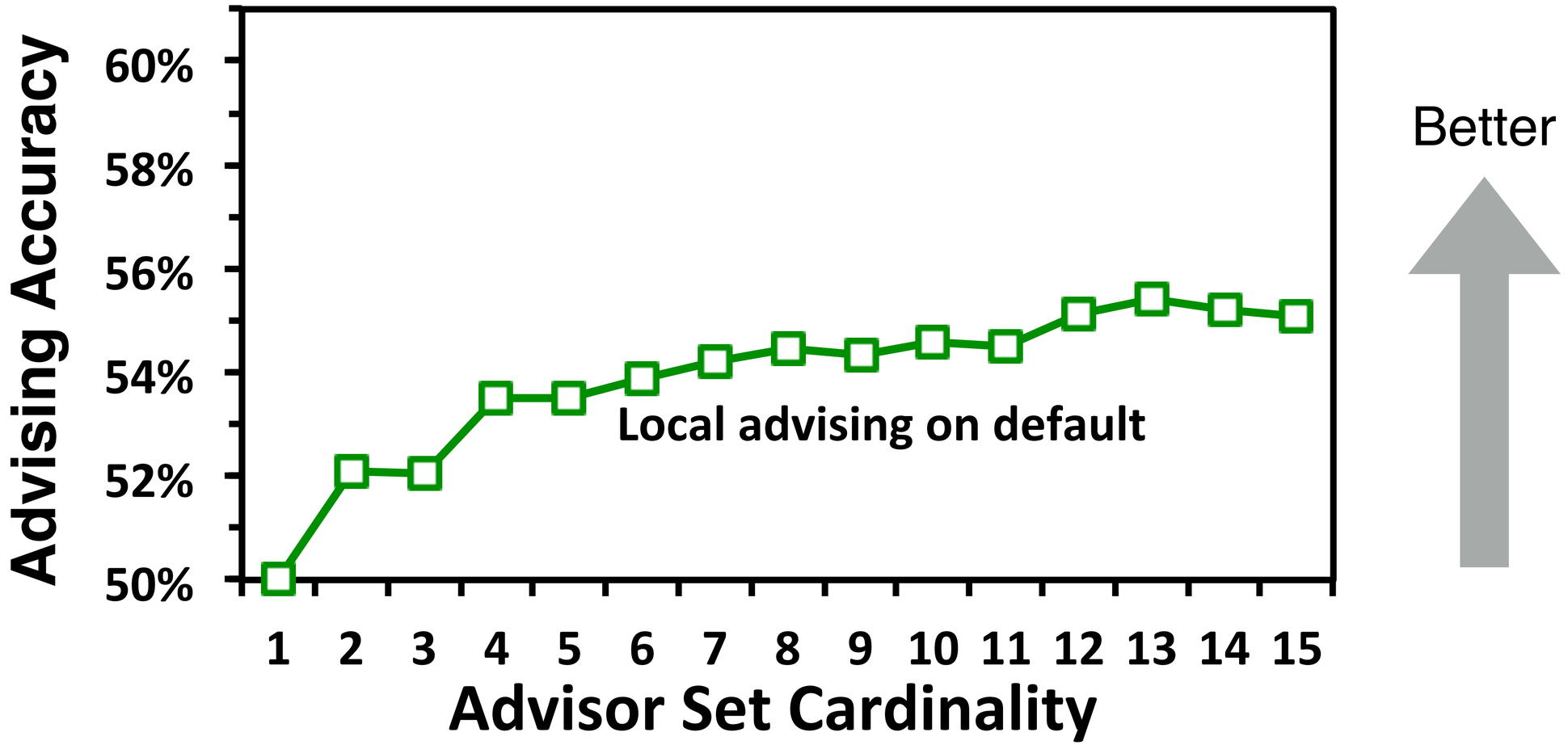
- Split the range of difficulties [0,1] into 10 bins.
- Report advisor accuracy uniformly averaged across bins.

The typical average accuracy is close to 50%.

Experimental results

Average accuracy of advisors versus set cardinality



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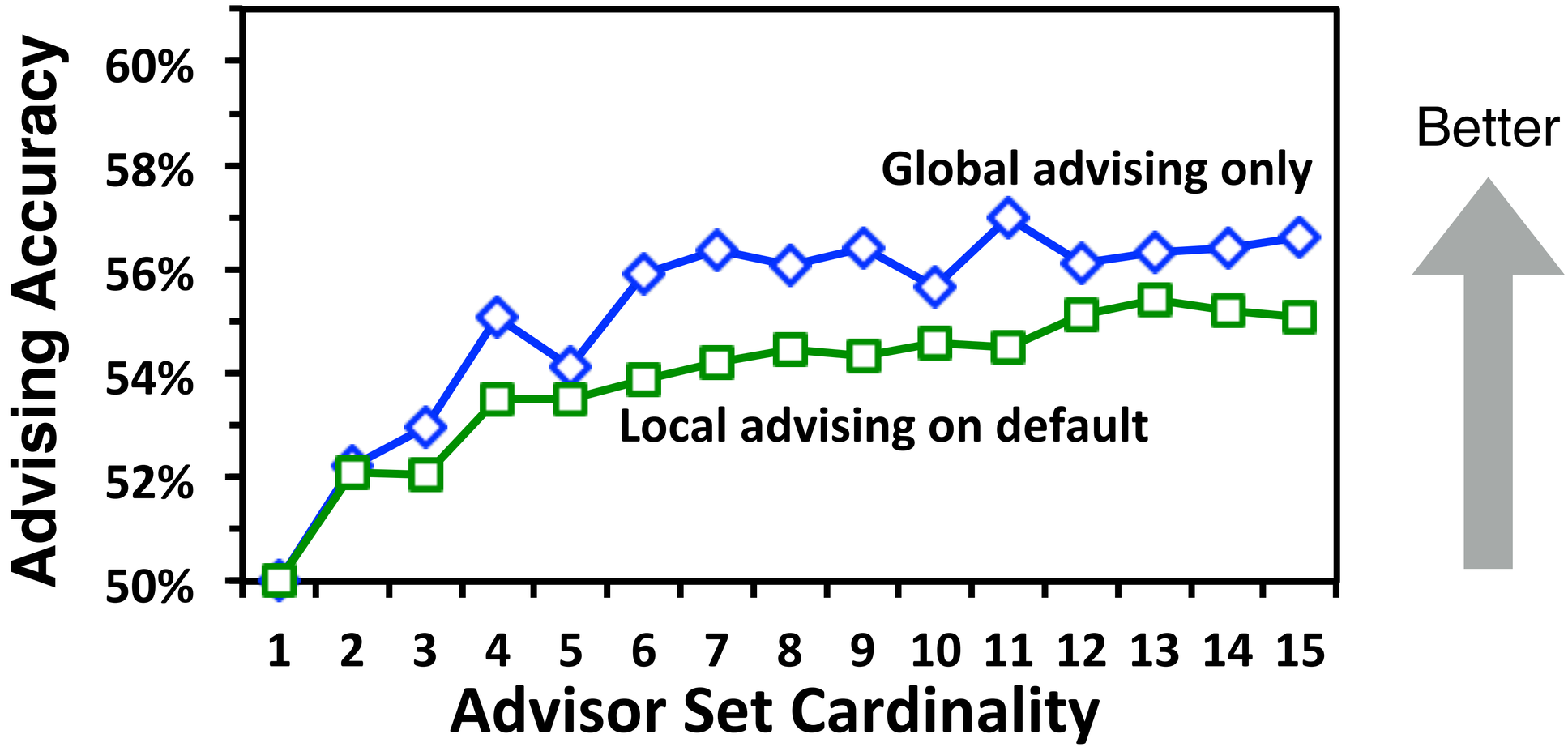

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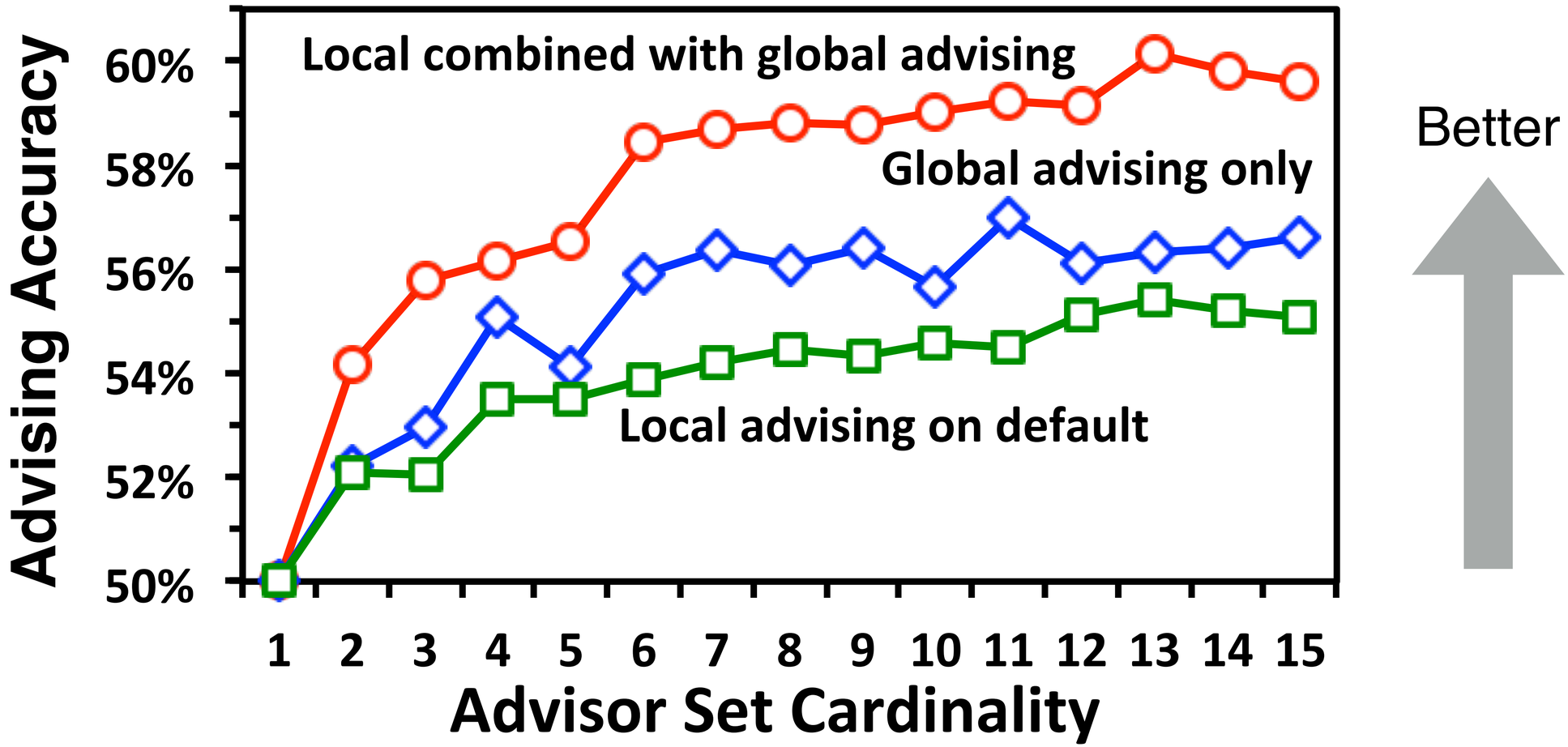

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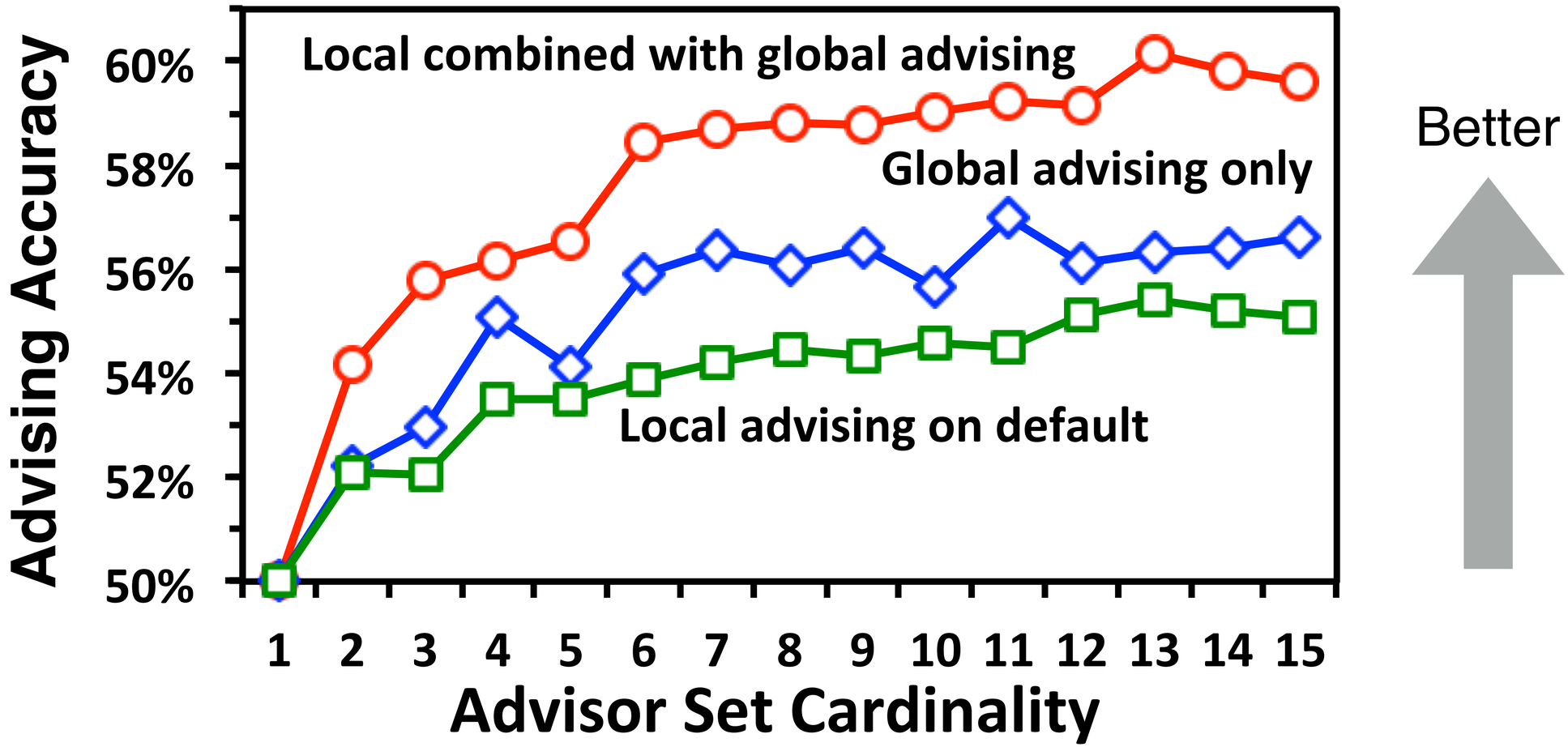
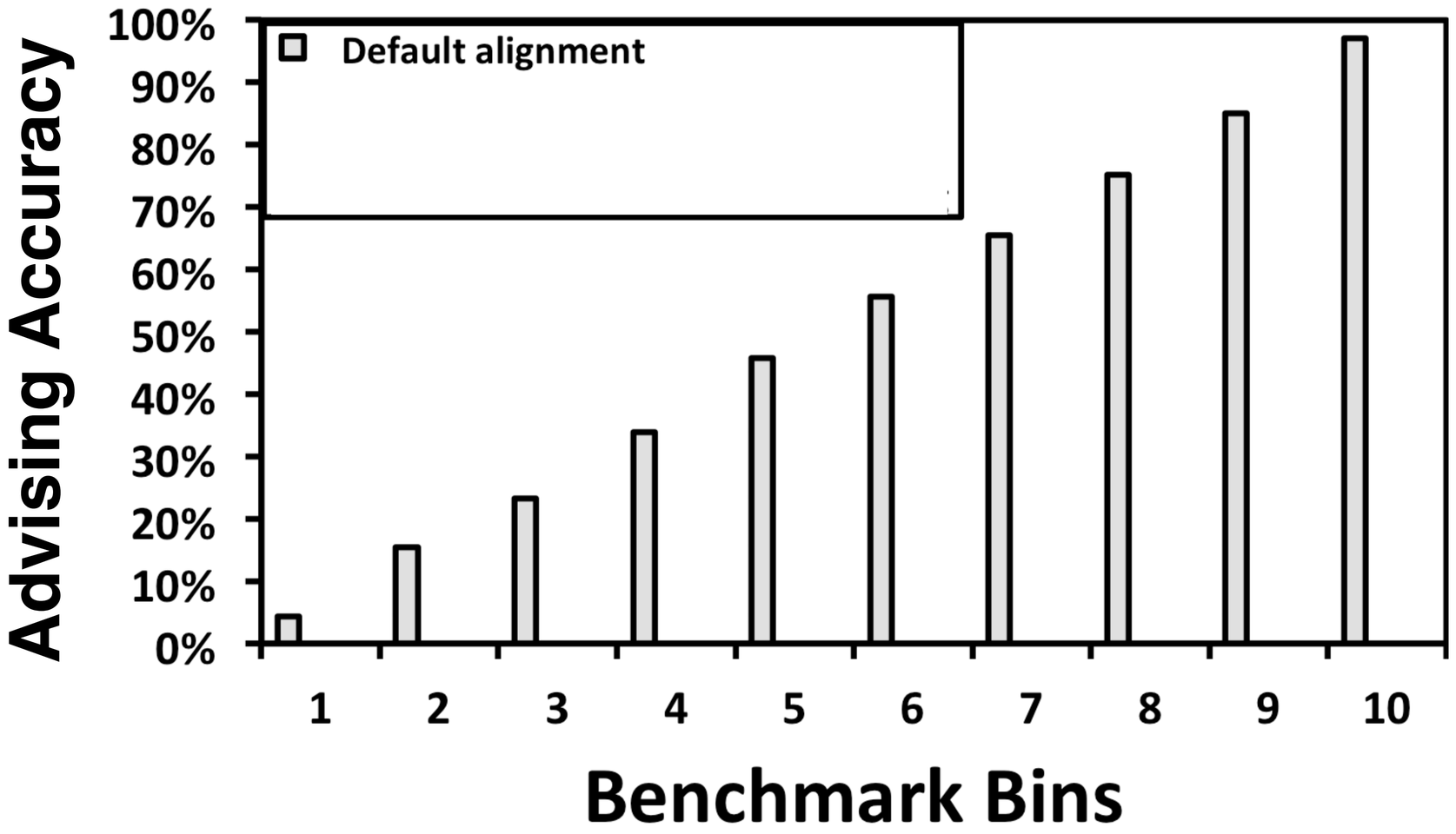


Boosts accuracy by 9% over default parameter choice

Experimental results

Average accuracy of advisors within difficulty bins

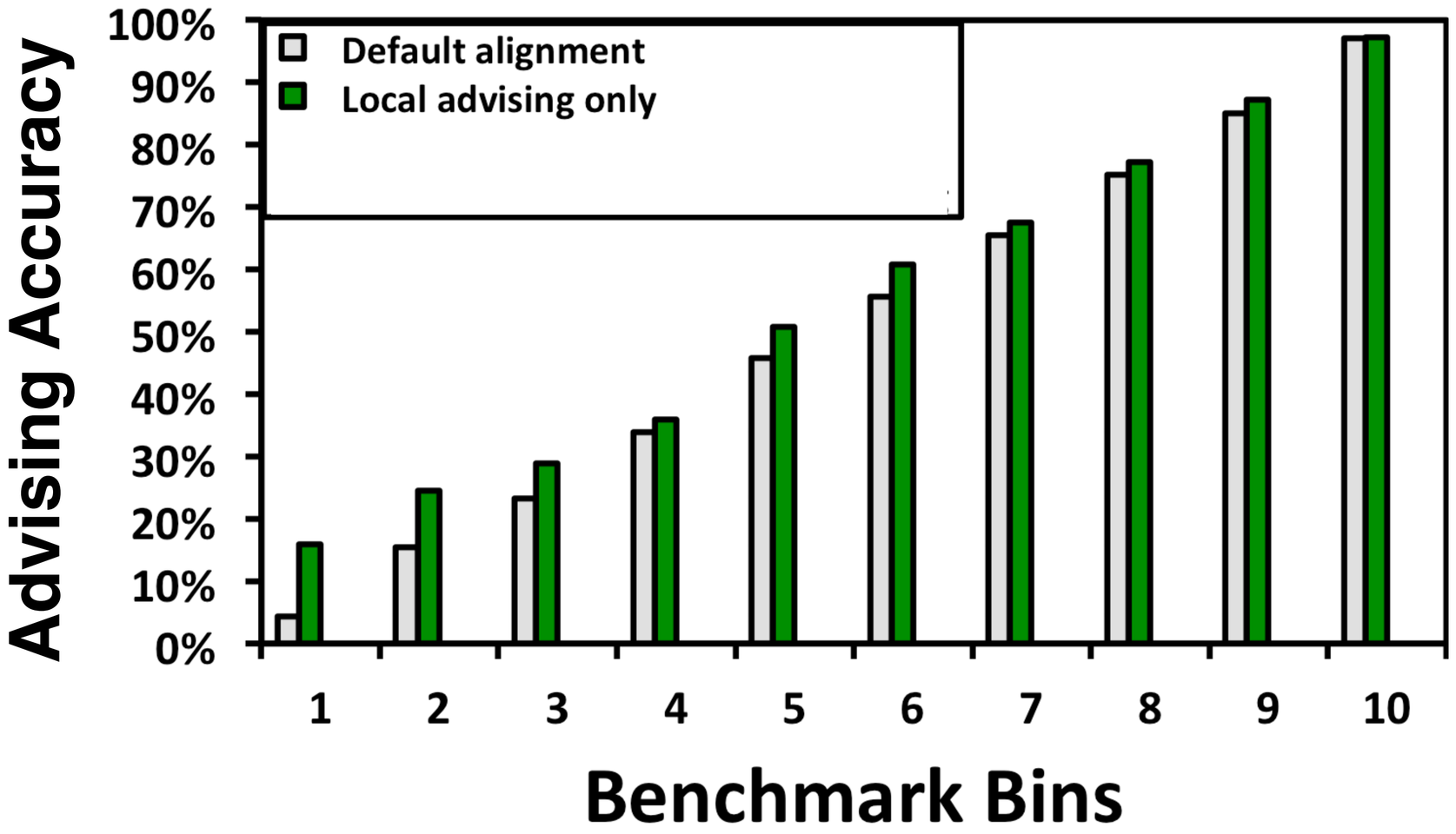


Better

oracle advising set
$k = 10$

Experimental results

Average accuracy of advisors within difficulty bins



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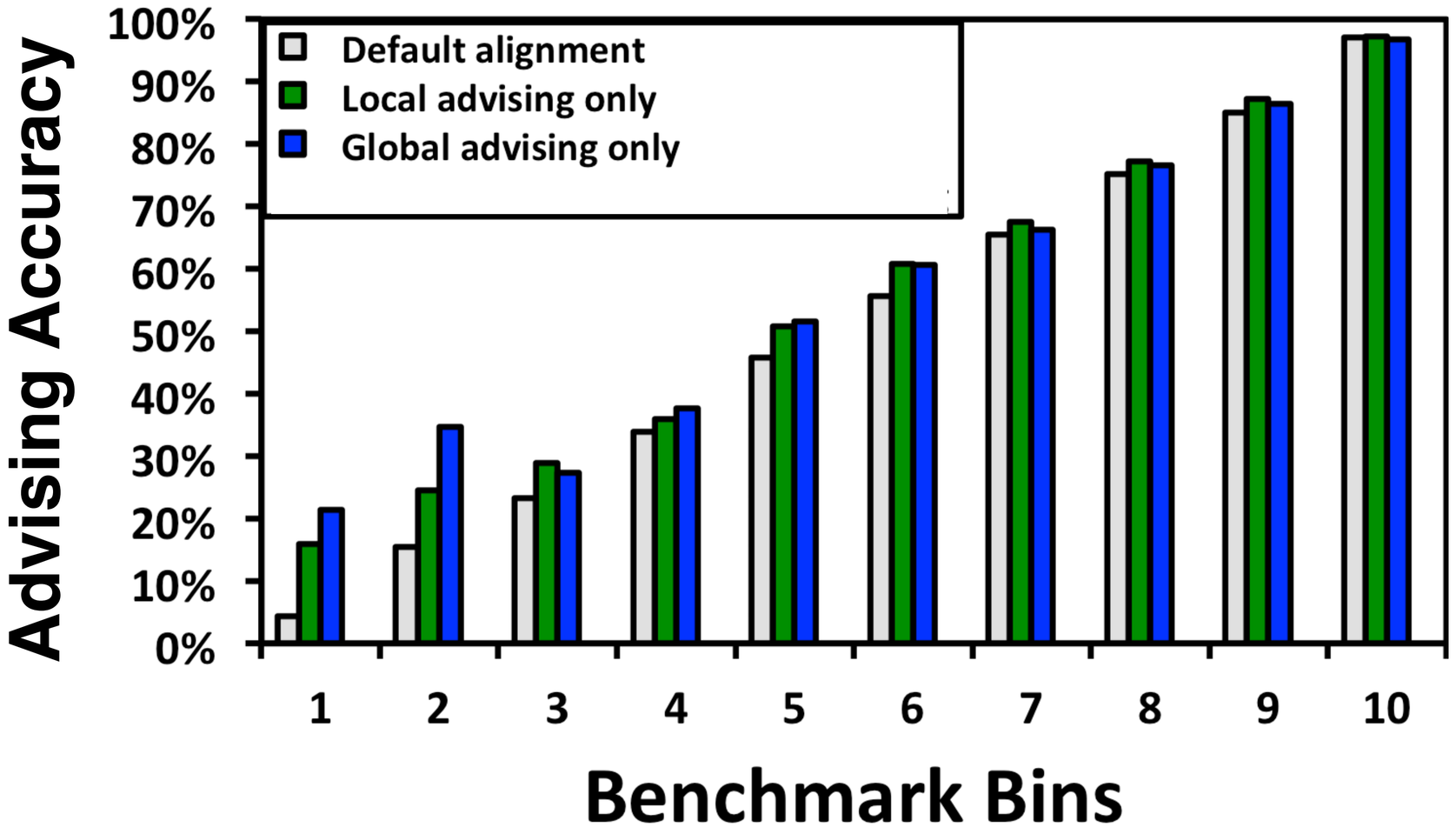

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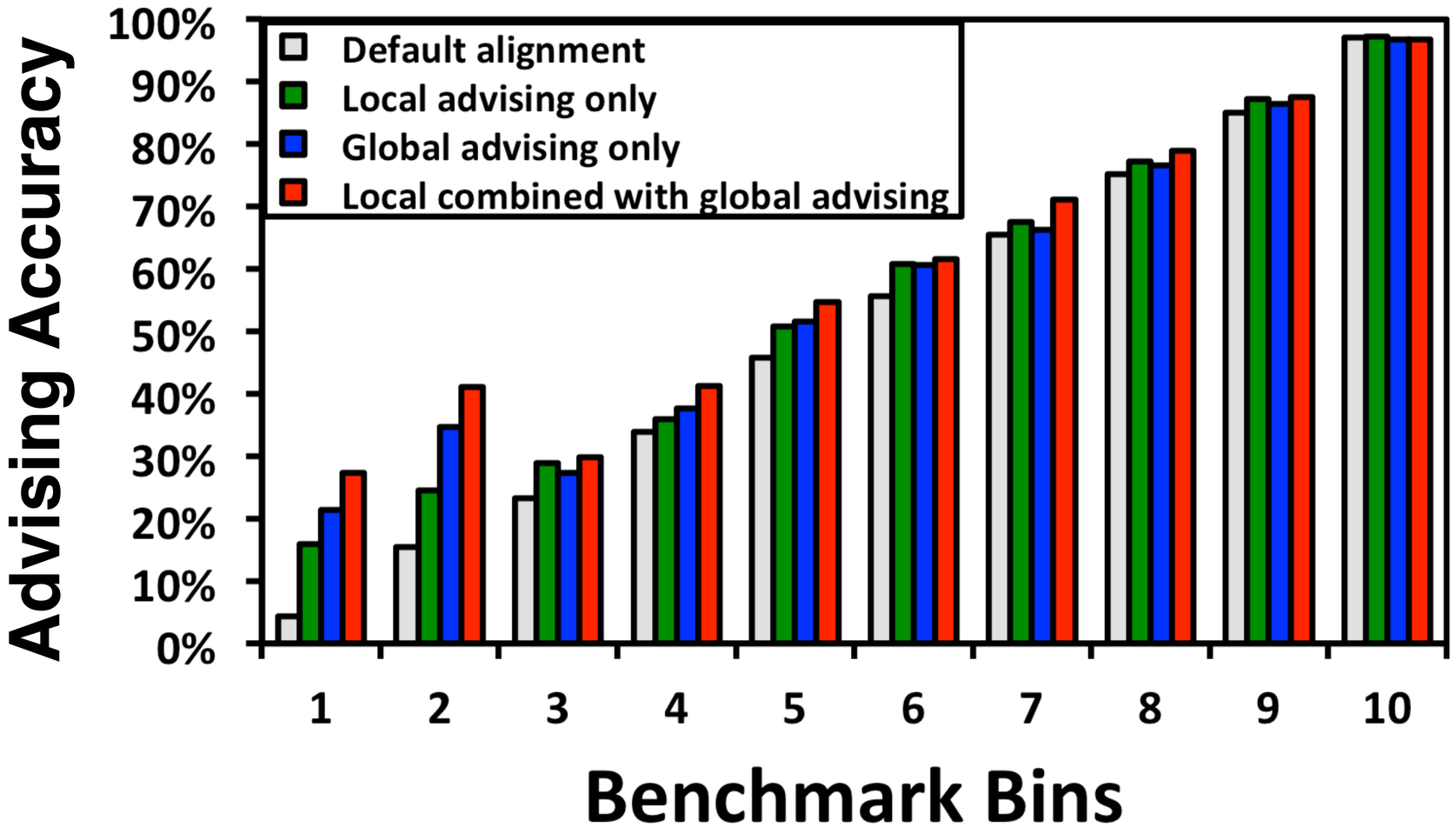

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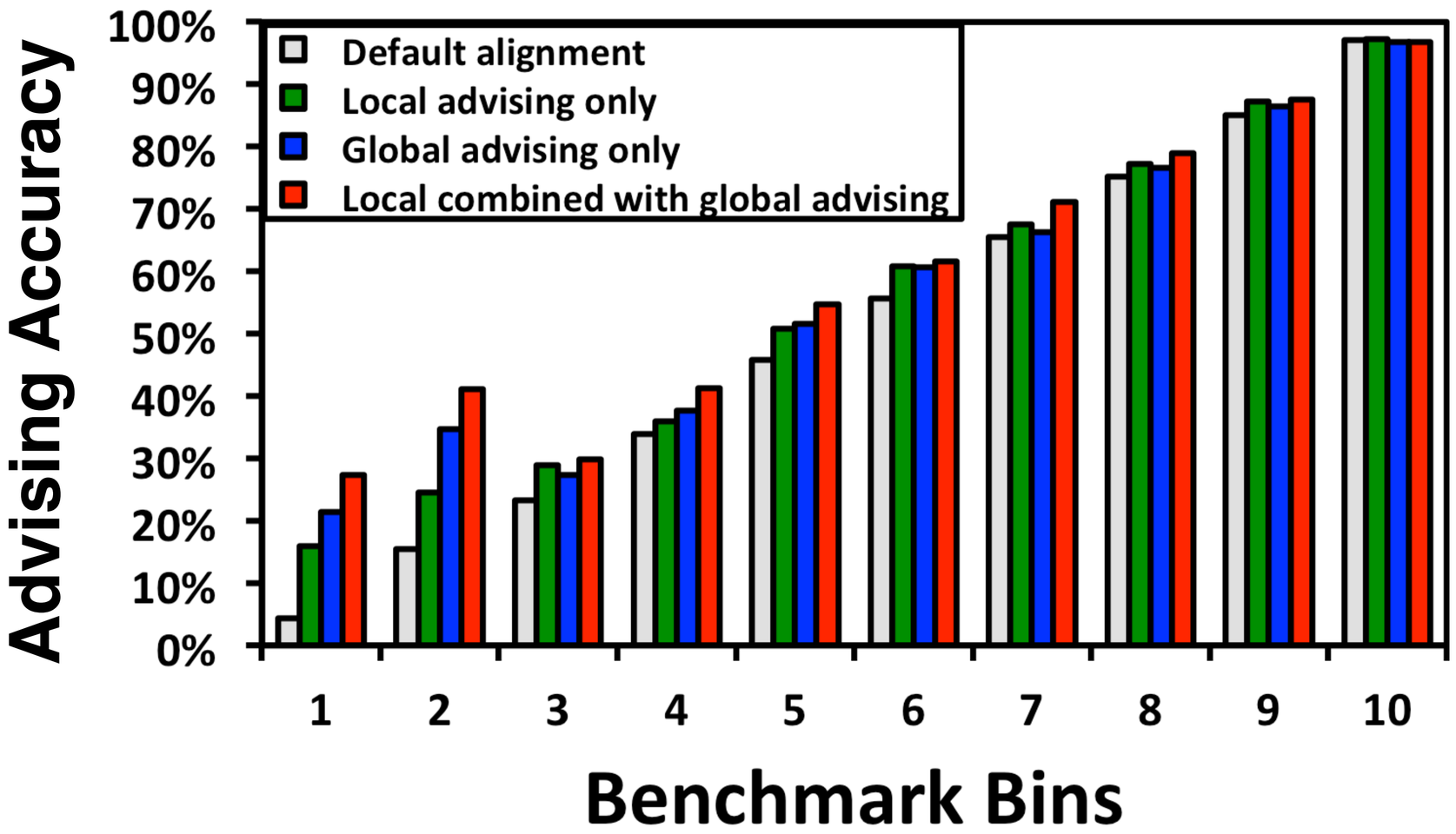

Better

oracle advising set
$k = 10$

Boosts accuracy on the hardest bins by almost 26%

Conclusions

Local adaptive realignment:

Conclusions

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- Uses diverse parameter choices for heterogeneous proteins.

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Conclusions

Local adaptive realignment:

- Uses diverse parameter choices for heterogeneous proteins.
- `Facet` estimator identifies misaligned regions.
- Misaligned regions are polished with parameter advising.
- With global advising, boosts accuracy by up to 26%.

Further research

Promising directions include:

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Promising directions include:

- Finding advisor sets tuned for local realignment.
- Improving the estimator by training on local examples.
- Using an ensemble of aligners to realign regions.

Software distribution

Available for download:

- `Facet` accuracy estimator
- `Opal` aligner with global and local parameter advising
- Parameter sets for advising

`facet.cs.arizona.edu`

Acknowledgments

People

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Travis Wheeler

Carl Kingsford

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- NIH Grant R01HG007104
- Gordon and Betty Moore Foundation Grant GBMF4554

THE UNIVERSITY OF ARIZONA | COMPUTER SCIENCE UASCIENCE

Computational Biology Department | Carnegie Mellon University School of Computer Science

NSF

NATIONAL INSTITUTES OF HEALTH

GORDON AND BETTY MOORE FOUNDATION

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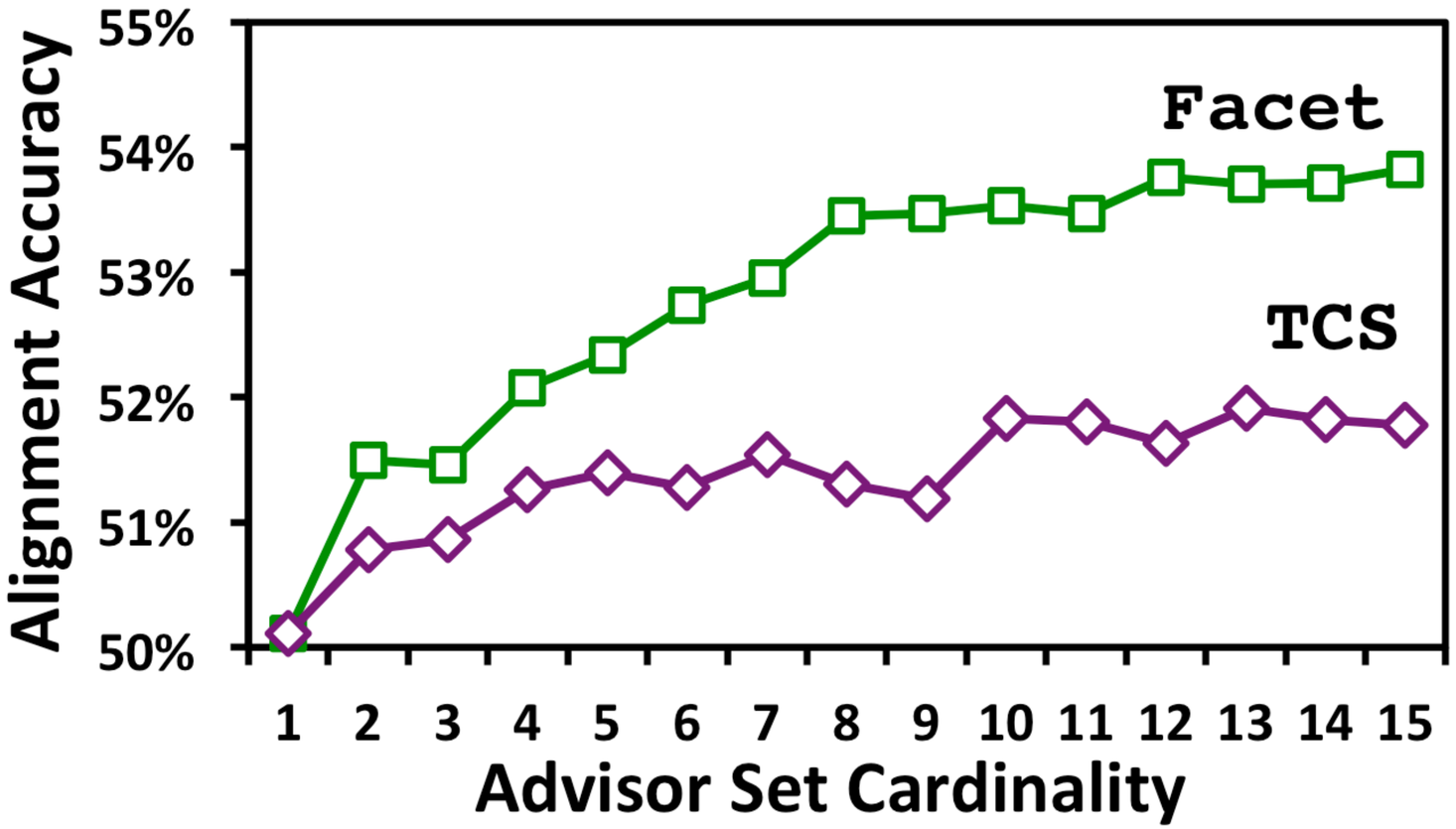
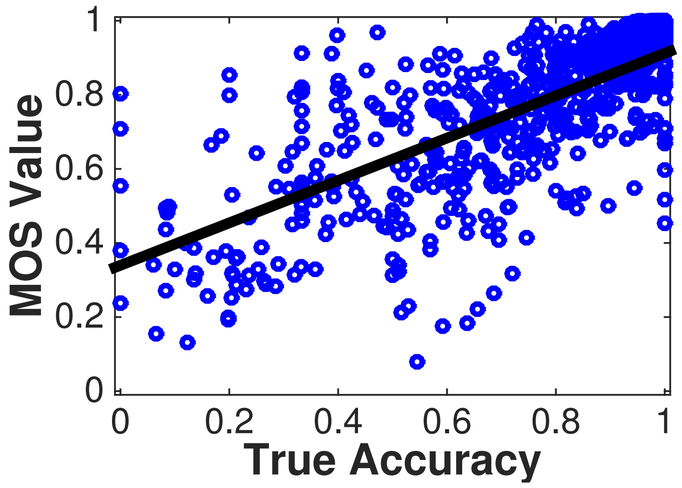


Better

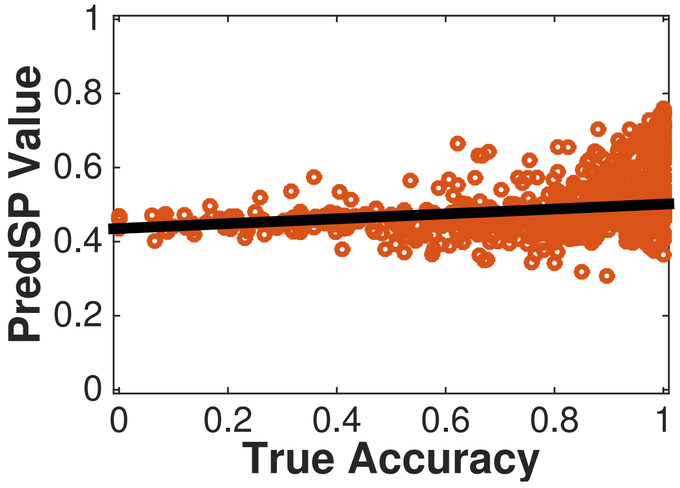
`Facet` outperforms `TCS` for adaptive local realignment

Accuracy estimation

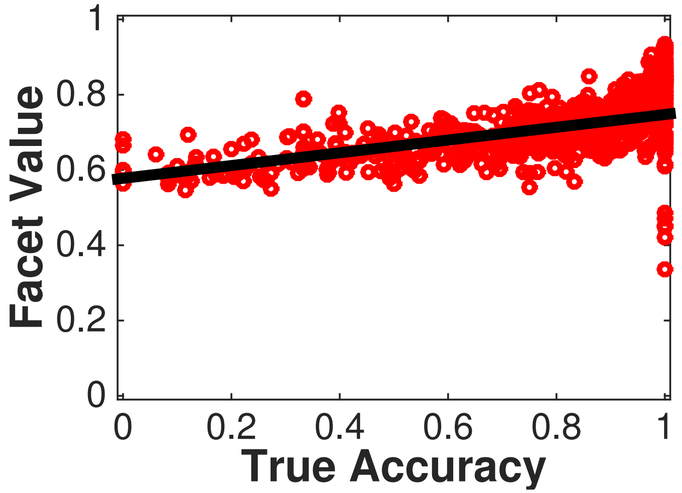
For parameter advising, an estimator should have high slope and low spread.



high slope,
high spread



low slope,
low spread



medium slope,
low spread

Facet's slope and spread is best for advising