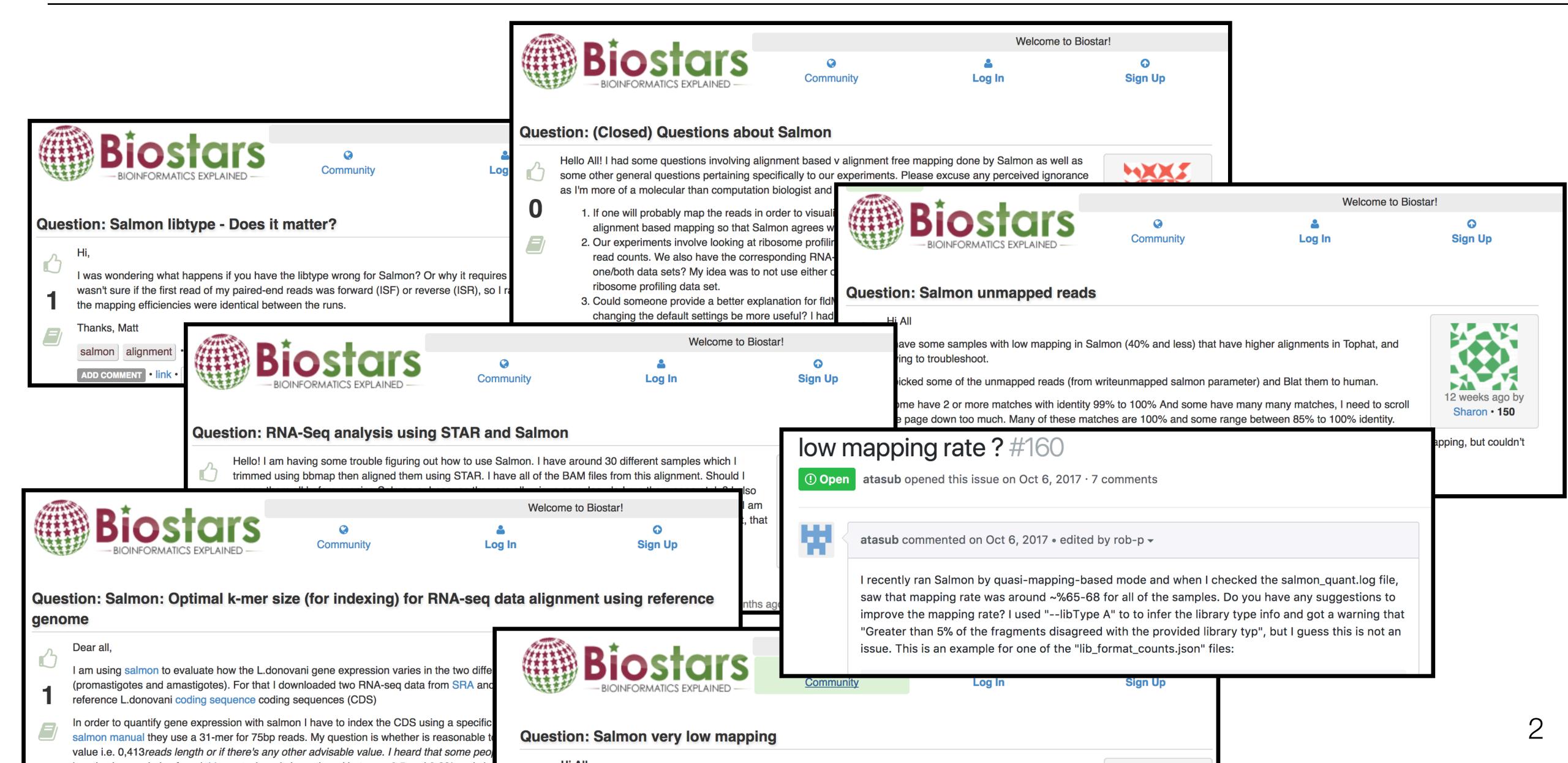
Building an automated bioinformatician: More accurate, large-scale genomic discovery using parameter advising

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School of Computer Science

Tunable parameters



Tunable parameters

```
Quant
Perform dual-phase, mapping-based estimation of
transcript abundance from RNA-seq reads
salmon quant options:
basic options:
  -v [ --version ]
                                       print version string
  -h [ --help ]
                                       produce help message
 -i [ --index ] arg
                                       Salmon index
 -l [ --libType ] arg
                                       Format string describing the library type
 -r [ --unmatedReads ] arg
                                       List of files containing unmated reads of (e.g. single-end reads)
 -1 [ --mates1 ] arg
                                       File containing the #1 mates
 -2 [ --mates2 ] arg
                                       File containing the #2 mates
 -o [ --output ] arg
                                       Output quantification file.
                                       [Quasi-mapping mode only] : Discard orphan mappings in quasi-mapping mode. If this flag is passed then only paired mappings
  --discardOrphansQuasi
                                       will be considered toward quantification estimates. The default behavior is to consider orphan mappings if no valid paired
                                       mappings exist. This flag is independent of the option to write the orphaned mappings to file (--writeOrphanLinks).
                                       [FMD-mapping mode only] : Consider orphaned reads as valid hits when performing lightweight-alignment. This option will
  --allowOrphansFMD
                                       increase sensitivity (allow more reads to map and more transcripts to be detected), but may decrease specificity as orphaned
                                       alignments are more likely to be spurious.
                                       Perform sequence-specific bias correction.
  --seqBias
  --gcBias
                                       [beta for single-end reads] Perform fragment GC bias correction
  -p [ --threads ] arg
                                       The number of threads to use concurrently.
  --incompatPrior arg
                                       This option sets the prior probability that an alignment that disagrees with the specified library type (--libType) results
                                       from the true fragment origin. Setting this to 0 specifies that alignments that disagree with the library type should be
                                       "impossible", while setting it to 1 says that alignments that disagree with the library type are no less likely than those
                                       that do
 -g [ --geneMap ] arg
                                       File containing a mapping of transcripts to genes. If this file is provided Salmon will output both quant.sf and
                                       quant.genes.sf files, where the latter contains aggregated gene-level abundance estimates. The transcript to gene mapping
                                       should be provided as either a GTF file, or a in a simple tab-delimited format where each line contains the name of a
                                       transcript and the gene to which it belongs separated by a tab. The extension of the file is used to determine how the file
                                       should be parsed. Files ending in '.gtf', '.gff' or '.gff3' are assumed to be in GTF format; files with any other extension
                                       are assumed to be in the simple format. In GTF / GFF format, the "transcript_id" is assumed to contain the transcript
                                       identifier and the "gene_id" is assumed to contain the corresponding gene identifier.
  -z [ --writeMappings ] [=arg(=-)]
                                       If this option is provided, then the quasi-mapping results will be written out in SAM-compatible format. By default, output
                                       will be directed to stdout, but an alternative file name can be provided instead.
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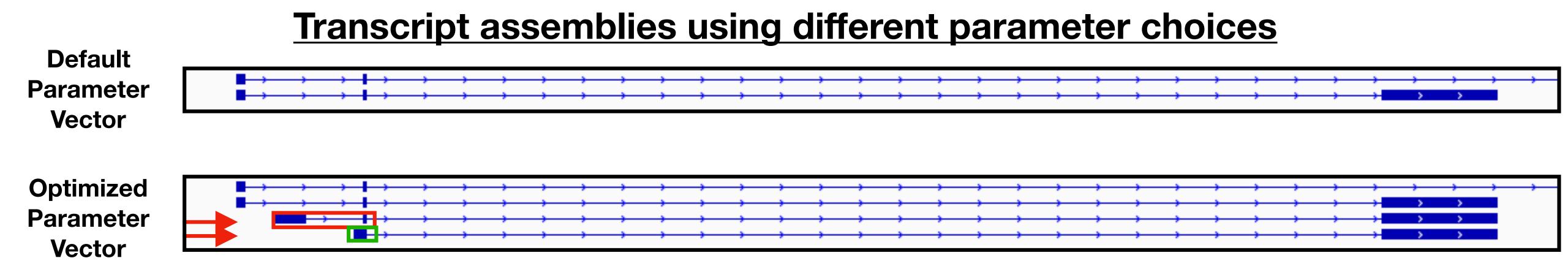
If you're using Salmon on a metagenomic dataset, consider setting this flag to disable parts of the abundance, estimation model

--reduceGCMemory If this option is selected, a more memory efficient (but slightly slower) representation is used to compute fragment GC content. Enabling this will reduce memory usage, but can also reduce speed. However, the results themselves will remain the same. --biasSpeedSamp arg The value at which the fragment length PMF is down-sampled when evaluating sequence-specific & GC fragment bias. Larger values speed up effective length correction, but may decrease the fidelity of bias modeling results. --strictIntersect Modifies how orphans are assigned. When this flag is set, if the intersection of the quasi-mappings for the left and right is empty, then all mappings for the left and all mappings for the right read are reported as orphaned quasi-mappings --fldMax arg The maximum fragment length to consider when building the empirical distribution --fldMean arg The mean used in the fragment length distribution prior --fldSD arg The standard deviation used in the fragment length distribution prior -f [--forgettingFactor] arg The forgetting factor used in the online learning schedule. A smaller value results in quicker learning, but higher variance and may be unstable. A larger value results in slower learning but may be more stable. Value should be in the interval (0.5, 1.0]. -m [--maxOcc] arg (S) MEMs occurring more than this many times won't be considered. --initUniform initialize the offline inference with uniform parameters, rather than seeding with online parameters. -w [--maxReadOcc] arg Reads "mapping" to more than this many places won't be considered. --noLengthCorrection [experimental]: Entirely disables length correction when estimating the abundance of transcripts. This option can be used with protocols where one expects that fragments derive from their underlying targets without regard to that target's length (e.g. QuantSeq) --noEffectiveLengthCorrection Disables effective length correction when computing the probability that a fragment was generated from a transcript. If this flag is passed in, the fragment length distribution is not taken into account when computing this probability. [experimental]: Don't consider concordance with the learned fragment length distribution when trying to determine the probability --noFragLengthDist that a fragment has originated from a specified location. Normally, Fragments with unlikely lengths will be assigned a smaller relative probability than those with more likely lengths. When this flag is passed in, the observed fragment length has no effect on that fragment's a priori probability. --noBiasLengthThreshold [experimental] : If this option is enabled, then no (lower) threshold will be set on how short bias correction can make effective lengths. This can increase the precision of bias correction, but harm robustness. The default correction applies a threshold. --numBiasSamples arg Number of fragment mappings to use when learning the sequence-specific bias model. --numAuxModelSamples arg The first <numAuxModelSamples> are used to train the auxiliary model parameters (e.g. fragment length distribution, bias, etc.). After ther first <numAuxModelSamples> observations the auxiliary model parameters will be assumed to have converged and will be fixed. --numPreAuxModelSamples arg The first <numPreAuxModelSamples> will have their assignment likelihoods and contributions to the transcript abundances computed without applying any auxiliary models. The purpose of ignoring the auxiliary models for the first <numPreAuxModelSamples> observations is to avoid applying these models before thier parameters have been learned sufficiently well. --useVBOpt Use the Variational Bayesian EM rather than the traditional EM algorithm for optimization in the batch passes. Factorizes the likelihood used in quantification by adopting a new notion of equivalence classes based on the conditional probabilities --rangeFactorizationBins arg with which fragments are generated from different transcripts. This is a more fine-grained factorization than the normal rich equivalence classes. The default value (0) corresponds to the standard rich equivalence classes, and larger values imply a more fine-grained factorization. If range factorization is enabled, a common value to select for this parameter is 4. Number of Gibbs sampling rounds to perform. --numGibbsSamples arg --numBootstraps arg Number of bootstrap samples to generate. Note: This is mutually exclusive with Gibbs sampling. Number of steps to discard for every sample kept from the Gibbs chain. The larger this number, the less chance that subsequent samples --thinningFactor arg are auto-correlated, but the slower sampling becomes. -q [--quiet] Be quiet while doing quantification (don't write informative output to the console unless something goes wrong). The prior (either the default or the argument provided via --vbPrior) will be interpreted as a transcript-level prior (i.e. each --perTranscriptPrior transcript will be given a prior read count of this value) --vbPrior arg The prior that will be used in the VBEM algorithm. This is interpreted as a per-nucleotide prior, unless the --perTranscriptPrior flag is also given, in which case this is used as a transcript-level prior --writeOrphanLinks Write the transcripts that are linked by orphaned reads. --writeUnmappedNames Write the names of un-mapped reads to the file unmapped_names.txt in the auxiliary directory. -x [--quasiCoverage] arg [Experimental]: The fraction of the read that must be covered by MMPs (of length >= 31) if this read is to be considered as "mapped". This may help to avoid "spurious" mappings. A value of 0 (the default) denotes no coverage threshold (a single 31-mer can yield a mapping). Since coverage by exact matching, large, MMPs is a rather strict condition, this value should likely be set to something low, if used.

Tunable parameters

Most users rely on the default parameter settings,

- which are meant to work well on average,
- but the most interesting examples are not typically "average".



The default parameter choices miss two transcripts that are supported by the data and in the reference transcriptome.

Tunable parameters

It's not just a problem in computational biology!

SATzilla: Portfolio-based Algorithm Selection for SAT

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Concertio

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Concertio Launches Optimizer Studio to Help Performance Engineers and IT Professionals Achieve Peak System Performance

by admin | Feb 22, 2018 | News | 0 comments

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ParamILS: An Automatic Algorithm Configuration Framework

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Swarm and Evolutionary Computation 1 (2011) 19-31



Contents lists available at ScienceDirect

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Invited paper

Parameter tuning for configuring and analyzing evolutionary algorithms

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ARTICLE INFO

ABSTRACT

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Almost all pieces of scientific software have tunable parameters.

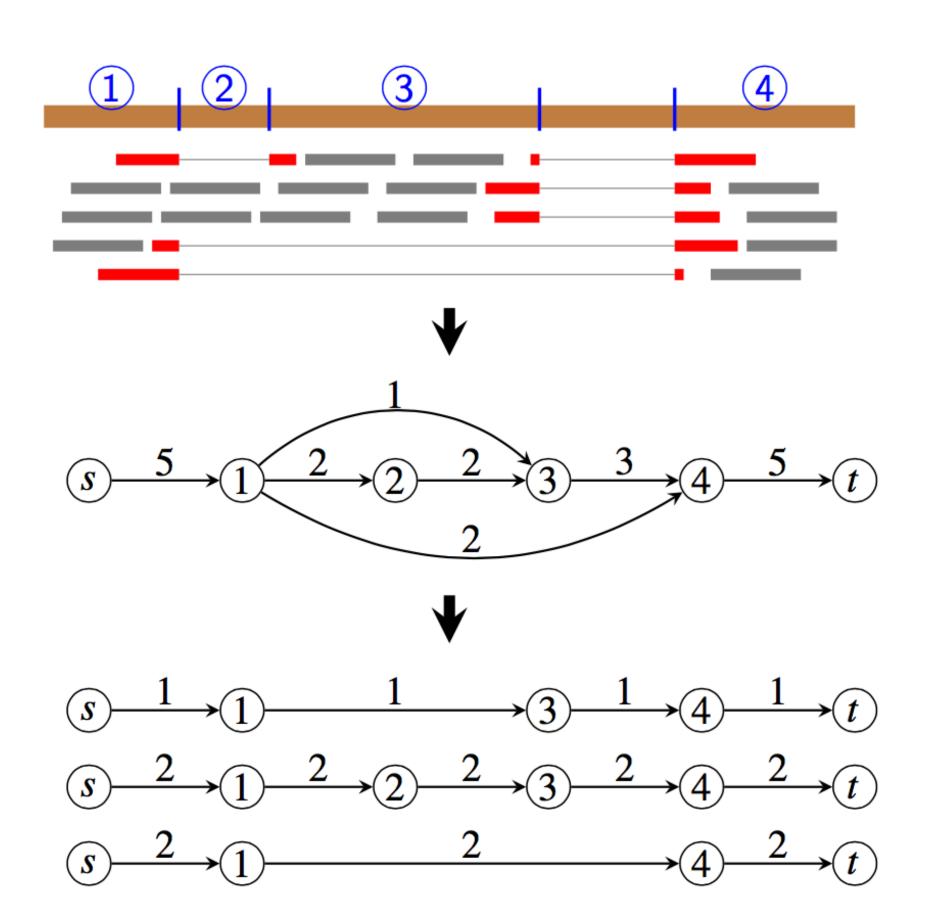
- Their settings can greatly impact the quality of output.
- Default parameters are best on average but may be bad in general.
- Mis-configuration can lead to missed or incorrect conclusions.

Can we remove parameter choice as a source of error in transcriptome analysis?

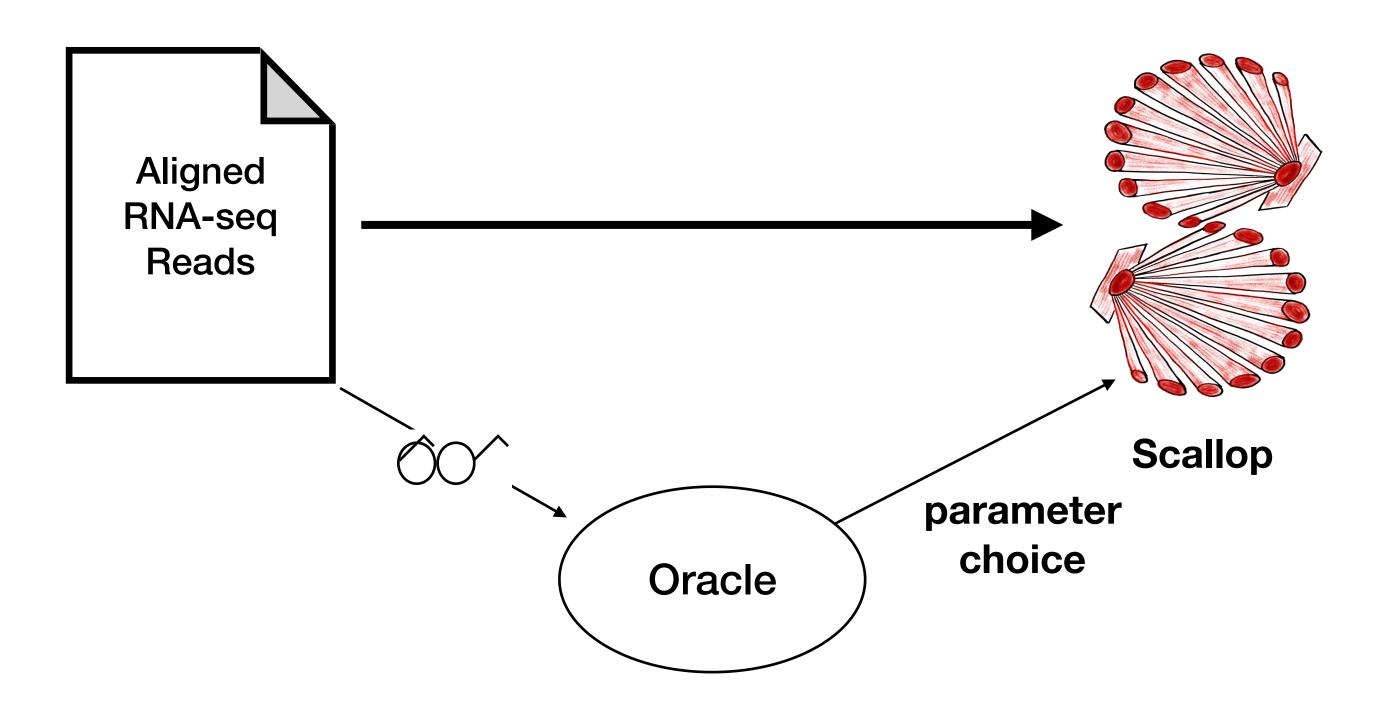
Transcript assembly

- is a fundamental problem in transcriptomics
- but is computationally difficult
- and easily impacted by choices of parameters.
- We will focus on the Scallop assembler.

Scallop was presented yesterday at the Computational RNA Biology COSI



The goal is to find the parameter choice for a given input.



In machine learning, this is the hyper-parameter tuning problem

- multi-armed bandit
- simulated annealing
- bayesian frameworks
- etc.

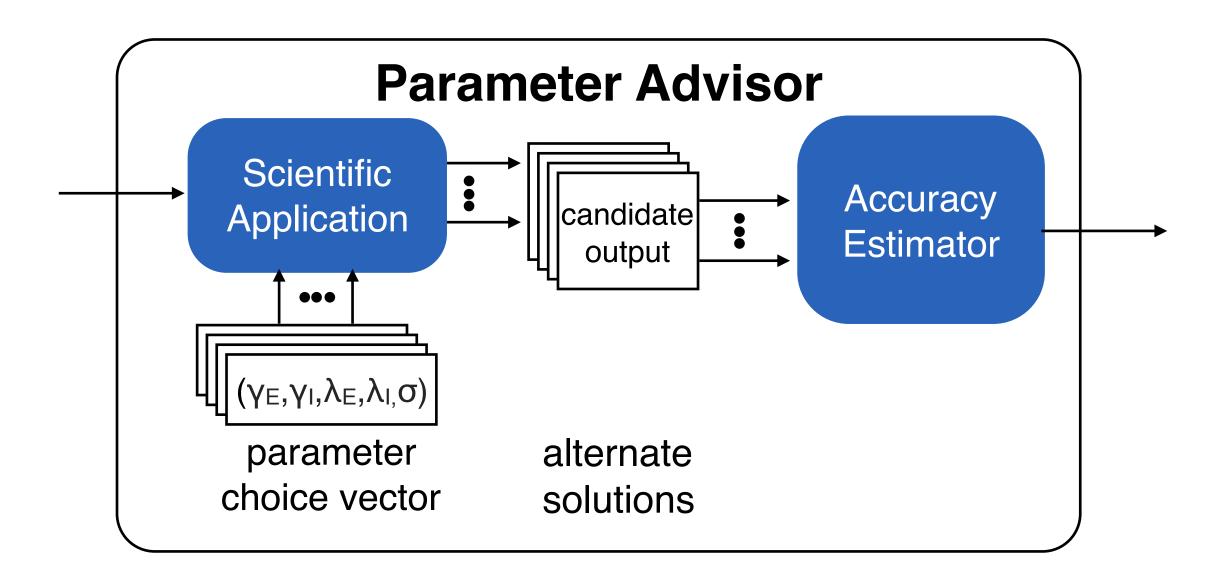
Issue is that running time is increased greatly since

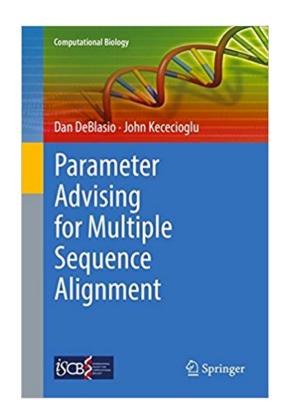
- the application needs to be run multiple times, and
- those instances need to be sequential

Parameter advising

Given an input an advisor

- uses an advisor set of parameter choice vectors to obtain candidates, then
- returns the most accurate of these solutions based on the accuracy estimation.

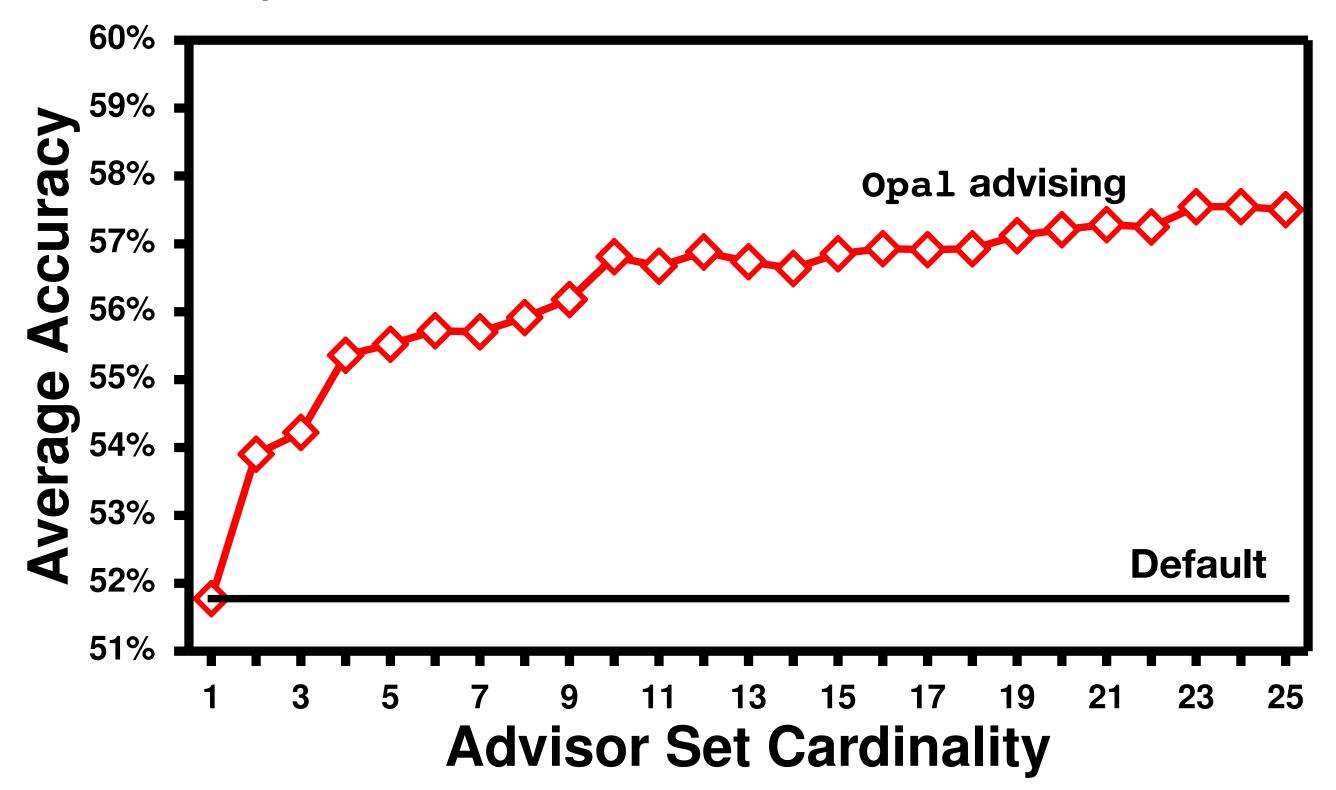


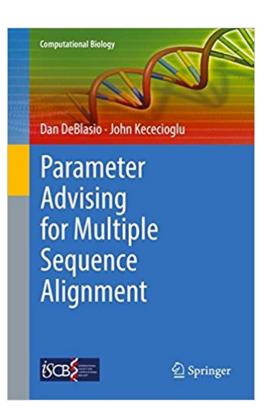


Parameter advising

Increases accuracy for multiple sequence alignment by

- choosing a parameter choice for each input and
- accuracy increases with advisor set size, but
- so does the resource requirement.

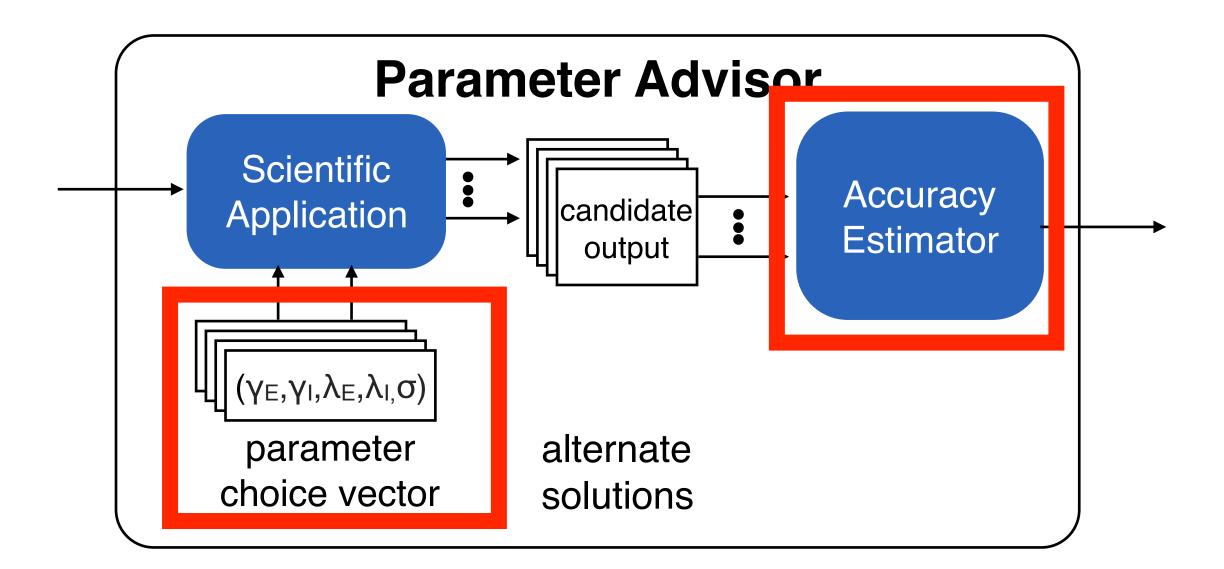




Parameter advising

Given an input an advisor

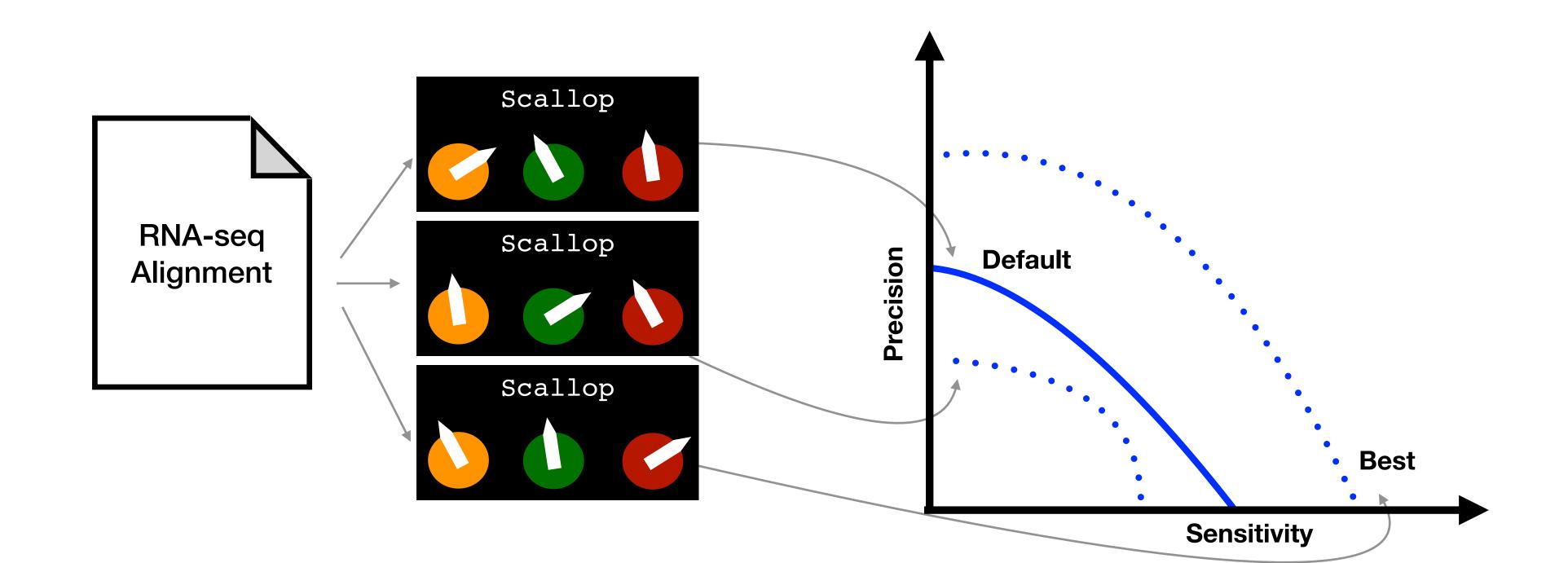
- uses an advisor set of parameter choice vectors to obtain candidates, then
- returns the most accurate of these solutions based on the accuracy estimation.



Steps to applying advising to a new domain defining:
(1) the advisor set, and
(2) an accuracy estimator

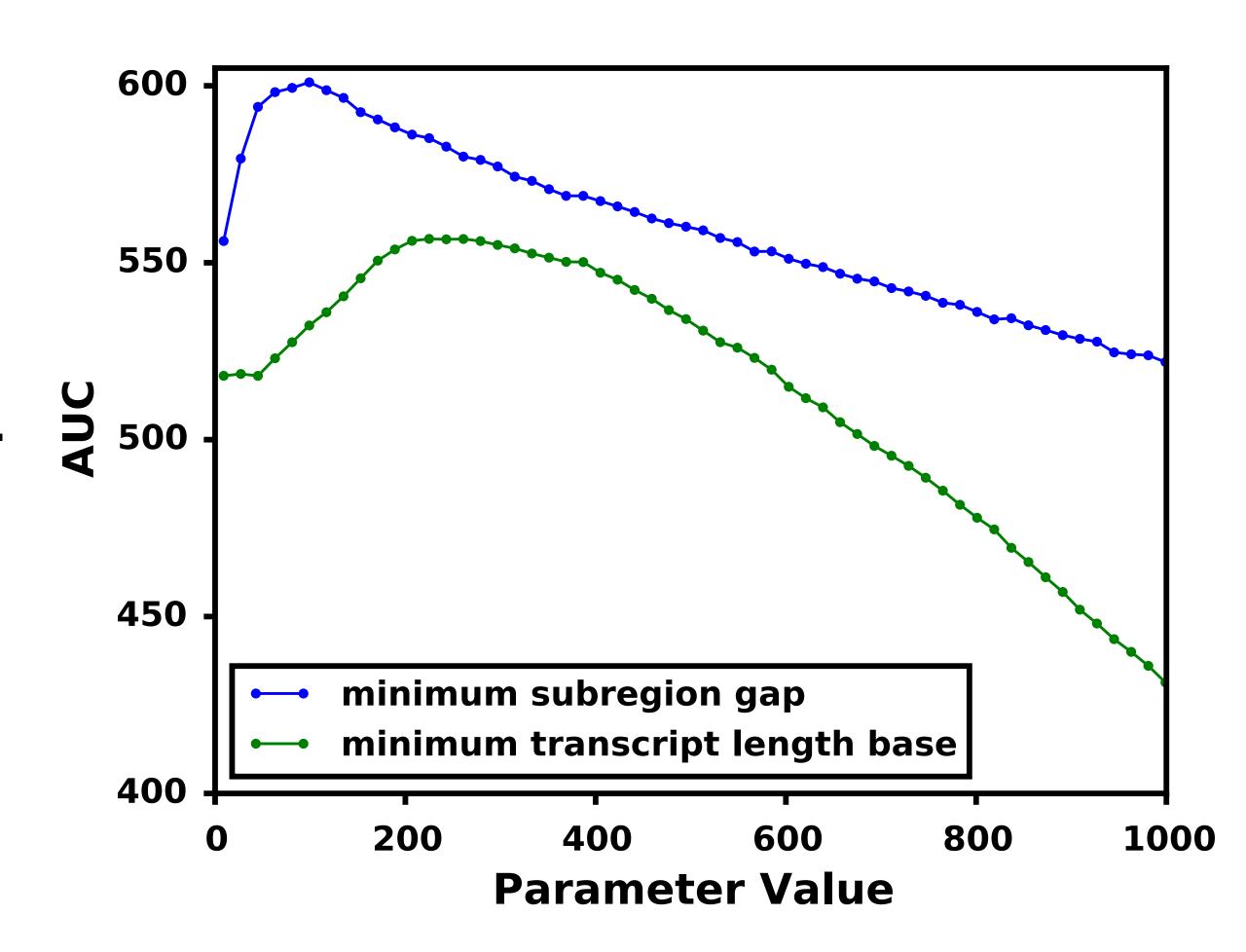
Advising for transcript assembly is different from previous implementations;

- the reference transcriptome is available so
- the area under the receiver operating characteristic curve can be used as both a measure and an objective, but
- the number of tunable parameters is very large.

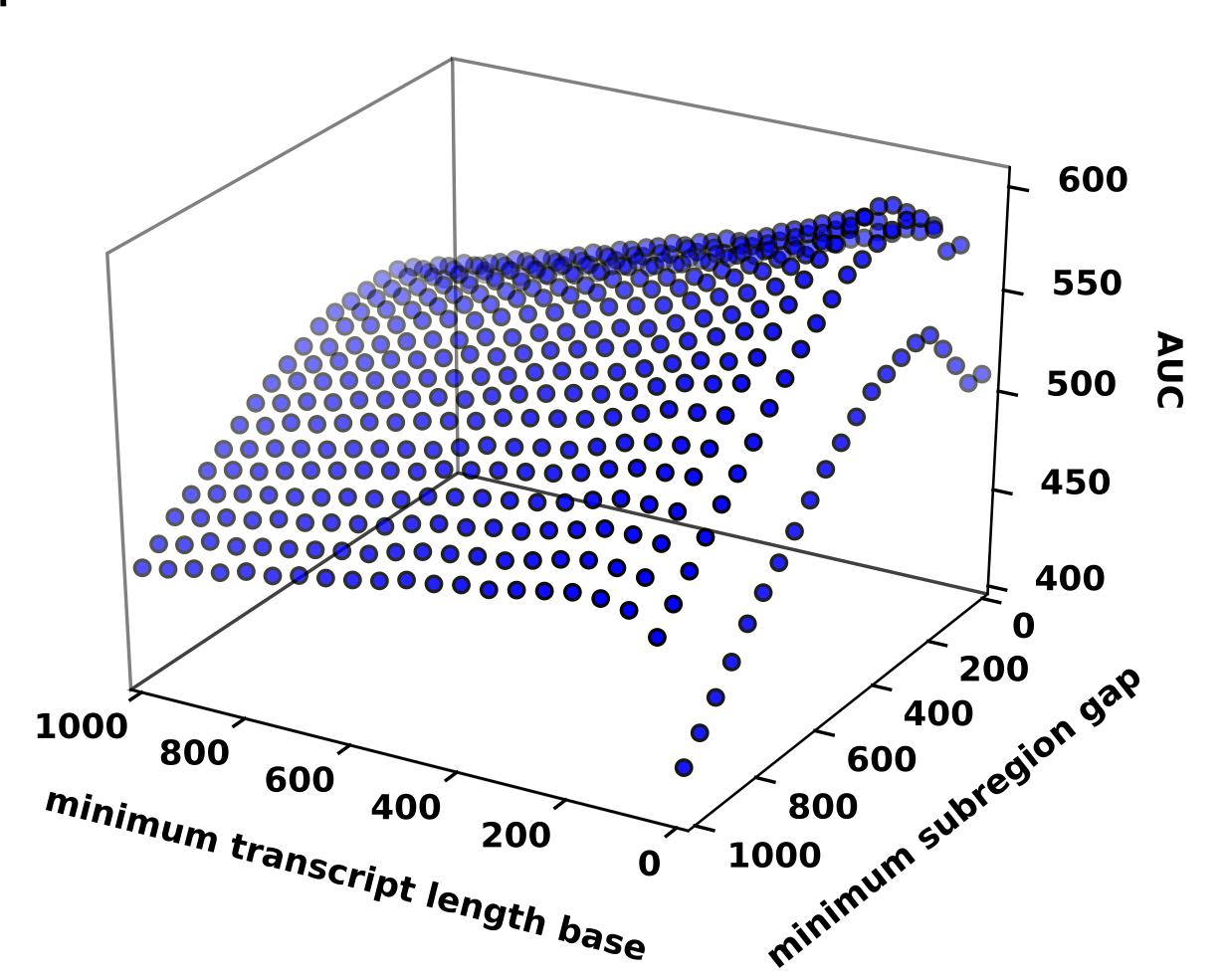


Cannot test all combinations of parameter values.

- Tested the behavior of each parameter in isolation.
- Each parameter had a single global maximum on the large regions tested.
- In general, we did not see non-global local maxima.

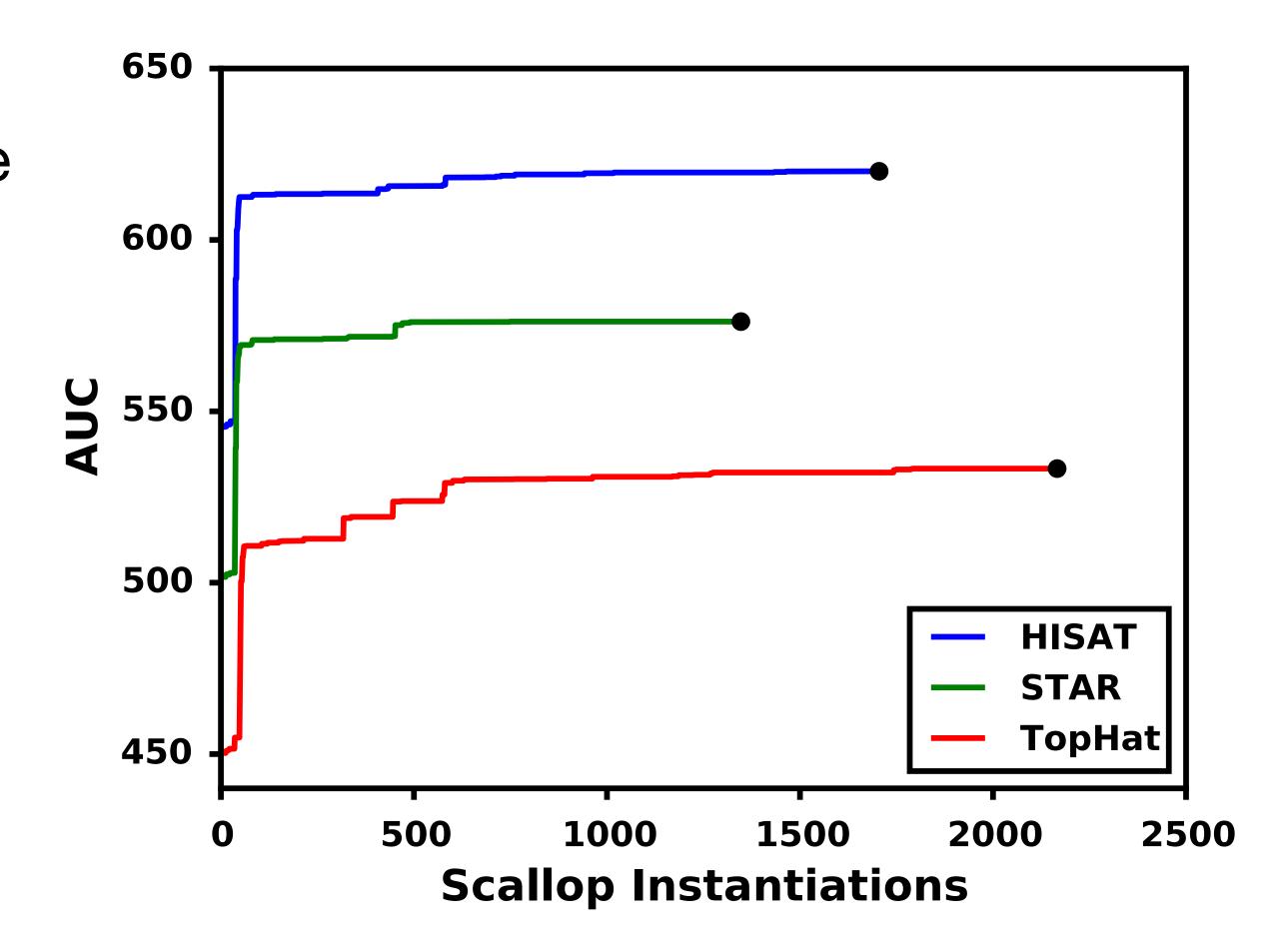


Pairs of parameters, tested in isolation also have one maxima.



Parameter curve smoothness means

- coordinate ascent will work well
- but is slow since Scallop's running time is significant.

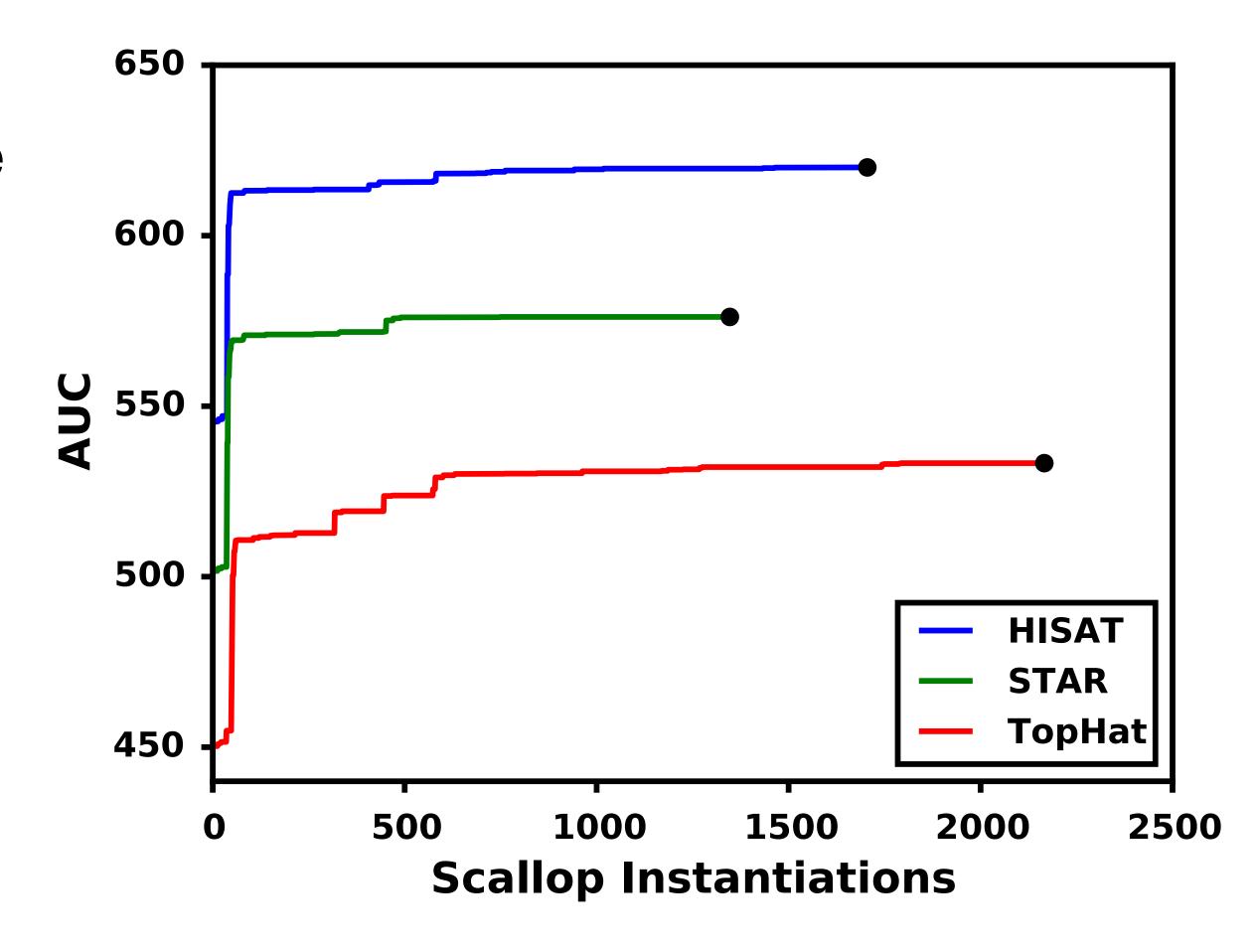


Parameter curve smoothness means

- coordinate ascent will work well
- but is slow since Scallop's running time is significant.

We can use coordinate ascent

- on a set of training samples
- to find settings for all 18 tunable parameters
- which can be used as a set for parameter advising.
- That set is precomputed and doesn't impact the advising time.



ID	Experiment	Aligner	ICC	NE	BG	EL	FL	MQ	NH	SBH	SG	SL	SO	TLB	TLI	UM	US
1	SRR545723	TopHat	2	1000	1359	20	3	11	20	1	39	11	1.5	454	8	false	false
2	SRR307911	TopHat	2	1000	1032	20	2	11	21	1	52	15	1.5	432	19	false	false
3	SRR534291	TopHat	0.75	51	785	25	3	1	9	1	121	16	1.51	503	8	false	false
4	SRR387661	TopHat	0.22	1000	999	20	3	11	20	1	53	15	1.5	429	19	false	false
5	SRR315334	TopHat	1.5	1000	1425	20	3	11	20	1	50	16	1.5	528	1	false	false
6	SRR307903	TopHat	1.61	250	733	2	0	11	2	1	23	26	0.75	521	2	false	false
7	SRR545695	TopHat	2	1000	852	20	2	2	104	1	5	7	1.5	432	19	false	false
8	SRR534319	TopHat	2.27	1000	306	20	0	1	20	1	7	11	1.5	346	21	false	false
9	SRR315323	TopHat	0.22	205	945	20	0	2	20	1	39	15	1.16	409	8	true	true
10	SRR534307	TopHat	2.22	1000	78	32	3	11	16	2	0	32	1.5	512	8	false	false
11	SRR545723	HISAT	1.75	11000	628	20	3	11	20	2	8	7	1.5	408	8	false	false
12	SRR307911	HISAT	99.66	1000	1828	3	5	11	3	1	43	15	0.17	392	8	false	false
13	SRR534291	HISAT	1	11000	851	22	5	11	3	1	120	3	0.17	267	30	false	false
14	SRR387661	HISAT	1.05	454	130	26	4	11	38	1	23	0	0.17	880	0	false	false
15	SRR315334	HISAT	0	282	870	20	4	11	1	1	48	8	1.28	307	21	false	false
16	SRR307903	HISAT	1.42	168	745	9	5	11	2	1	23	6	0.17	396	0	false	false
17	SRR545695	HISAT	5.56	1000	778	26	2	11	25	2	0	0	1.5	360	8	false	false
18	SRR534319	HISAT	2	1000	1669	20	0	11	81	1	4	7	1.5	150	73	false	false
19	SRR315323	HISAT	2	685	782	15	0	11	14	1	40	7	1.5	180	50	false	false
20	SRR534307	HISAT	2	146	309	41	8	11	10	3	2	0	1.17	370	4	false	false
21	SRR545723	STAR	2	11000	455	22	6	11	3	1	3	21	1.26	252	16	false	false
22	SRR307911	STAR	0.22	1000	490	20	3	11	8	1	53	26	0.5	289	24	false	false
23	SRR534291	STAR	0.22	11000	481	24	0	2	11	1	123	26	0.24	352	8	false	false
24	SRR387661	STAR	2	1000	734	20	4	11	35	2	42	29	1.5	411	1	false	false
25	SRR315334	STAR	0.5	1000	1070	8	0	11	8	1	41	29	0.75	267	33	false	false
26	SRR307903	STAR	2	1000	976	8	5	11	20	1	35	35	0.17	433	8	false	false
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28	SRR534319	STAR	2	800	1574	17	4	2	20	1	8	18	1.5	307	4	false	false
29	SRR315323	STAR	2	11000	1043	20	3	7	20	1	33	35	1.5	150	50	true	true
30	SRR534307	STAR	1.58	292	54	20	0	11	9	3	0	29	1.5	320	8	false	false
	Default		2.00	1,000	50	20	3	1	20	1	3	15	1.50	150	50	false	false
	Initial step size		10.00	10,000	100	100	10	10	100	10	10	20	10.00	500	100	n/a	n/a

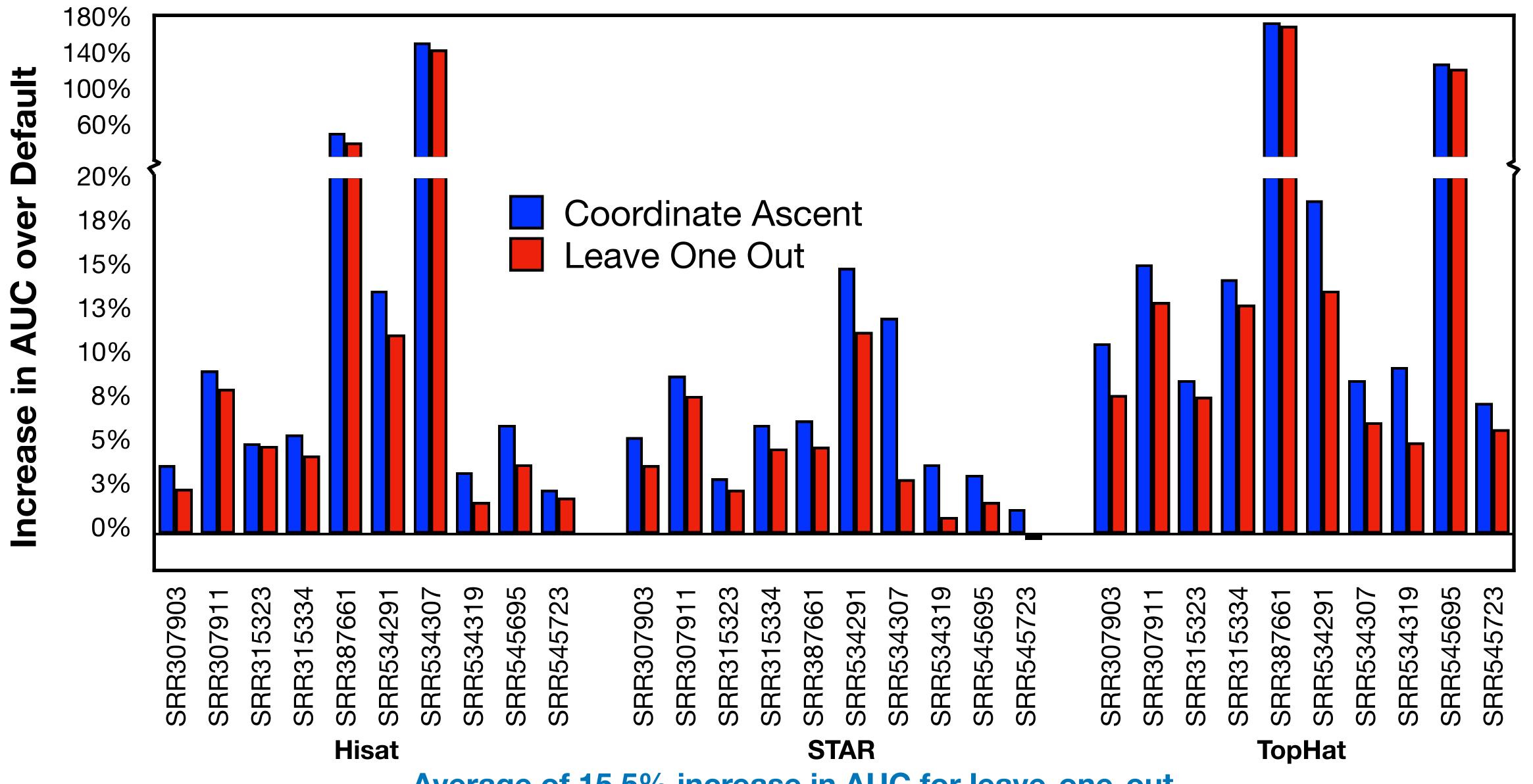
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- maximum edit distance (ED)
- maximum intron contamination coverage (ICC)
- maximum number of exons (NE)
- minimum bundle gap (BG)
- minimum exon length (EL)
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- minimum mapping quality (MQ)
- minimum number or hits in a bundle (NH)
- minimum router count (RC)
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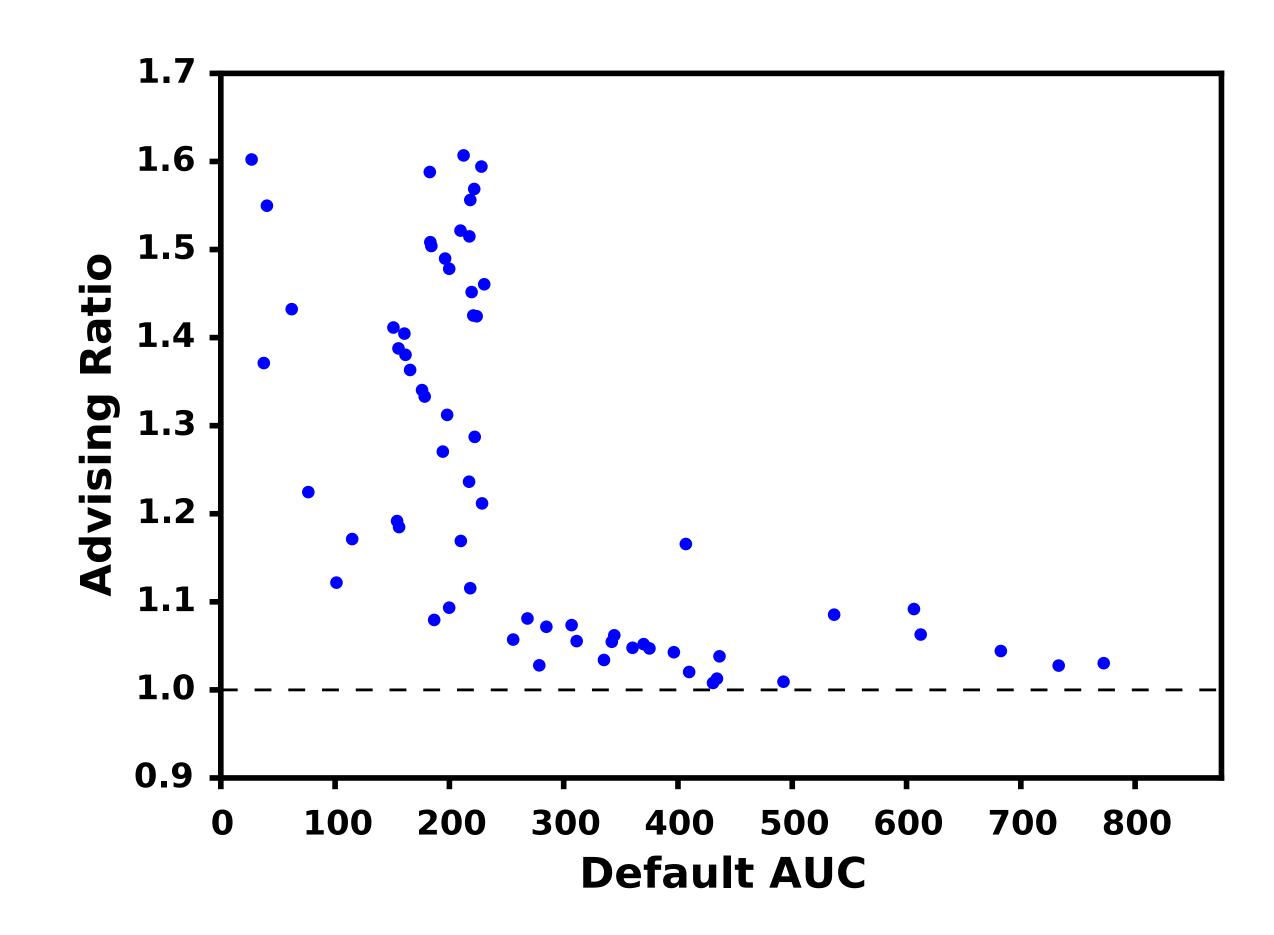
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6	SRR307903	TopHat	1.61	250	733	2	()	11	2	1	23	26	0.75	521	2	false	false
7	SRR545695	TopHat	2	1000	852	20	2	2	104	1	5	7	1.5	432	19	false	false
8	SRR534319	TopHat	2.27	1000	306	20	()	1	20	1	7	11	1.5	346	21	false	false
9	SRR315323	TopHat	0.22	205	945	20	()	2	20	1	39	15	1.16	409	8	true	true
10	SRR534307	TopHat	2.22	1000	78	32	3	11	16	2	0	32	1.5	512	8	false	false
11	SRR545723	HISAT	1.75	11000	628	20	3	11	20	2	8	7	1.5	408	8	false	false
12	SRR307911	HISAT	99.66	1000	1828	3	5	11	3	1	43	15	0.17	392	8	false	false
13	SRR534291	HISAT	1	11000	851	22	5	11	3	1	120	3	0.17	267	30	false	false
14	SRR387661	HISAT	1.05	454	130	26	4	11	38	1	23	()	0.17	880	()	false	false
15	SRR315334	HISAT	0	282	870	20	4	11	1	1	48	8	1.28	307	21	false	false
16	SRR307903	HISAT	1.42	168	745	9	5	11	2	1	23	6	0.17	396	0	false	false
17	SRR545695	HISAT	5.56	1000	778	26	2	11	25	2	0	()	1.5	360	8	false	false
18	SRR534319	HISAT	2	1000	1669	20	()	11	81	1	4	7	1.5	150	73	false	false
19	SRR315323	HISAT	2	685	782	15	()	11	14	1	40	7	1.5	180	50	false	false
20	SRR534307	HISAT	2	146	309	41	8	11	10	3	2	0	1.17	370	4	false	false
21	SRR545723	STAR	2	11000	455	22	6	11	3	1	3	21	1.26	252	16	false	false
22	SRR307911	STAR	0.22	1000	490	20	3	11	8	1	53	26	0.5	289	24	false	false
23	SRR534291	STAR	0.22	11000	481	24	()	2	11	1	123	26	0.24	352	8	false	false
24	SRR387661	STAR	2	1000	734	20	4	11	35	2	42	29	1.5	411	1	false	false
25	SRR315334	STAR	0.5	1000	1070	8	()	11	8	1	41	29	0.75	267	33	false	false
26	SRR307903	STAR	2	1000	976	8	5	11	20	1	35	35	0.17	433	8	false	false
27	SRR545695	STAR	2	1000	388	20	8	11	89	2	20	23	1.5	307	19	false	false
28	SRR534319	STAR	2	800	1574	17	4	2	20	1	8	18	1.5	307	4	false	false
29	SRR315323	STAR	2	11000	1043	20	3	7	20	1	33	35	1.5	150	50	true	true
30	SRR534307	STAR	1.58	292	54	20	()	11	9	3	0	29	1.5	320	8	false	false
	Default		2.00	1,000	50	20	3	1	20	1	3	15	1.50	150	50	false	false
	Initial step size		10.00	10,000	100	100	10	10	100	10	10	20	10.00	500	100	n/a	n/a

- maximum dynamic programming table size (DP)
- maximum edit distance (ED)
- maximum intron contamination coverage (ICC)
- maximum number of exons (NE)
- minimum bundle gap (BG)
- minimum exon length (EL)
- minimum flank length (FL)
- minimum mapping quality (MQ)
- minimum number or hits in a bundle (NH)
- minimum router count (RC)
- minimum splice boundary hits (SBH)
- minimum subregion gap (SG)
- minimum subregion length (SL)
- minimum subregion overlap (SO)
- minimum transcript length base (TLB)
- minimum transcript length increase (TLI)
- uniquely mapped reads only (UM)
- use the secondary alignment (US)



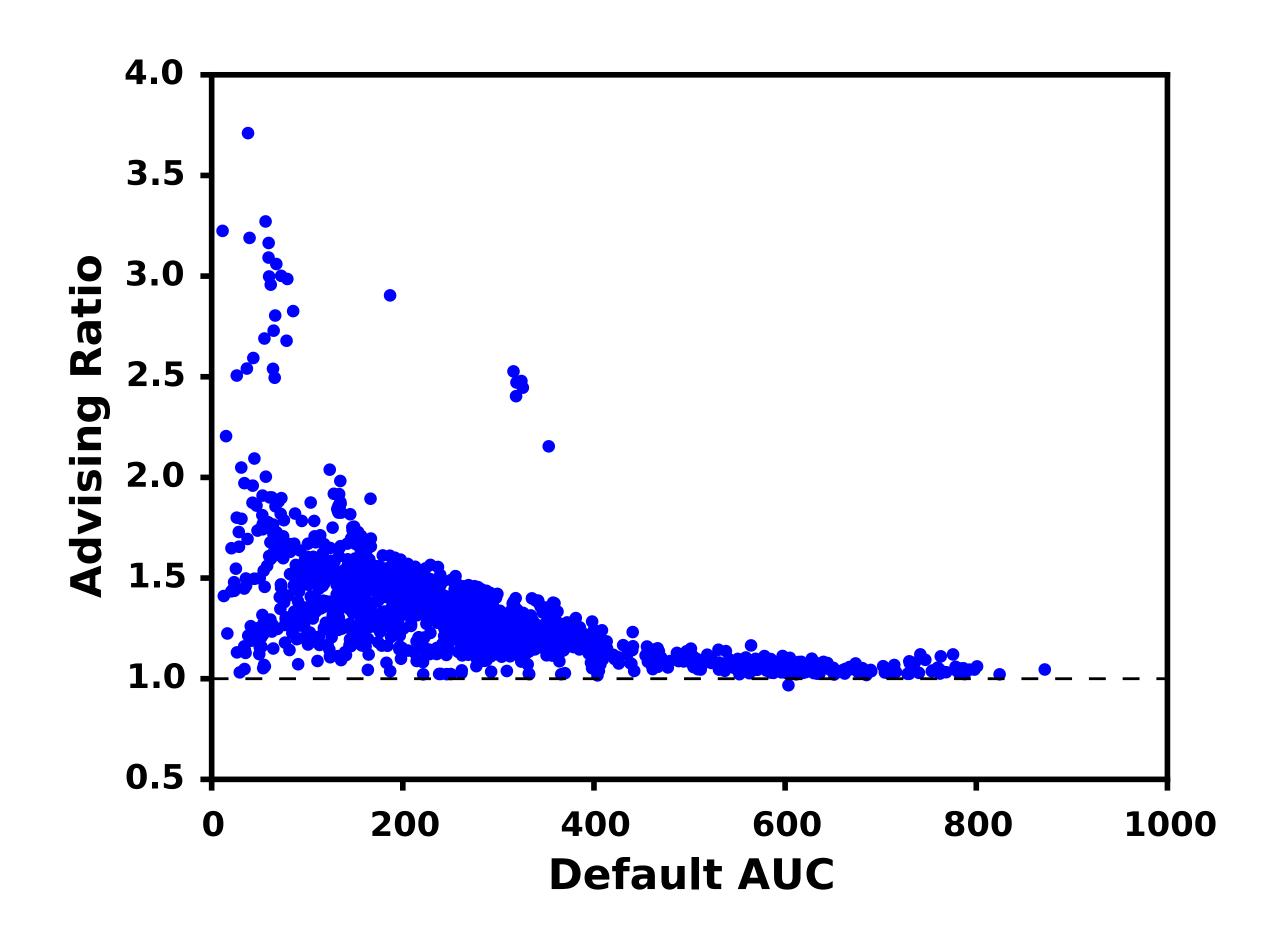
65 ENCODE dataset

- all of the aligned RNA-seq experiments from ENCODE
- aligned using a variety of aligners
- using either the current or legacy reference genome
- stands in for the performance of advising on generic input
- average 25.7% increase in AUC

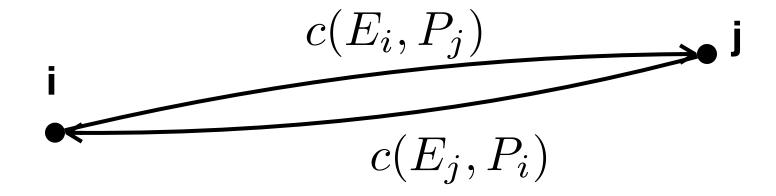


SRA dataset

- all 1595 RNA-Seq experiments from the SRA
- aligned using STAR to the same reference genome
- represents performance of advising in a high-throughput experiment
- average of 38.2% increase in AUC



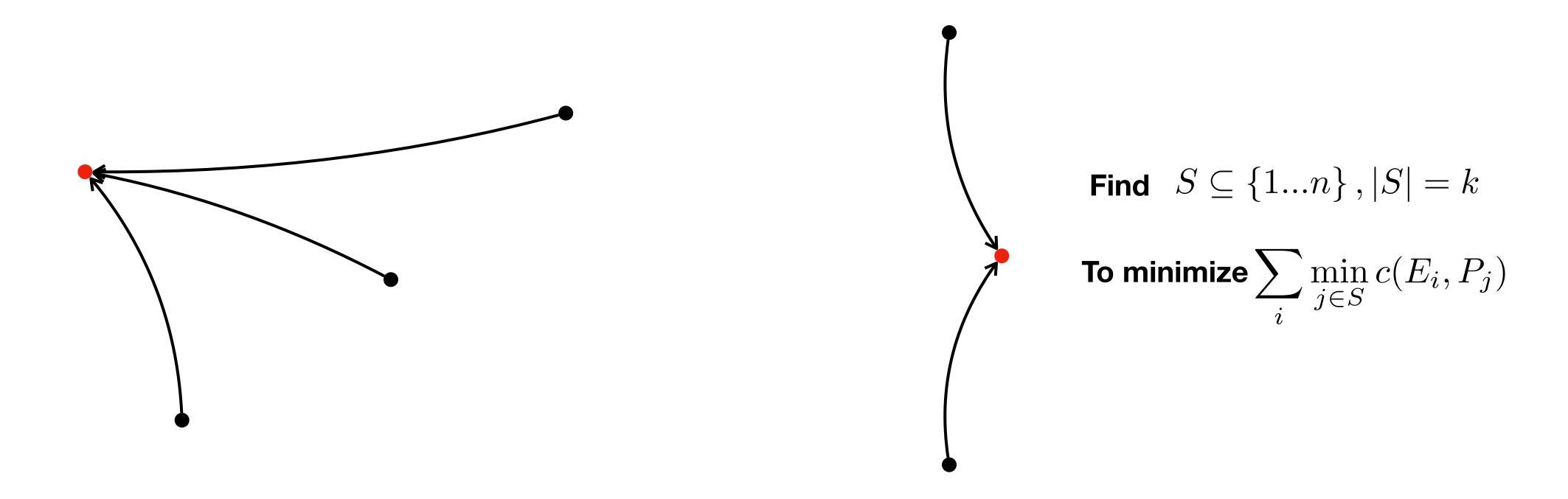
- 31 parameters may be too many to run in parallel
 - parameter subsets were found using the oracle set method for advising
 - parameters are meant to cover the range of inputs



31 parameters may be too many to run in parallel

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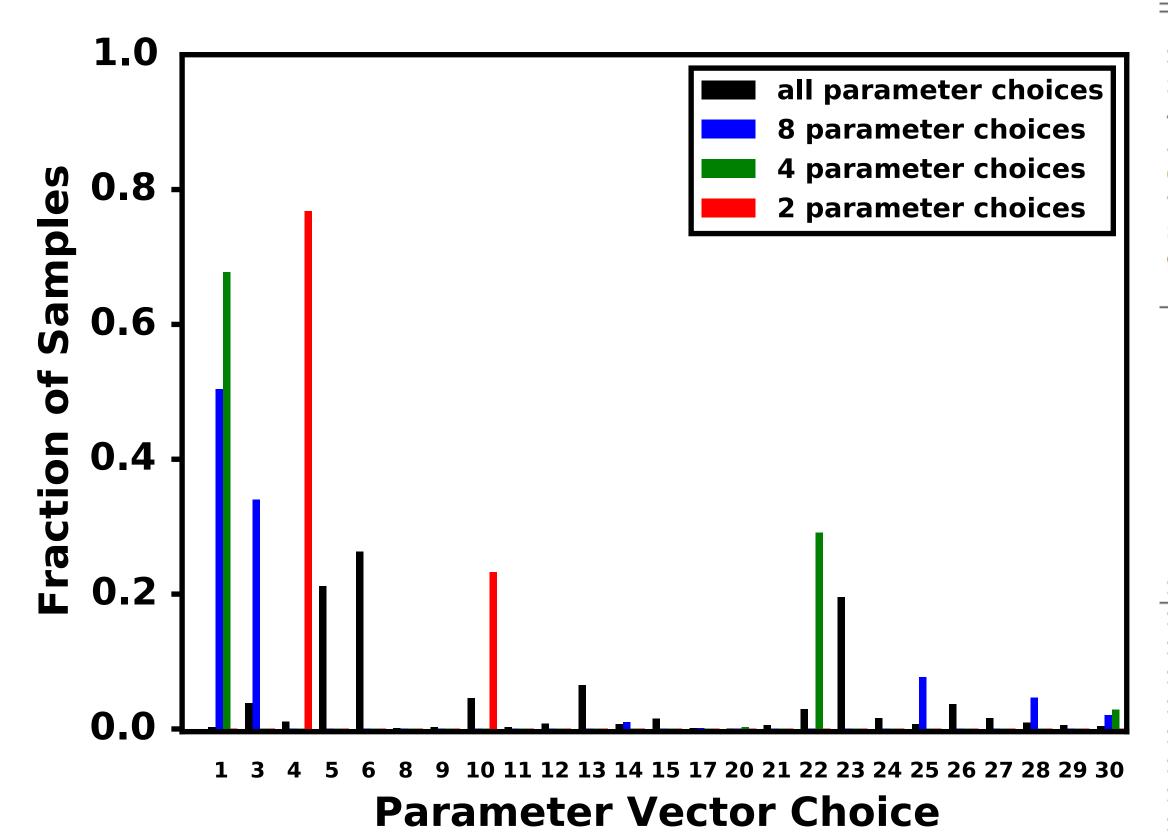
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31 parameters may be too many to run in parallel

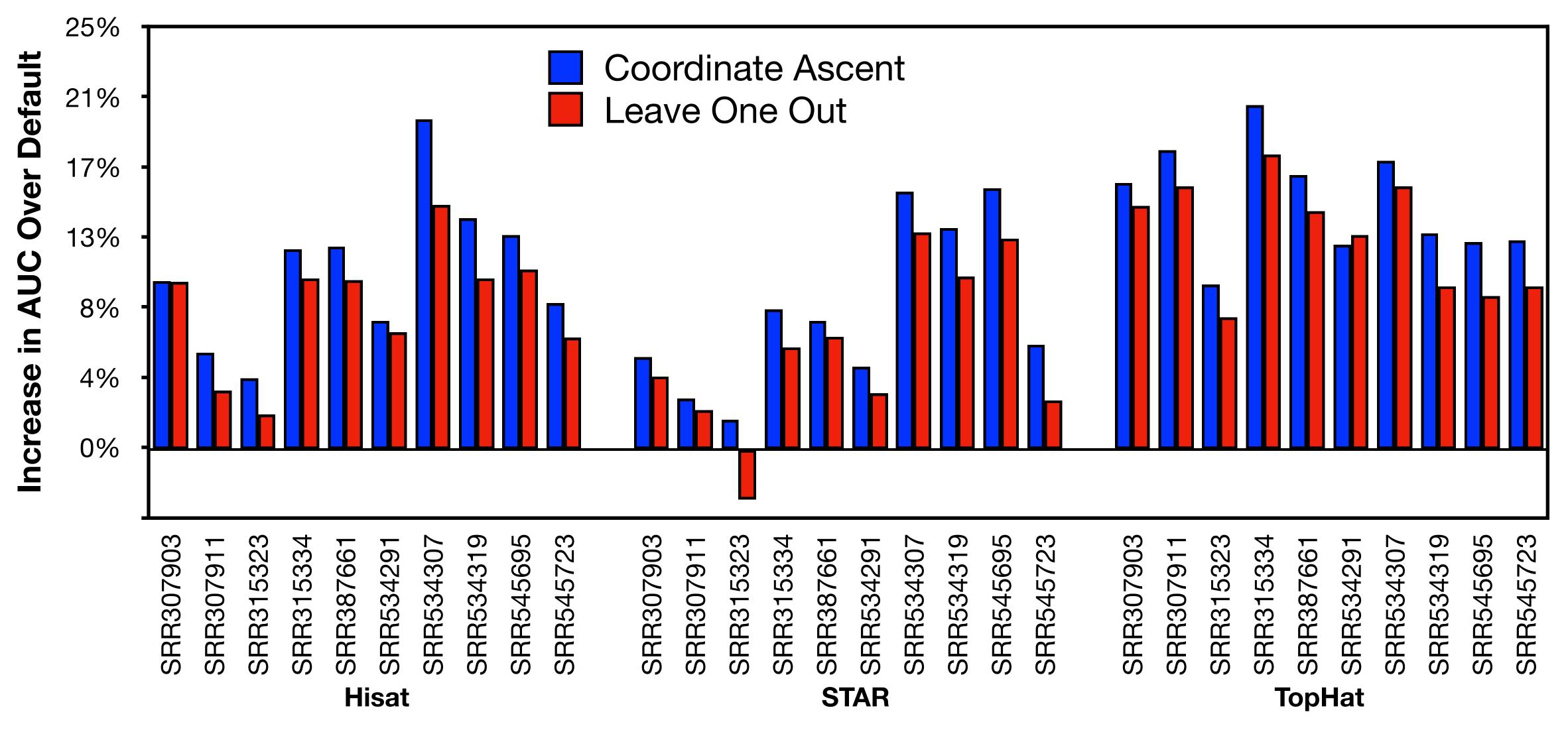
- parameter subsets were found using the *oracle set* method for advising
- parameters are meant to cover the range of inputs

Not all parameters are used when available



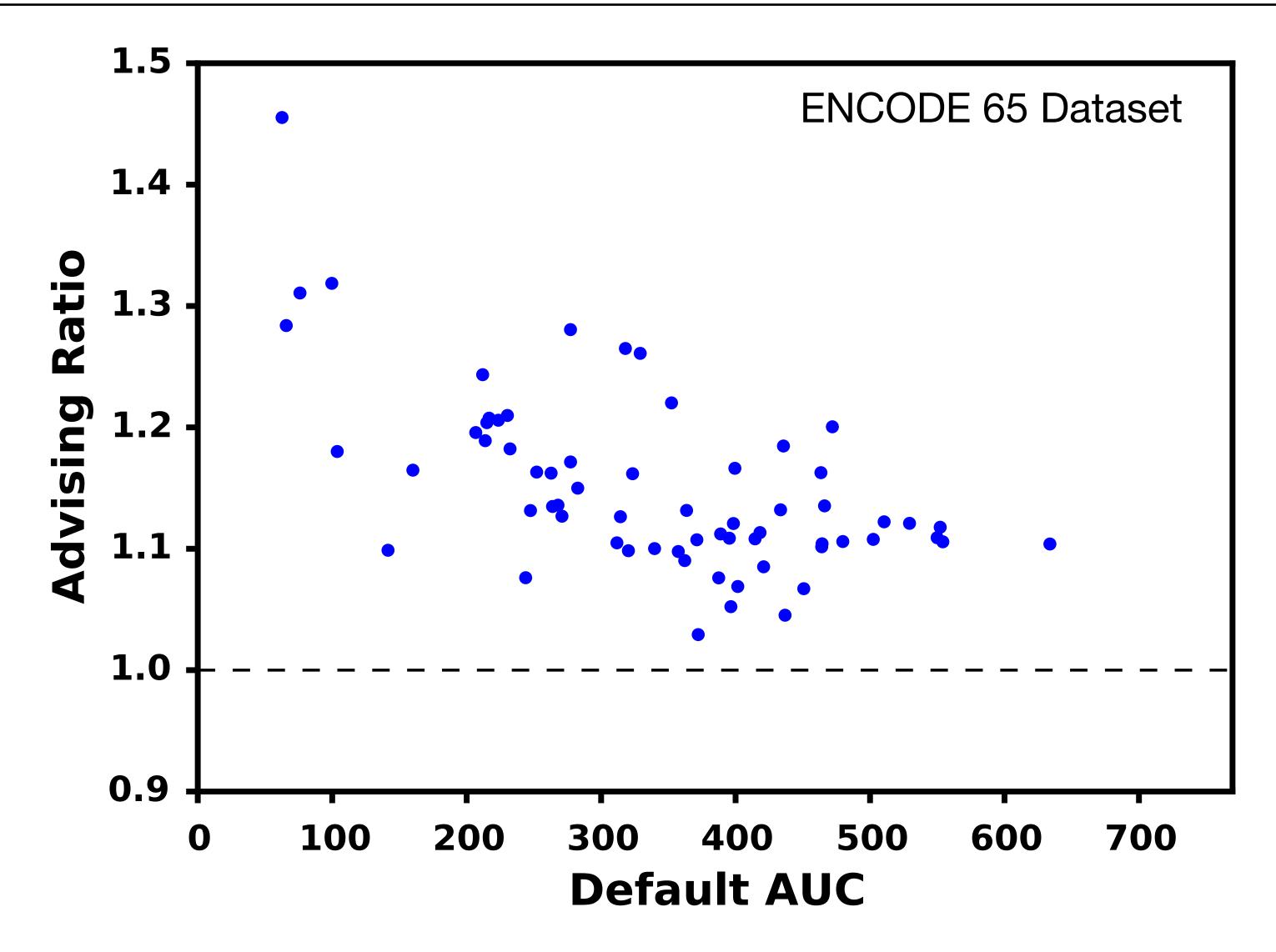
ID	Experiment	Aligner	2	4	8
1	SRR545723	TopHat		X	X
2	SRR307911	TopHat			
3	SRR534291	TopHat			\mathbf{X}
4	SRR387661	TopHat	X		
5	SRR315334	TopHat			
6	SRR307903	TopHat			
7	SRR545695	TopHat			
8	SRR534319	TopHat			
9	SRR315323	TopHat			
10	SRR534307	TopHat	X		
11	SRR545723	HISAT			
12	SRR307911	HISAT		X	
13	SRR534291	HISAT			
14	SRR387661	HISAT			X
15	SRR315334	HISAT			
16	SRR307903	HISAT			
17	SRR545695	HISAT			X
18	SRR534319	HISAT			
19	SRR315323	HISAT			
20	SRR534307	HISAT		X	X
21	SRR545723	STAR			
22	SRR307911	STAR			
23	SRR534291	STAR			
24	SRR387661	STAR			
25	SRR315334	STAR			X
26	SRR307903	STAR			
27	SRR545695	STAR			
28	SRR534319	STAR			X
29	SRR315323	STAR			
30	SRR534307	STAR		X	X

StringTie advising



11.1% and 9.0% average increase in accuracy for Coordinate Ascent and Leave One Out

StringTie advising



Summary

Parameter advising increases AUC for transcript assembly.

- Coordinate ascent is a novel method for advisor set construction.
- Advisor subsets can be used to reduce the resource requirements.
- Improvements are seen for both Scallop and StringTie.

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Poster this evening B-655

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