Actual behavior of a Gibbs sampler

(thanks to Stephen Altschul)

Behavior of the Objective Function
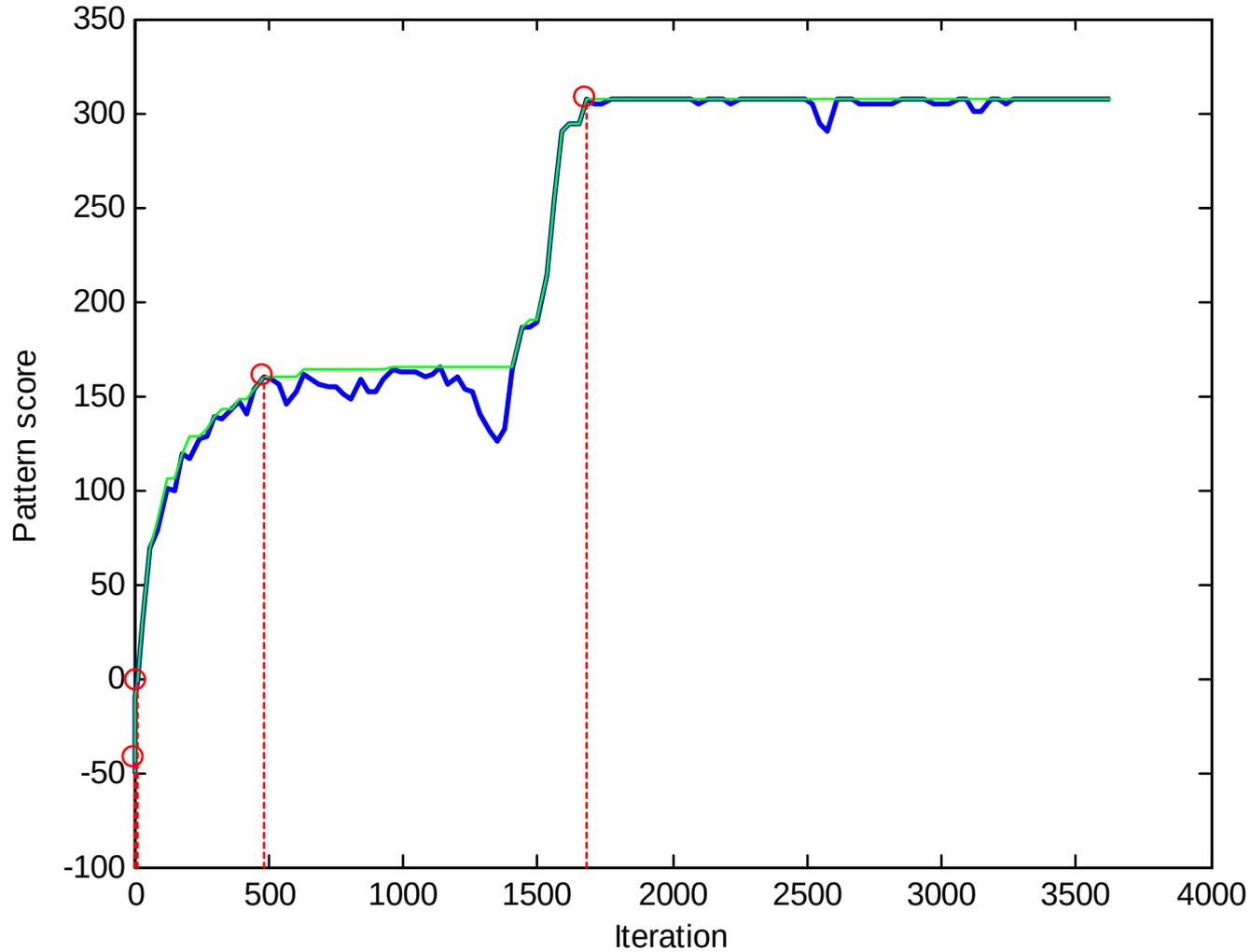
The Evolving Multiple Alignment

|			
MTQPSKTTKLTKDEV	SKTTKLTKDEVDRLI	GISQMHVSRLQRKAV	ETGDILGISQMHVSR
MPPLFVMNNEILMHL	FVMNNEILMHLRALK	GISRSYVSRIEKRAL	EIAKELGISRSYVSR
VVFNQLLVDRRVSIT	QLLVDRRVSITAENL	TVRDSSMSLMQALQN	ITAENLGLTQPAVSN
WFQNRRMKWKKENKT	RYLTRRRIEIAHAL	GVPQQQQQQQQPSQ	EIAHALCLTERQIKI
SGTGKELVARALHDY	KELVARALHDYGRRR	KLDAQALERLKQHRW	RAADLLGLNRNTLRK
RIRYRRKNLKHTQRS	RRKNLKHTQRSLAKA	PESEQDTQLAEMRAR	SLAKALKISHVSVSQ
ALDAGVSVHIVRDYL	GVSVHIVRDYLLRGL	VLRQFVERREALAN	RAAFEAGIGLGALAR
QLNGQDVNDLYELVL	QDVNDLYELVLAEVE	PLRDSVKQALKNYFA	RAALMMGINRGTLRK
LEIYHHIKKEKSPKG	HHIKKEKSPKGKSSI	FIMESNLTKVEQHTL	EVAKKCGITPLQVRV
SQISRWKRDWIPKFS	RWKRDWIPKFSMLLA	GVDKSQISRWKRDWI	KTAEAVGVDKSQISR
GSVAVLIKDEEGKEM	VLIKDEEGKEMILSY	RIAQTLLNLAKQPDA	EIGQIVGCSRETVGR
TINADGSVYAEEVKP	QTKTAKDLGVYQSAI	GVYQSAINKAIHAGR	KTAKDLGVYQSAINK
EIVTAGALKYQENAY	AGALKYQENAYRQAA	GISDAAVSQWKEVIP	AVAKALGISDAAVSQ
QLLLRRMEAINESLH	RRMEAINESLHPPMD	LLEQLLLRRMEAINE	SVAQHVCLSPSRLSH
DLSGKMPNLRQQMMR	QDMILLLSKKNAEER	NLRQQMMRLMSGEIK	DIGNYLGLTVETISR
GGLDSYIRAANAWPM	SYIRAANAWPMLSAD	RVRQLEKNAMKKLRA	ELADRYGVSAERVRQ
TRLAWPGNVRQLENT	RLARHFLQIAARELG	MLPDSWATLLGQWAD	EAARLLGWGRNTLTR
ETAATMKDVALKAKV	TMKDVALKAKVSTAT	KVSQATRNRVEKAAR	DVALKAKVSTATVSR
PRSASHYLLSDQKSR	LVEEKRRAAKLAATL	LLSDQKSRLVEEKRR	DAAALLGVSEMTIRR
YHNEQKERQAIEQLI	QKERQAIEQLIRHRC	KERQAIEQLIRHRCA	DVARLAGVSVATVSR
RLLQLSQGQAVKGNQ	AMLVANDQMALGAMR	ALADSLMQLARQVSR	DVAEYAGVSYQTVSR
TRPTEKQYETLENQL	KNKRALLDALAIEML	VLEDQEHQVAKEERE	KLAQKLGVEQPTLYW
SNSLKAAPVELRQWL	KAAPVELRQWLEEVL	YSAAMAEQRHQEWLR	ELKNELGAGIATITR
AFVKFNCAALPDNLL	FNCAALPDNLLESEL	LSRATEASKTLQEVL	KAARLLGMTPRQVAY
EQLNEREKQIMELRF	EREKQIMELRFGLVG	GISQSYISRLEKRII	DVADMMGISQSYISR
EDKISGTKSERPGLK	SGTKSERPGLKKLLR	MERELIVERTKAGLE	KVAIIYDVGVSTLYK
TIHPKDSLGETAFN	PKDSLGETAFNMLLD	FEPESGYRAMQQILS	DVAKRANVSTTTVSH
FIGGEDEPGKADIRE	EDEPGKADIREVAFA	FSSSSGYELAKQMLA	DIAIEAGVSLATVSR
ARQQEVFDLIRDHIS	EVFDLIRDHISQTGM	HISQTGMPPTRAEIA	EIAQRLGFRSPNAAE
EDEELAELAKKVAHL	LAELAKKVAHLLTKE	GINESQISRWKGDFI	KVADALGINESQISR
1 iteration	10 iterations	480 iterations	1680 iterations

Phase Shifts

The Gibbs sampling algorithm may easily converge on a local optimum that is a "phase-shifted" version of the global optimum. **Why?**

Optimal solution:
Solution found:
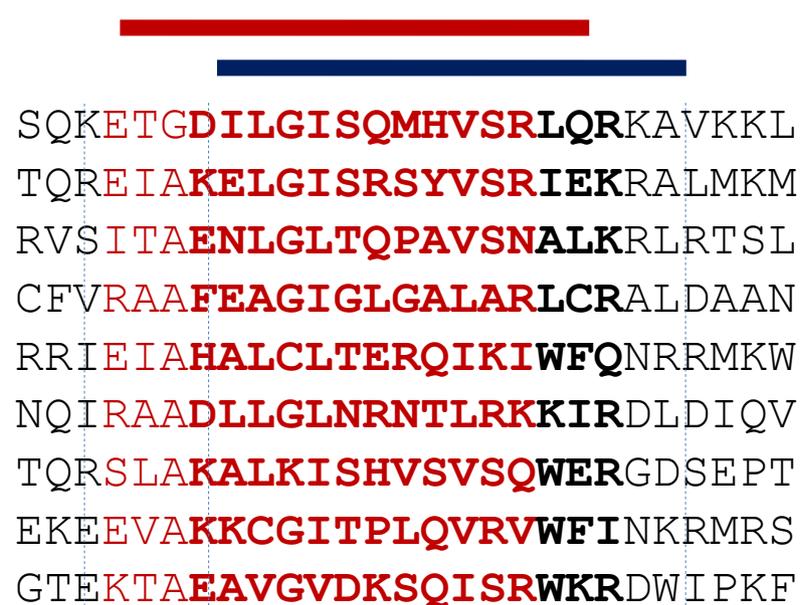
```
SQKETGDILGISQMHVSRLQRKAVKKL
TQREIAKELGISRSYVSRIEKRALMKM
RVSITAENLGLTQPAVSNALKRLRTSL
CFVRAAFEAGIGLGALARLCRALDAAN
RRIEIAHALCLTERQIKIWFQNRRMKW
NQIRAADLLGLNRNTLRKKIRDLDIQV
TQRSLAKALKISHVSVSQWERGDSEPT
EKEEVAKKCGITPLQVRVWFINKRMRS
GTEKTAEAVGVDKSQISRWKRDWIPKF
```

• • •   • • •

One remedy is to add a separate "phase-shift sampling step".

No segments are removed, but likelihoods are calculated for the current alignment and several phase-shifted alternatives.

This can be understood as changing the topology, of definition of distance, on the underlying "alignment space."