BMI/CS 776
Lecture 26
Parametric Inference

Colin Dewey

2007.04.26

Polytope algebra

- Natural to define addition and multiplication of polytopes: $\mathit{polytope\ algebra}\ \left(\mathcal{P}_d, \oplus, \odot\right)$

$$
\begin{aligned}
P \oplus Q \quad &:= \quad \mathrm{conv}(P \cup Q) \\
&= \quad \left\{ \lambda p + (1-\lambda) q \in \mathbb{R}^d \ : \ p \in P,\, q \in Q,\, 0 \leq \lambda \leq 1 \right\}.
\end{aligned}
$$

(convex hull of union)

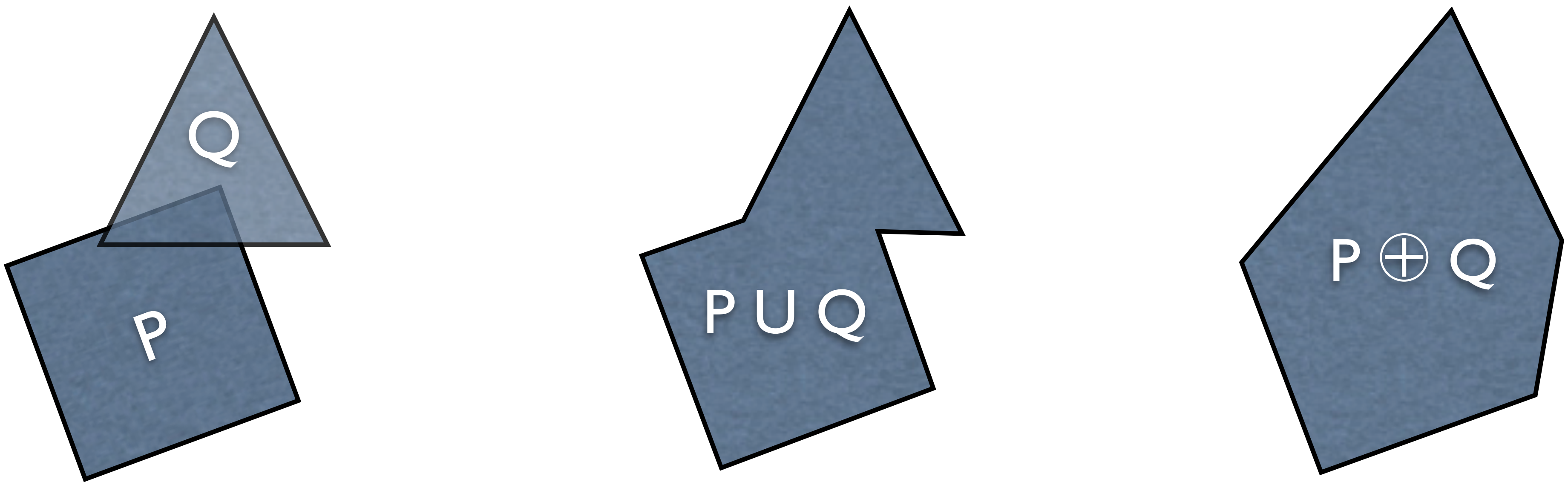
$$
\begin{aligned}
P \odot Q \quad &:= \quad P + Q \\
&= \quad \left\{ p + q \in \mathbb{R}^d \ : \ p \in P,\, q \in Q \right\}.
\end{aligned}
$$

(Minkowski sum)

Polytope addition

$$\begin{aligned} P \oplus Q \quad &:= \quad \mathrm{conv}(P \cup Q) \\ &= \quad \left\{ \lambda p + (1-\lambda) q \in \mathbb{R}^d \ : \ p \in P, \, q \in Q, \, 0 \le \lambda \le 1 \right\}. \end{aligned}$$

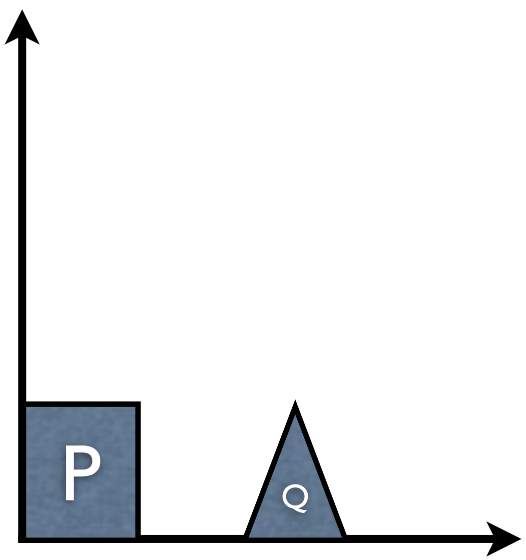
(convex hull of union)

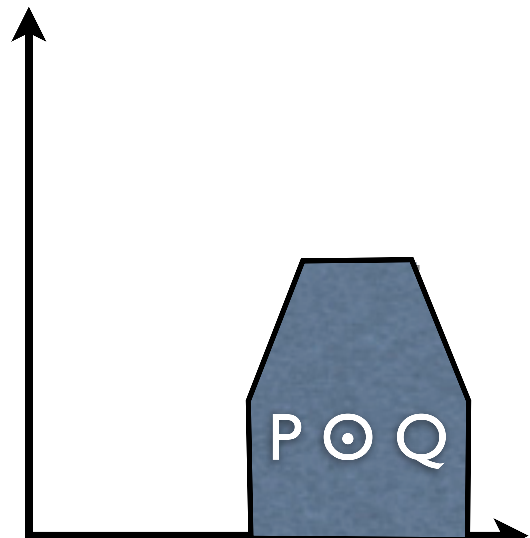


Polytope multiplication

$$\begin{aligned} P \odot Q \quad &:= \quad P + Q \\ &= \quad \{\, p + q \in \mathbb{R}^d \;:\; p \in P,\, q \in Q \,\}. \end{aligned}$$

(Minkowski sum)





Properties of polytope algebra

- Addition and multiplication both commutative
- Distributive property also holds

Proposition *If P, Q, R are polytopes in $\mathbb{R}^d$ then*

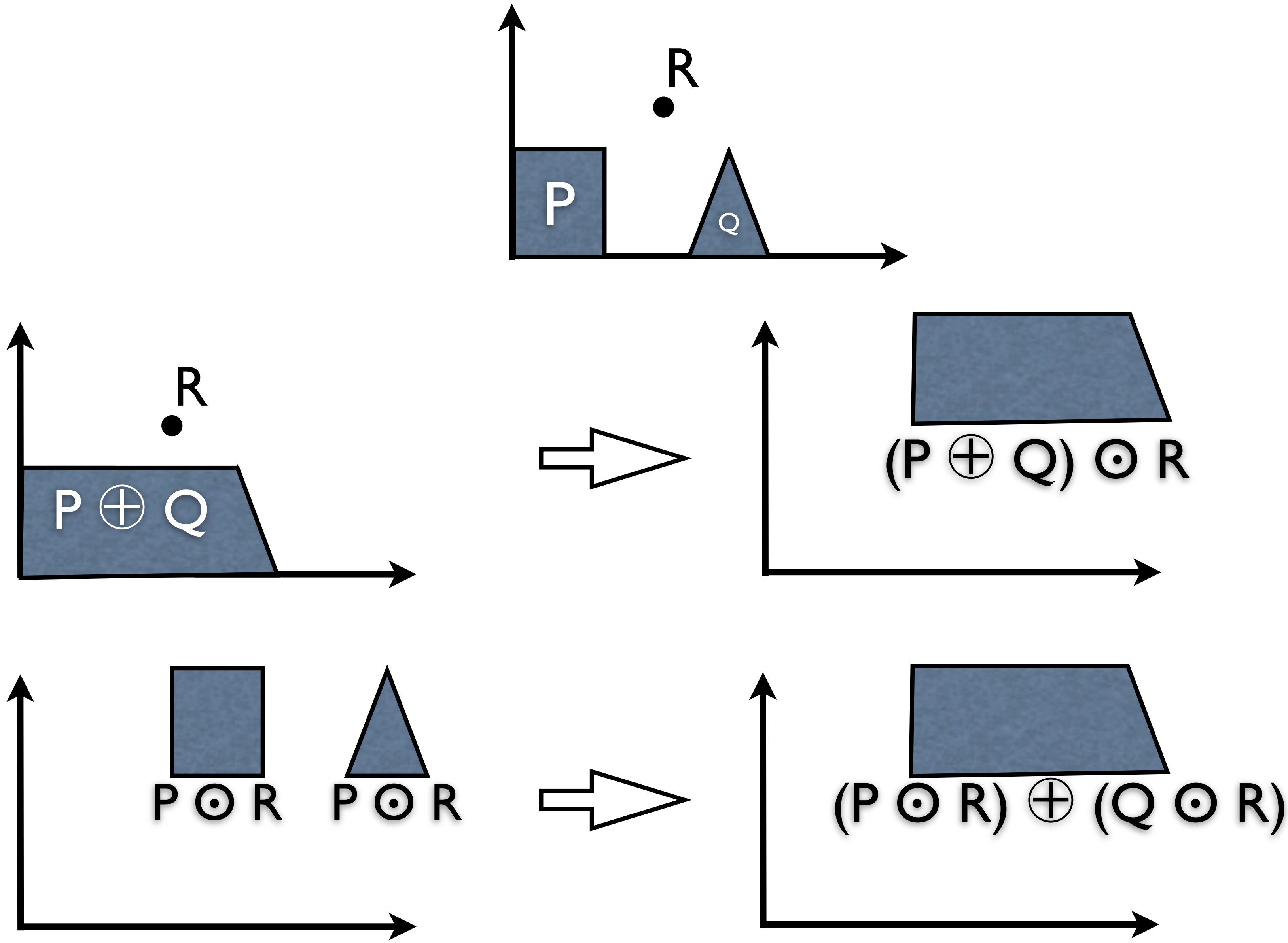
$$(P \oplus Q) \odot R \quad = \quad (P \odot R) \oplus (Q \odot R). \qquad (1)$$

Proof Consider points $p \in P$, $q \in Q$ and $r \in R$. For $0 \leq \lambda \leq 1$ note that

$$(\lambda p + (1-\lambda)q) + r \quad = \quad \lambda(p+r) + (1-\lambda)(q+r).$$

The left hand side represents an arbitrary point in the left hand side of (1), and the right hand side represents a point in the right hand side of (1) $\square$

Distributive property



Newton polytope

- Every polynomial has a corresponding polytope called the *Newton polytope*

Polynomial in d variables, $\theta_1, \theta_2, \dots, \theta_d$:

$$f = \sum_{i=1}^{n} c_i \cdot \theta_1^{v_{i1}} \theta_2^{v_{i2}} \cdots \theta_d^{v_{id}}$$

$$c_i \in \mathbb{R},$$

exponent vector of *i*th monomial: $v_i = (v_{i1}, v_{i2}, \dots, v_{id}) \in \mathbb{N}^d, \forall i$

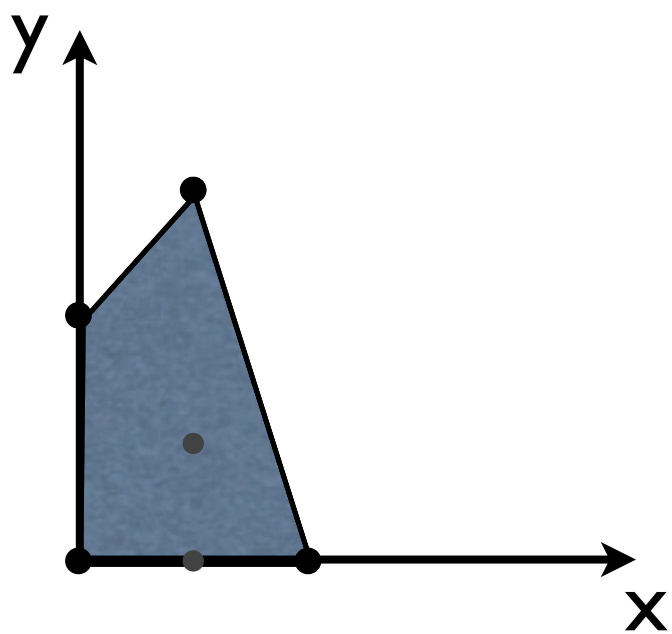
- The newton polytope is the convex hull of the exponent vectors of the monomials

$$\mathrm{NP}(f) := \mathrm{conv}\{v_1, v_2, \dots, v_n\} \subset \mathbb{R}^d.$$

Example Newton polytope

$$f = 1 + 3x + 9xy + 2x^2 + 5y^2 + xy^3$$

exponent vectors: $(0,0), (1,0), (1,1), (2,0), (0,2), (1,3)$



Newton polytope algebra

Theorem 2.25 *Let f and g be polynomials in $\mathbb{R}[\theta_1, \ldots, \theta_d]$. Then*

$$\mathrm{NP}(f \cdot g) = \mathrm{NP}(f) \odot \mathrm{NP}(g) \quad \textit{and} \quad \mathrm{NP}(f+g) \subseteq \mathrm{NP}(f) \oplus \mathrm{NP}(g).$$

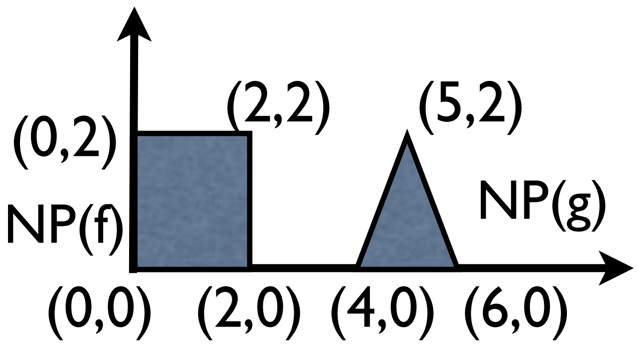
If all coefficients of f and g are positive then $\mathrm{NP}(f+g) = \mathrm{NP}(f) \oplus \mathrm{NP}(g)$.

(for proof, see book "Algebraic Statistics for Computational Biology")

Example Newton polytope algebra

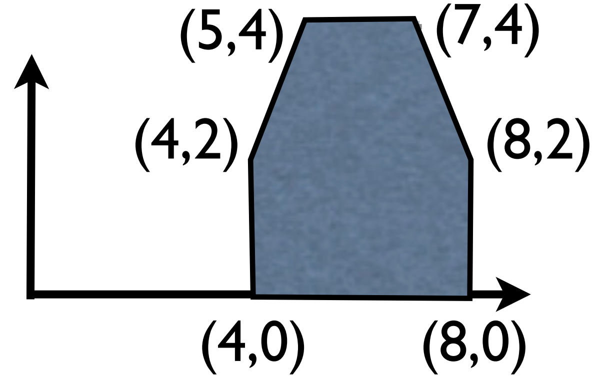
$$f = 3 + x^2 + 2x^2y^2 + 5y^2$$

$$g = 3x^4 + x^5y^2 + 2x^6$$

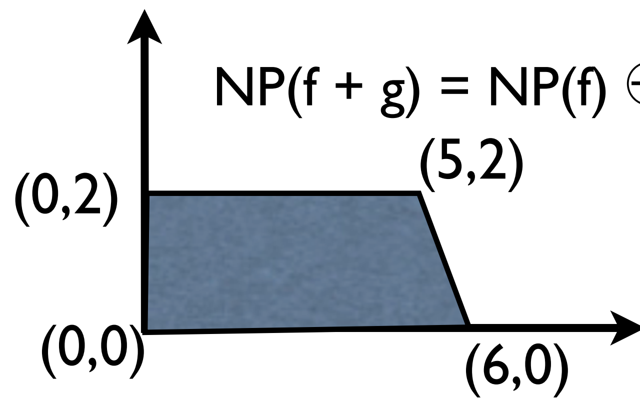


$$f \cdot g = 9x^4 + 6x^6 + 2x^8 + 15x^4y^2 + 3x^5y^2 + 16x^6y^2 + x^7y^2 + 5x^5y^4 + 4x^8y^2 + 2x^7y^4$$

NP(f · g) = NP(f) ⊙ NP(g)



$$f + g = 3 + x^2 + 2x^2y^2 + 5y^2 + 3x^4 + x^5y^2 + 2x^6$$



Probabilistic models and newton polytopes

- HMM example

$$\text{Prob}(\tau) = \sum_{\sigma} p_{\sigma,\tau}$$

$$p_{\sigma,\tau} = \frac{1}{l}\theta'_{\sigma_1,\tau_1}\theta_{\sigma_1,\sigma_2}\theta'_{\sigma_2,\tau_2}\theta_{\sigma_2,\sigma_3}\dots\theta'_{\sigma_n,\tau_n}$$

The probability of each parse is of the form $x_1^{v_1} x_2^{v_2} \cdots x_d^{v_d}$

We wish to find the MAP parse: $\bar{\sigma} = \text{argmax}_\sigma\{p_{\sigma,\tau}\}$

equivalently

$$\bar{\sigma} = \text{argmax}_\sigma \log p_{\sigma,\tau}$$

Recursive decomposition

- Inference function can be decomposed
- Allow for efficient computation

$$\mathrm{Prob}(\tau) = \sum_{\sigma} p_{\sigma,\tau}$$

$$p_{\tau} = \sum_{\sigma_n=1}^{l} \theta'_{\sigma_n,\tau_n} \left(\sum_{\sigma_{n-1}=1}^{l} \theta_{\sigma_{n-1},\sigma_n} \theta'_{\sigma_{n-1},\tau_{n-1}} \left(\cdots \left(\sum_{\sigma_1=1}^{l} \theta_{\sigma_1,\sigma_2} \theta'_{\sigma_1,\tau_1} \right) \cdots \right) \right)$$

Polytope propagation algorithm

- Sum-product algorithm (e.g., forward algorithm for HMMs) with:
  - Parameters replaced by unit vectors
  - Sum replaced convex hull of union
  - Product replaced by Minkowski sum
  - That is, we are running the algorithm with the polytope algebra instead of $(+,\times)$
- Output is the Newton polytope of the inference function

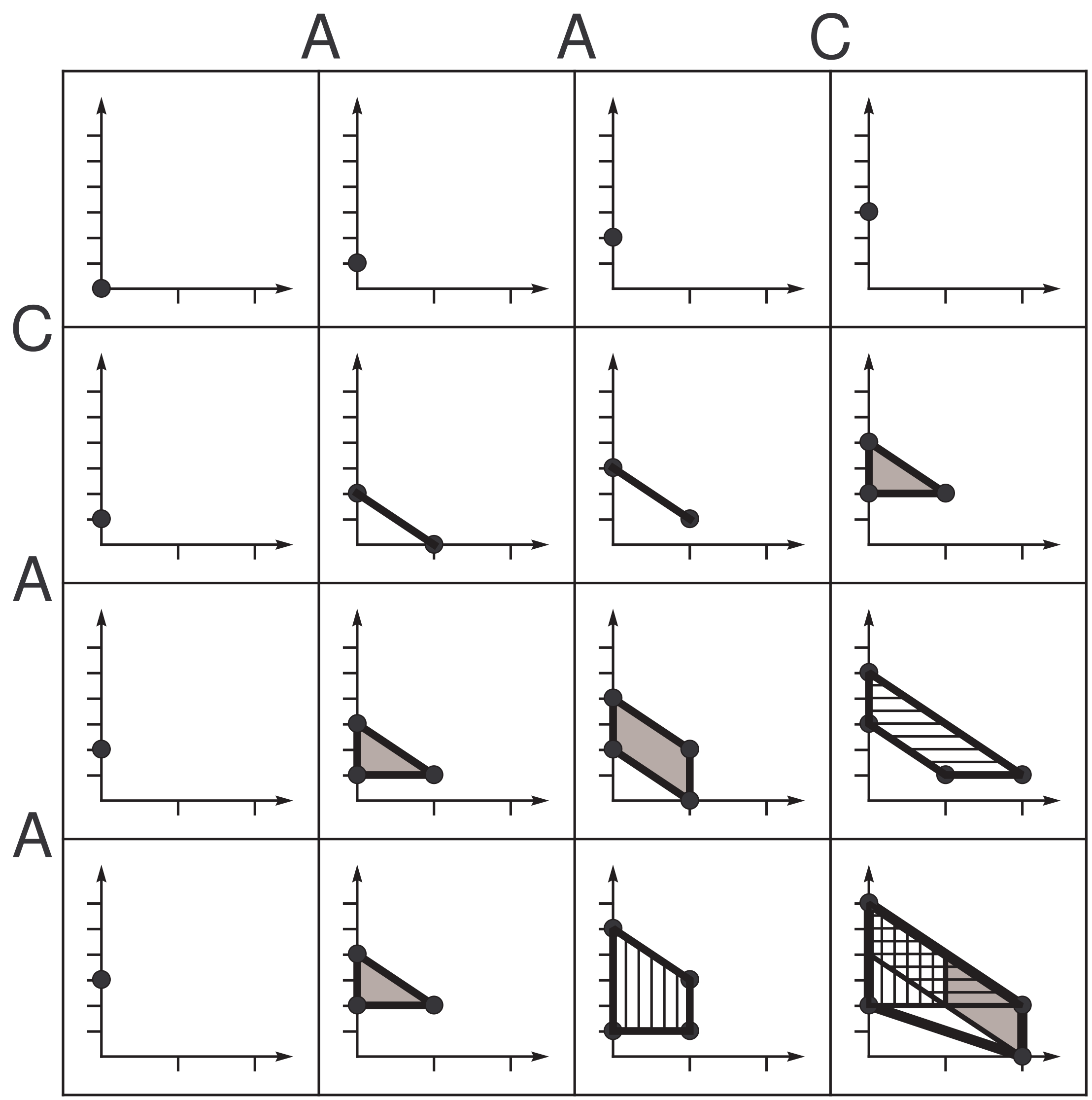
Parametric alignment

- Use same recurrences as Needleman-Wunsch
- Entries are now polytopes not numbers
- Parameters are vectors

$$P[i,j] = \mathrm{conv}\left(\begin{array}{l} P[i-1,j-1] \odot v(\sigma_i^1, \sigma_j^2) \quad \cup \\ P[i-1,j] \odot \{(0,1)\} \quad \cup \\ P[i,j-1] \odot \{(0,1)\} \end{array} \right)$$

(for simple mismatch, space scoring scheme)

Parametric alignment



Implementation

```
template<typename SemiRing>
void
alignGlobalLastRow(const string& seq1,
                   const string& seq2,
                   const typename SemiRing::Element match,
                   const typename SemiRing::Element mismatch,
                   const typename SemiRing::Element gap,
                   vector<typename SemiRing::Element>& row);
```

Implementation

```
const Element one = SemiRing::multiplicativeIdentity;
// Initialize row
row.resize(seq2.size() + 1);
row[0] = one;
// Calculate first row
for (size_t j = 1; j <= seq2.size(); ++j)
    row[j] = gap * row[j - 1];
// Calculate remaining rows
Element up, diag;
for (size_t i = 1; i <= seq1.size(); ++i) {
    diag = row[0];
    row[0] *= gap;
    for (size_t j = 1; j <= seq2.size(); ++j) {
        up = row[j];
        if (seq1[i - 1] == seq2[j - 1]) {
            row[j] = match * diag + gap * (up + row[j - 1]);
        } else {
            row[j] = mismatch * diag + gap * (up + row[j - 1]);
        }
        diag = up;
    }
}
```

Hemoglobin alignment

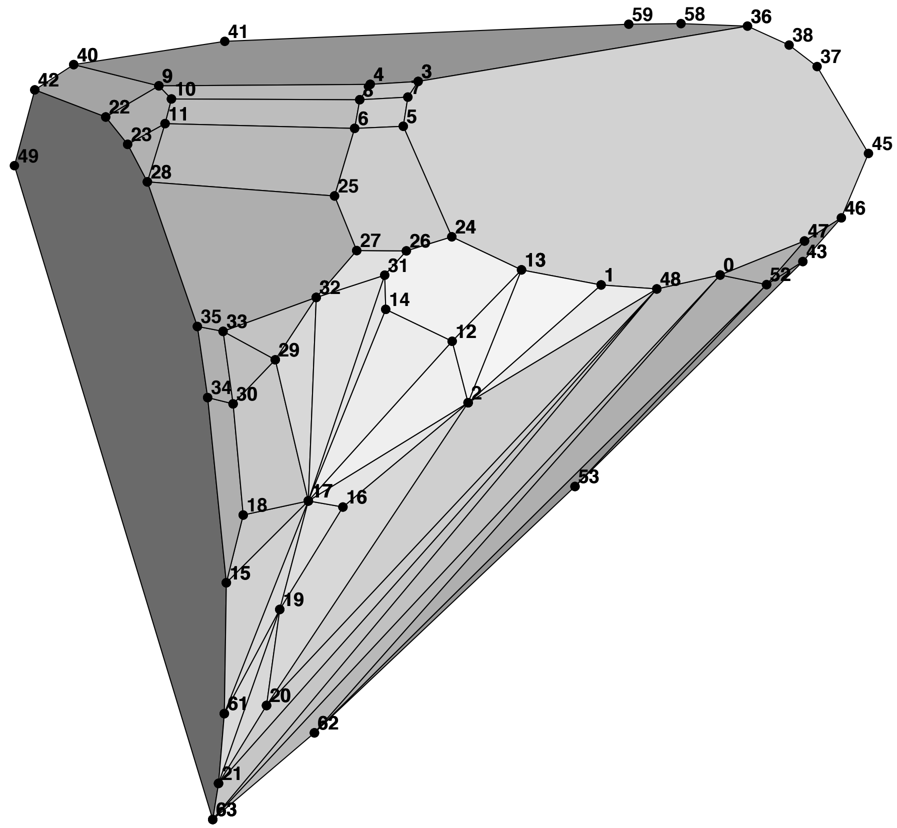
β FASFGNLSSPTAILGNPMV
α FPHF-DLSH-----GSAQI.

h_1
β UUUGCGUCCUUUGGGAACCUCUCCAGCCCCACUGCCAUCCUUGGCAACCCCAUGGUC
α UUUCCCACUUC---GAUCUGUCACAC---------------GGCUCCGCUCAAAUC.

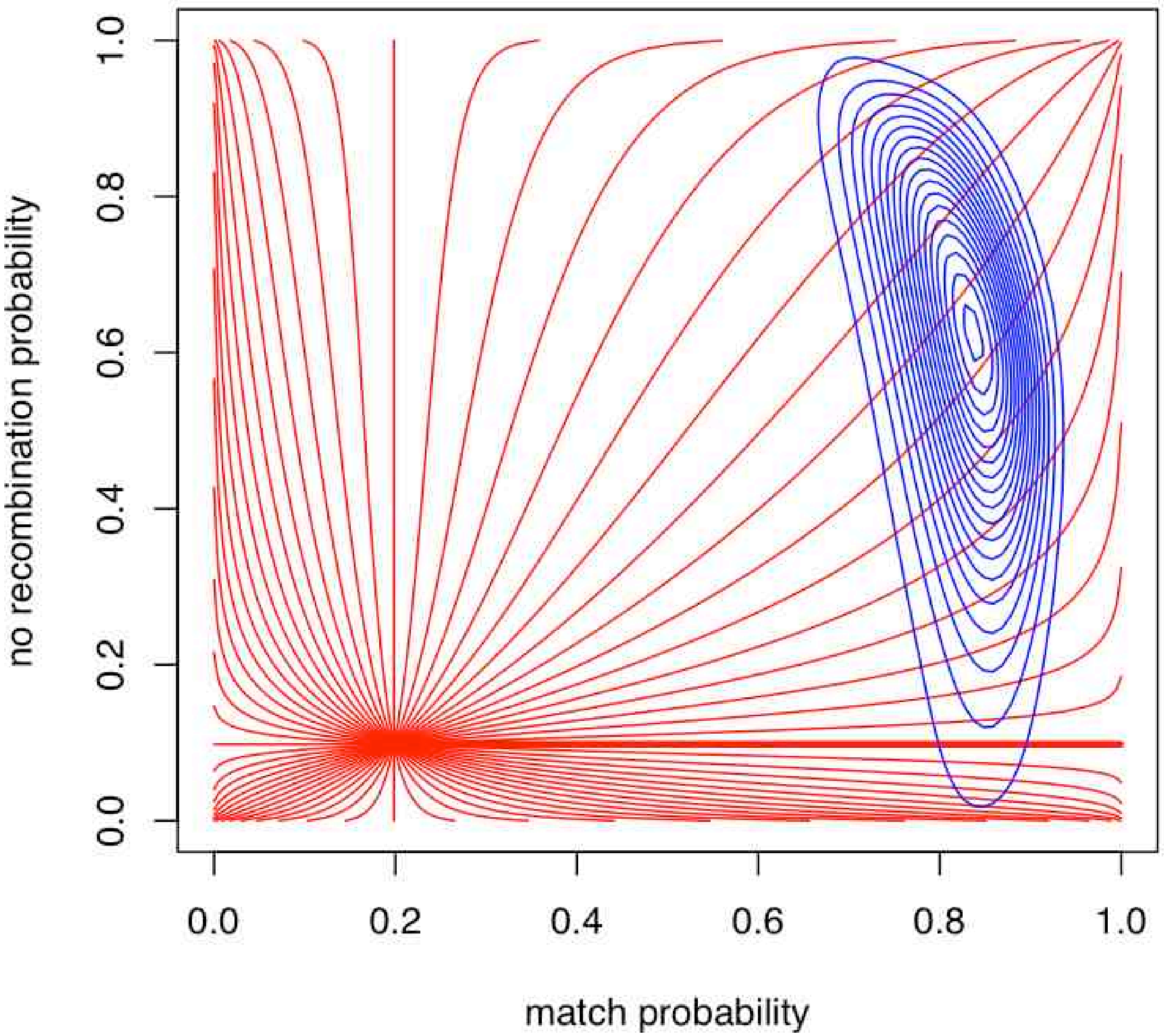
h_2
β UUUGCGUCCUUUGGGAACCUCUCCAGCCCCACUGCCAUCCUUGGCAACCCCAUGGUC
α UUUCCCACUUCG---AUCUGUCACAC---------------GGCUCCGCUCAAAUC,

Two possible alignments of mRNA

Hemoglobin alignment polytope



Normal cones and likelihood surfaces



Blue: Likelihood surface

Red: Subdivision of parameter space into regions with same MAP estimate