BMI/CS 776
Lecture 26
Parametric Inference

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Polytope algebra

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

\[
P \oplus Q := \text{conv}(P \cup Q)
= \{ \lambda p + (1 - \lambda)q \in \mathbb{R}^d : p \in P, q \in Q, 0 \leq \lambda \leq 1 \}.
\]

(convex hull of union)

\[
P \odot Q := P + Q
= \{ p + q \in \mathbb{R}^d : p \in P, q \in Q \}.
\]

(Minkowski sum)
Polytope addition

\[ P \oplus Q := \text{conv}(P \cup Q) \]
\[ = \{ \lambda p + (1 - \lambda)q \in \mathbb{R}^d : p \in P, q \in Q, 0 \leq \lambda \leq 1 \}. \]

(convex hull of union)
Polytope multiplication

\[ P \odot Q := P + Q \]

\[ = \{ p + q \in \mathbb{R}^d : p \in P, q \in Q \} . \]

(Minkowski sum)

\[ \begin{array}{c}
P \odot Q \\
\end{array} \]

\[ \begin{array}{c}
P \oplus Q \\
\end{array} \]
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

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

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

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

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). \qed
Distributive property

\[(P \oplus Q) \odot R = (P \odot R) \oplus (Q \odot R)\]
Newton polytope

- Every polynomial has a corresponding polytope called the Newton polytope

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

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

exponent vector of $i$th monomial:

$$v_i = (v_{i1}, v_{i2}, \ldots, v_{id}) \in \mathbb{N}^d, \forall i$$

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

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

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

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

(for proof, see book “Algebraic Statistics for Computational Biology”)

Example Newton polytope algebra

\[ f = 3 + x^2 + 2x^2y^2 + 5y^2 \]
\[ g = 3x^4 + x^5y^2 + 2x^6 \]

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

\[ \text{NP}(f \cdot g) = \text{NP}(f) \otimes \text{NP}(g) \]

\[ f + g = 3 + x^2 + 2x^2y^2 + 5y^2 + 3x^4 + x^5y^2 + 2x^6 \]

\[ \text{NP}(f + g) = \text{NP}(f) \oplus \text{NP}(g) \]
Probabilistic models and newton polytopes

- HMM example

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

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

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: \( \tilde{\sigma} = \arg\max_{\sigma} \{ p_{\sigma, \tau} \} \)

equivalently

\( \tilde{\sigma} = \arg\max_{\sigma} \log p_{\sigma, \tau} \)
Recursive decomposition

- Inference function can be decomposed
- Allow for efficient computation

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

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

- 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

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

(for simple mismatch, space scoring scheme)
Parametric alignment

Fig. 7.2. $P[i, j]$ with $\sigma_1 = CAA$ and $\sigma_2 = AAC$. 

(max, +) algebra (which is ... to determine $P[3, 3]$ from $P[2, 2]$, $P[2, 3]$, and $P[3, 2]$. Table 7.1 lists, for each vertex of the polytope...
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);
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

$\beta$ FASFGNLSSPTAILGNPMV
$\alpha$ FPHF-DLSH------GSAQI.

$h_1$

$\beta$ UUUGCGUCCUUUGGAACCUCUCCAGCCCCACUGCAAUCCUUUGGCAACCCCAUGGUC
$\alpha$ UUCCCCACUUC---GAUCUGUCACAC------------------------GGCUCCGCUCAAAUC.

$h_2$

$\beta$ UUUGCGUCCUUUGGAACCUCUCCAGCCCCACUGCAAUCCUUUGGCAACCCCAUGGUC
$\alpha$ UUCCCCACUUCG---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