Projection onto the Convex Hull of Point Cloud

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UGRC Presentation

Problem Setup

- We study quantum states represented by density matrices $X \in \mathbb{C}^{4\times 4}$.
- Goal: Determine whether a state P is **separable** or **entangled**.
- Separable set:

$$\mathrm{SEP} = \{X \succeq 0,\ \mathrm{Tr}(X) = 1,\ X^{T_B} \succeq 0\}.$$

- Key task: Project a given point P onto $\mathrm{conv}(S) = \mathrm{SEP}$.
- Access to an inner product oracle

$$\mathcal{O}_X(A) = \mathrm{Tr}(A^\dagger X),$$

PPT Criterion

- A two–qubit state is separable iff its partial transpose is positive semidefinite(PPT Criterion):

$$X \in \mathrm{SEP} \quad \Longleftrightarrow \quad X^{T_B} \succeq 0.$$

- Useful as a fast membership test.
- If X^{T_B} has a negative eigenvalue: state is entangled.

Reconstructing X from Pauli Inner Products

- The 4×4 Hermitian space is 16-dimensional with orthonormal basis

$$\{\sigma_\alpha \otimes \sigma_\beta : \alpha, \beta = 0, 1, 2, 3\},$$

  where $\sigma_0 = I$ and $\sigma_{1,2,3}$ are Pauli matrices.

- Compute coefficients by inner product:

$$c_{\alpha\beta} = \mathrm{Tr}[(\sigma_\alpha \otimes \sigma_\beta)\, X]\,.$$

- Since the basis is orthonormal,

$$X = \frac{1}{4} \sum_{\alpha,\beta=0}^{3} c_{\alpha\beta}\, (\sigma_\alpha \otimes \sigma_\beta).$$

- Thus: measure all 16 expectation values $\{c_{\alpha\beta}\}$ ⇒ fully reconstruct the operator P.

Projection as an SDP

- Want the Frobenius-norm projection of P onto SEP:

$$X^{\star} = \arg\min_{X} \|X - P\|_F^2$$

$$\text{s.t. } X \succeq 0,\ \mathrm{Tr}(X) = 1,\ X^{T_B} \succeq 0.$$

- Convex objective + convex (spectrahedral) constraints ⇒ globally solvable.

Geometric Interpretation

- The set SEP is the convex hull of product pure states.
- Projection problem becomes:

$$\min_{w \geq 0, \sum w_i = 1} \|S^\top w - P\|_F^2,$$

  where columns of S are generator vertices.
- projection is obtained by solving the above convex problem using CVXPY.

Generic Problem Statement

- Given a set of points S and a point P, comment on the membership of P in conv(S)
- if P lies outside conv(S) then also give projection and hence supporting hyperplane.

Convex Hull Feasibility Test

- Goal: Check whether a point $P \in \mathbb{R}^d$ lies in $\mathrm{conv}(S)$, where $S = \{x_1, \ldots, x_n\}$.
- Solve the LP in variables $\lambda_1, \ldots, \lambda_n$:

$$\min 0 \quad \text{s.t.}$$

  - Matching coordinates:

$$\sum_{i=1}^{n} \lambda_i \, x_i[j] = P[j], \quad j = 1, \ldots, d$$

  - Sum-to-one constraint:

$$\sum_{i=1}^{n} \lambda_i = 1$$

  - Non-negativity:

$$\lambda_i \geq 0 \quad \forall i$$

Method 1: Projection using Face-Walking

- Goal: compute the projection of a point p onto $\mathrm{conv}(S)$ without solving a global QP.
- Start from a boundary point x_0 on the convex hull.
- Repeatedly:
  - Identify the hull facet (simplex) containing current x.
  - Work entirely within that face's affine hull.
  - Move in the direction that decreases $\|x - p\|$.
- Algorithm transitions smoothly across faces until the projection is reached.

Face-Walking: Step Mechanics

- For current face with vertices $\{v_i\}$:
  - Compute gradient $g = x - p$.
  - Project g onto the tangent space of the face: $g_{\text{tan}} = \Pi_{\text{aff}(F)}(g)$.
  - Convert direction into barycentric update $\beta' = \beta + s\gamma$.
- Step size s: first time a barycentric coordinate hits zero:

$$s^{=\min_{j:\,\gamma_j<0}} \left(-\frac{\beta_j}{\gamma_j}\right).$$

- Move to the new point $x \leftarrow x + s^d$; transition to a lower-dimensional face if needed.

Termination & Output

- Algorithm stops when:
  - Projection of p onto the face's affine hull lies *inside* the face.
  - Or tangent gradient vanishes (stationary on face).
  - Or the minimizer is a vertex.
- Final results:
  - Approximate projection x_{proj}.
  - Sequence of visited boundary points (walk path).
  - Final supporting face and termination reason.

Method 2: Projection using Active Set

- Compute

$$x_{\text{proj}} = \arg \min_{x \in \mathrm{conv}(S)} \|x - P\|^2.$$

- Represent x as $S^\top w$ with $w \geq 0, \sum w = 1$.
- Maintain an active set A of vertices.
- Start at nearest vertex to P: $A = \{k\}, \ w = [1]$.
- Core tool: small QPs solved via OSQP → CVXOPT → SLSQP.

Active-Set Iterations

- Compute KKT directional tests $\Delta_i = (x - P)^\top (s_i - x)$.
- If all $\Delta_i \geq -\varepsilon$: optimal.
- Otherwise add violator $j = \arg\min \Delta_i$ to active set.
- Solve small QP:

$$\min_w \|V_A w - P\|^2, \quad w \geq 0, \ \sum w = 1.$$

- If solution has all $w \geq 0$: accept and update x.

Drop Step & Final Output

- If QP solution has negative weights:
  - Interpolate between old and new weights.
  - Compute $t^{=\min \frac{w_i^{\text{old}}}{w_i^{\text{old}}-w_i^{\text{new}}}}$.
  - Drop any vertex whose weight hits zero.
  - Re-solve QP on reduced active set.
- Final results:
  - Active vertices A.
  - Weights $w \geq 0, \ \sum w = 1$.
  - Projection: $x_{\text{proj}} = S^\top w$.

Charged Ball Method: Intuition & Goal

- Abbasov, 2017 (link to paper)
- Goal: Find the boundary point of $X = \{x : f(x) \leq 0\}$ closest to the origin (orthogonal projection).
- Physical analogy:
  - A positively charged ball moves inside X.
  - It is attracted to the origin by an inverse–square force.
  - Boundary reacts by cancelling the normal force, so motion becomes *tangential* on $\mathrm{bd}\, X$.
  - Viscous damping gradually reduces velocity.
- At equilibrium: tangential force vanishes $\Rightarrow$ ball stops at the closest boundary point.

Method 3: Charged Ball Method: Iteration Mechanics

- Each iteration updates:
  - **Position** via an Euler predictor: $\tilde{x} = x + \delta z$.
  - **Projection** back to boundary: $x_{\text{new}} = \mathrm{Proj}_{\mathrm{bd}X}(\tilde{x})$.
  - **Tangential driving direction** $\psi(x)$ (from Coulomb attraction).
  - **Curvature correction** $\chi(x, z)$ (accounts for boundary geometry).
- Velocity update:

$$z_{\text{new}} = z + \delta\big(p_1\psi - p_2 z - \chi\big).$$

- Step-size control: compare boundary-correction magnitude and adapt δ (increase, decrease, or accept).

Termination & Output

- Algorithm stops when:
    - Tangential driving force becomes small: $\|\psi(x)\| \leq \varepsilon$.
    - (Equivalently) the ball reaches equilibrium on the boundary.
- Final results:
    - Approximate projection point on $\mathrm{bd}X$.
    - Final velocity z (approximately zero at convergence).
    - Step-size history and visited boundary points.

Further directions

- dealing with higher dimension of tensor products, where there is no PPT condition to help?
- construct smooth function approximations circumscribing the convex hull and apply charged balls method.
- design an adaptive approach directly with supporting hyperplanes without involving projections.

Questions?