Exact Algebraic Computation of Learning Coefficients for Two-Dimensional Singular Statistical Models

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International Conference on Symbolic Computation and Machine Learning, 2026

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In This Talk

$$\mathrm{SC} \rightarrow \mathrm{ML}$$

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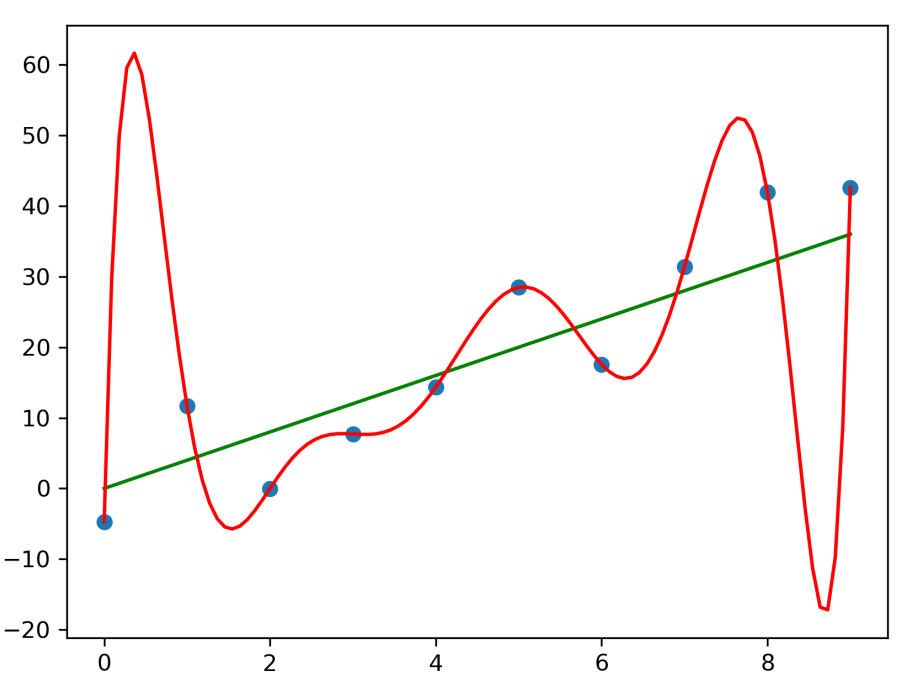
We give an application of Symbolic Computation to the analysis of Machine Learning models.

The Generalization Paradox



Model selection: choosing which model will best fit the data.

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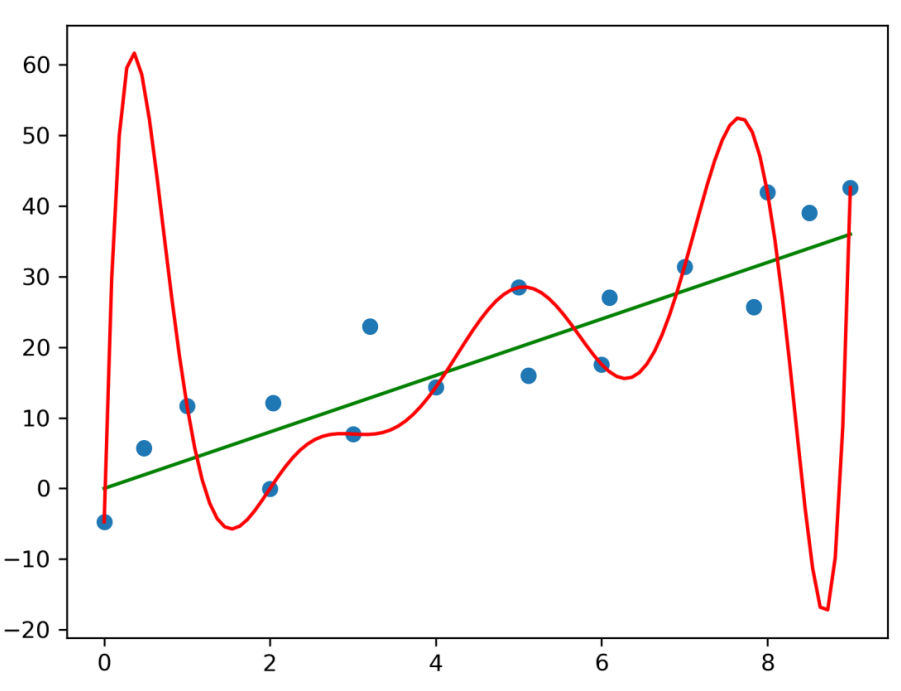

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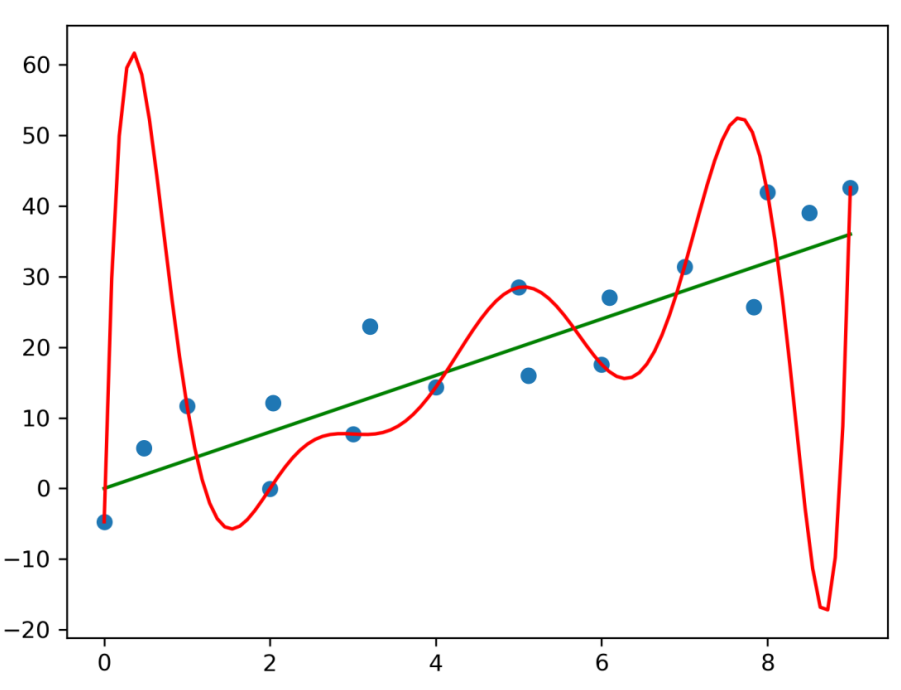
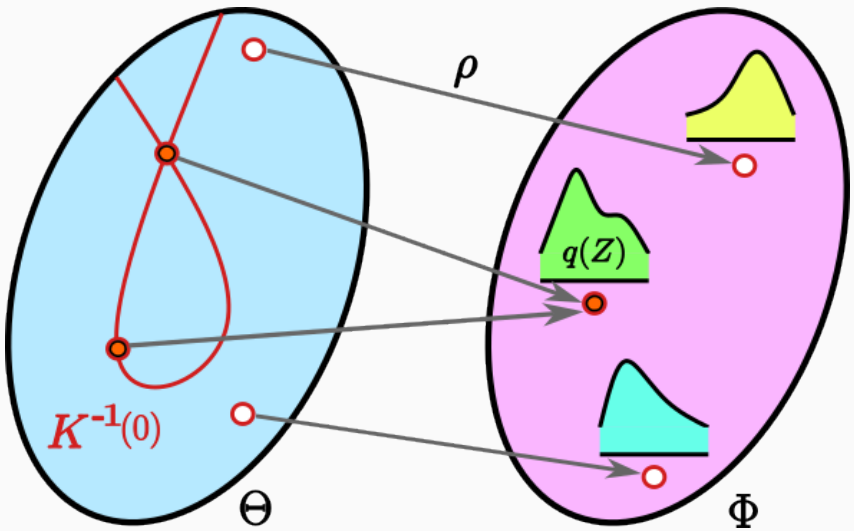


Model selection: choosing which model will best fit the data.

Deep learning (artificial neural networks, transformers) challenges the assumptions of **classical learning theory**. Why don't neural networks overfit when the number of layers is increased? Why do they generalize so well? Parameter count is not a good approach.

Parameterized Statistical Models



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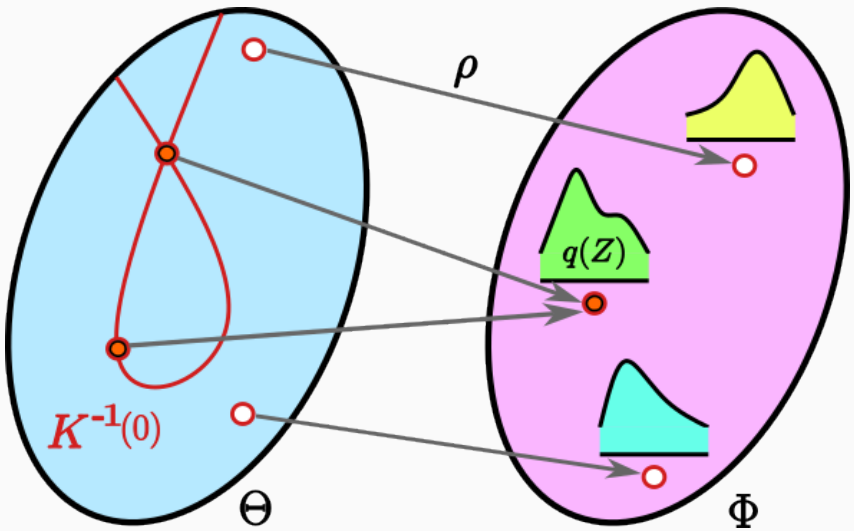

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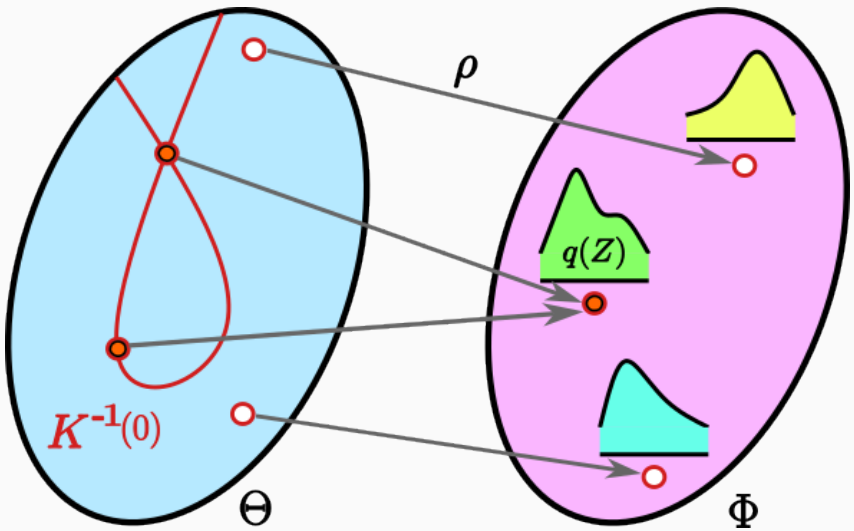

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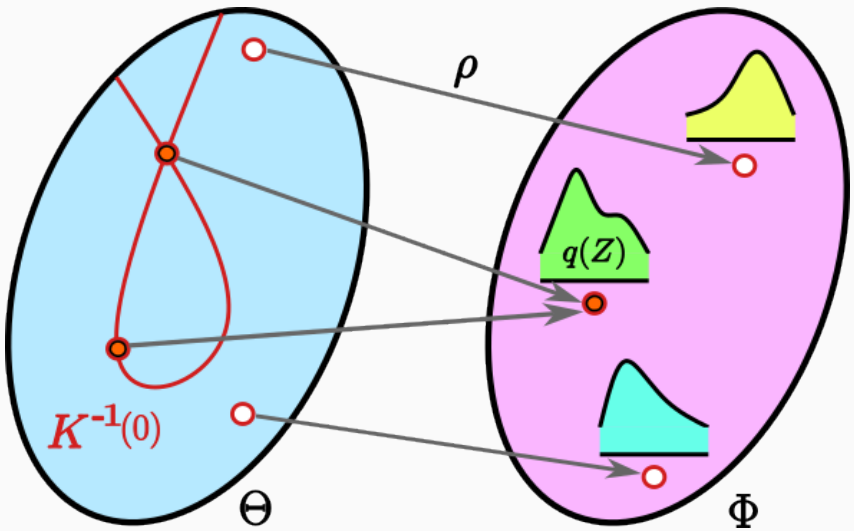

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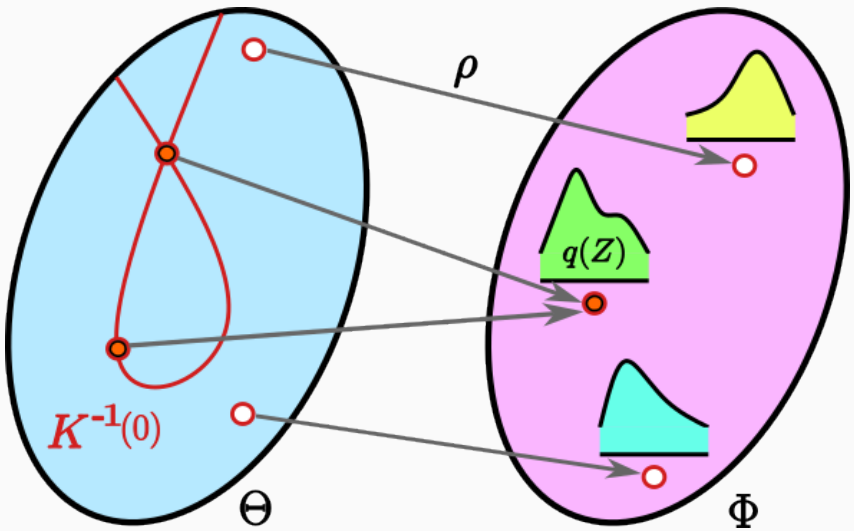

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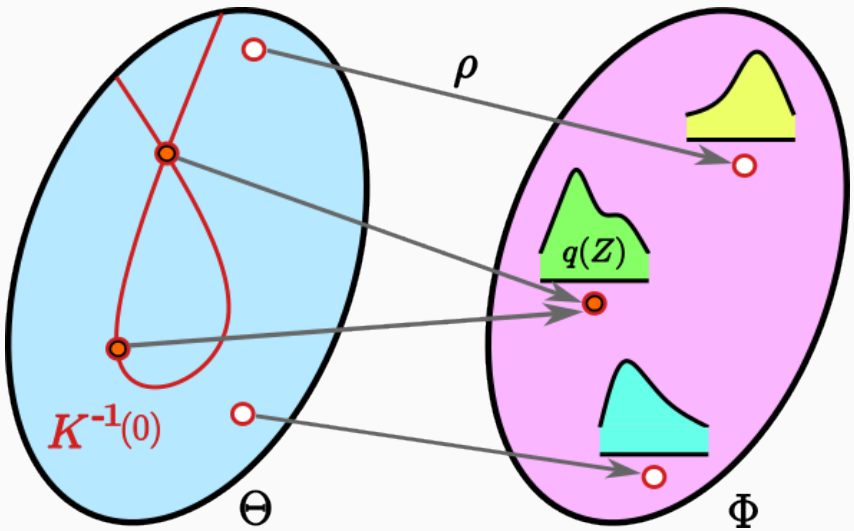

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Regular and singular models

A pair $(\Phi, q(Z))$ is **regular** if it satisfies:

1. (**Identifiability**) $\rho : \Theta \to \Phi$ is injective AND;
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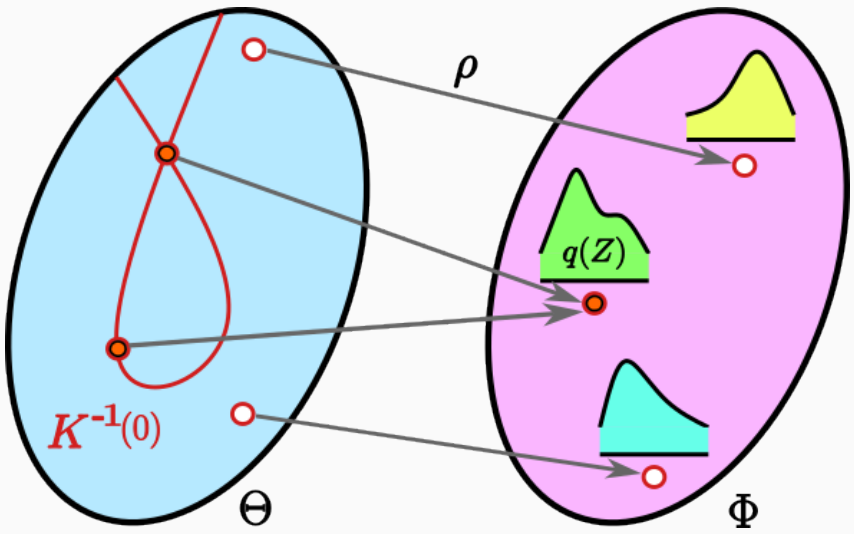

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Most models in the wild are singular.

Generalization, Model Selection & Information Criteria

Statistical Learning Theory:

- A **dataset** $D_n = \{z_1, \ldots, z_n\} \in (\mathbb{R}^m)^n$, sampled i.i.d. from $q(Z)$,

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Approach: Asymptotic approximation of the ML leads to the:

Bayesian Information Criterion [Schwarz'78]

$$\mathrm{BIC}(\Phi) = \underbrace{-nL_n(\theta_{\mathrm{MLE}})}_{\text{bias}} + \underbrace{\tfrac{d}{2}\log n}_{\text{variance}},$$

only when the model is regular!

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$$\mathrm{WBIC}(\Phi) = \underbrace{-nL_n(\theta_0)}_{\text{bias}} + \underbrace{\lambda \log n}_{\text{variance}},$$

where the **learning coefficient** $\lambda \leq \frac{d}{2}$, with equality for regular models.

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- But resolutions of singularities are notoriously hard to compute!

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This work

We modify the works of [V'76],[P et al'99],[C'18] to guarantee termination. This gives an exact algorithm to compute RLCTs in $d = 2$. We discuss its complexity.

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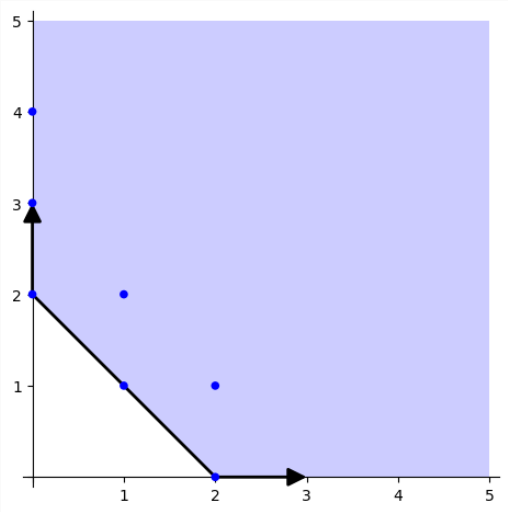

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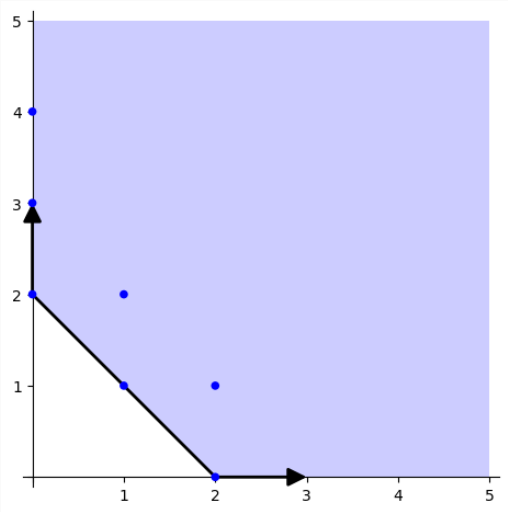

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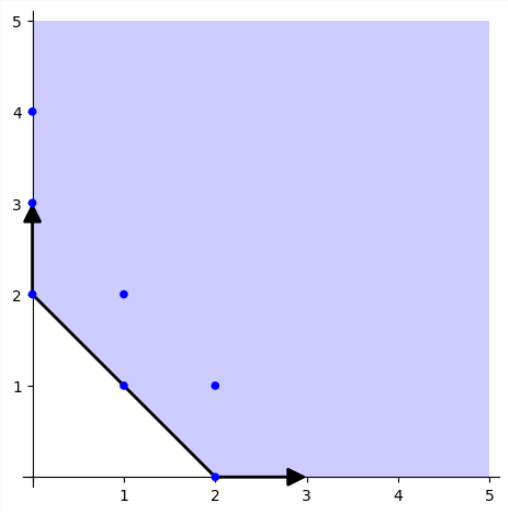

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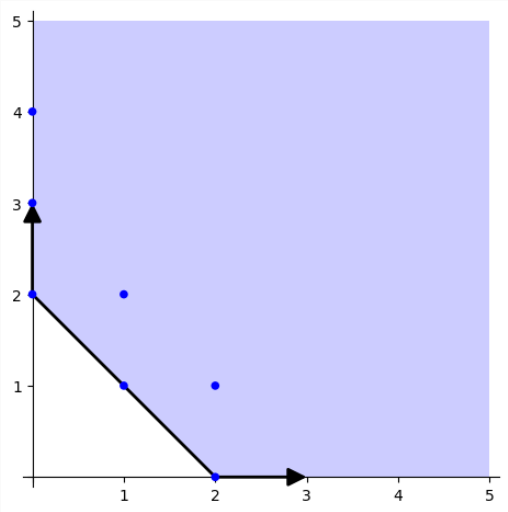

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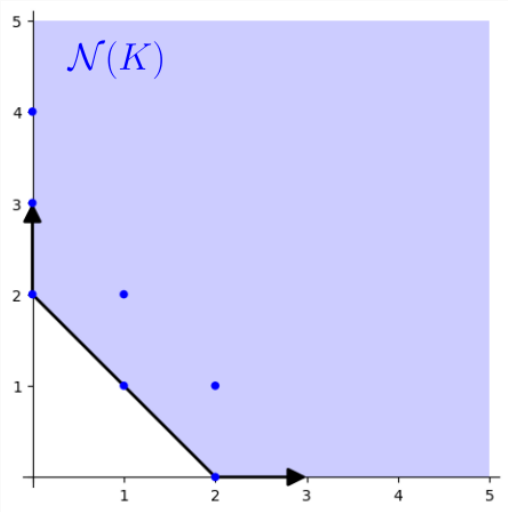

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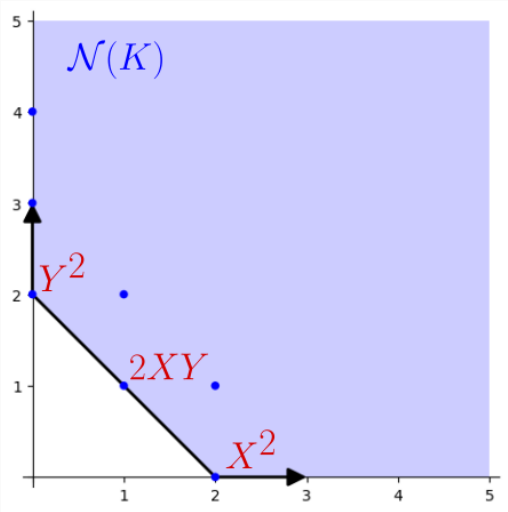

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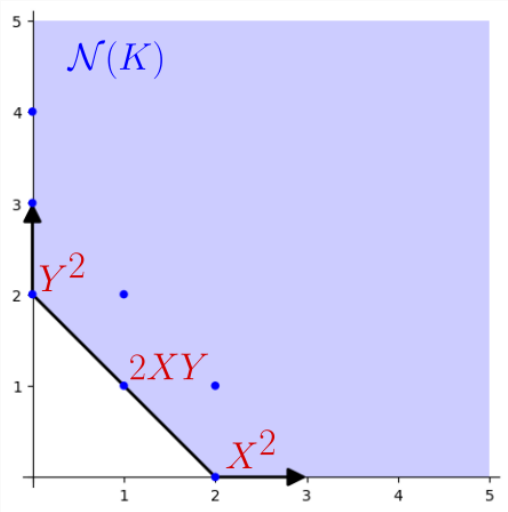

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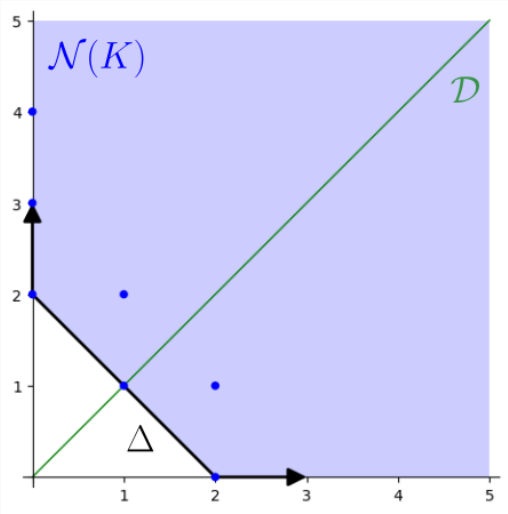

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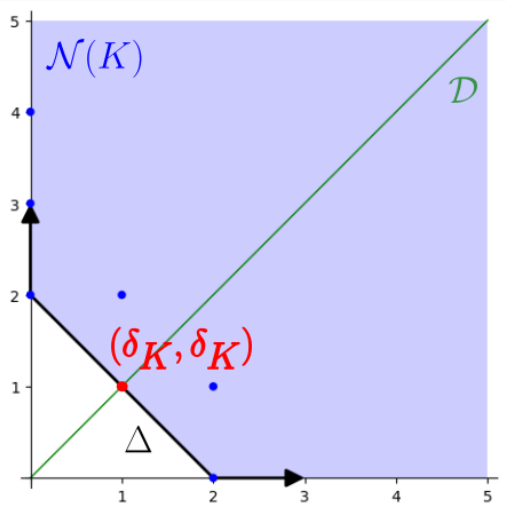

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- **Newton distance:** $\delta_K =$ coordinate of $\mathcal{D} \cap \partial\mathcal{N}(K)$.

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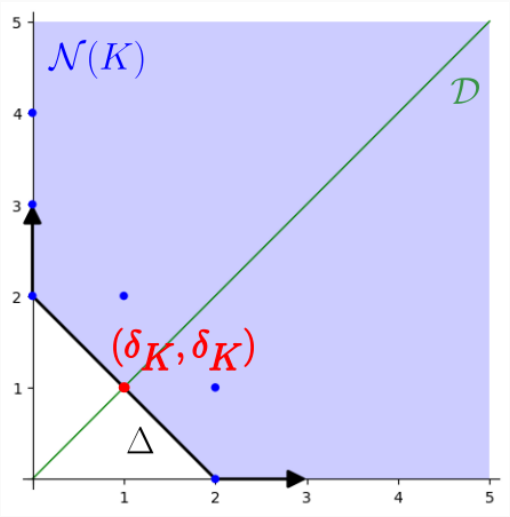

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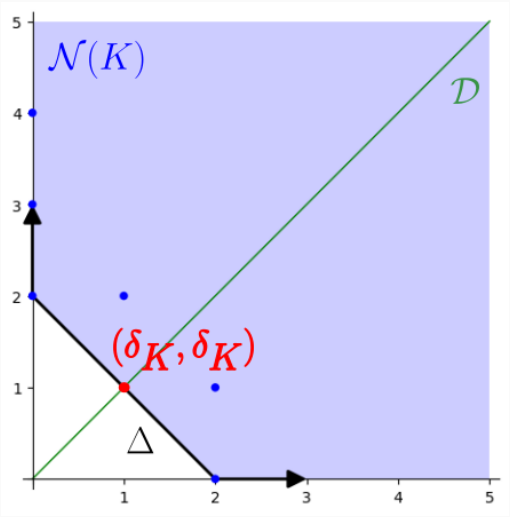
  - $K_\Delta = Y^2 + 2XY + X^2$
- **Main facet:** $\Delta =$ facet intersected by $\mathcal{D}$.
- **Newton distance:** $\delta_K =$ coordinate of $\mathcal{D} \cap \partial\mathcal{N}(K)$.
  - $\delta_K = 1$

Newton Polygon

Let $d = 2$, and $\theta = (X, Y)$. Let $K(\theta) = K(X, Y) = \sum a_{pq} X^p Y^q \in \mathbb{Q}[X][Y]$.



- $K(X, Y) = Y^2 + 2XY + X^2 + Y^3 + 4XY^2 + 3X^2Y + Y^4$
- **Support:** $S_K = \{(p, q) \mid a_{pq} \neq 0\} \subseteq \mathbb{N}^2$
  - $S_K = \{(0, 4), (0, 3), (0, 2), (1, 2), (1, 1), (2, 1), (2, 0)\}$
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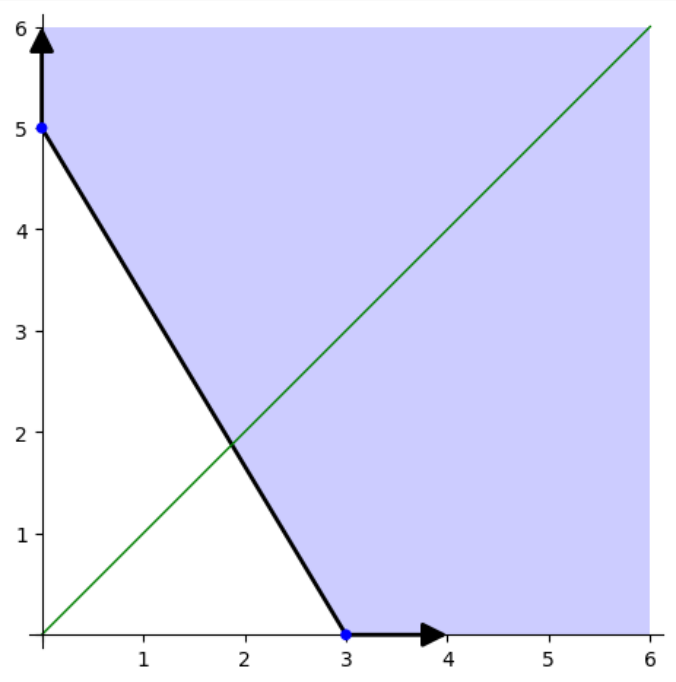

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We say that K is normalized if K_Δ has no factor in $\bar{\mathbb{Q}}[X, Y]$ of multiplicity $m > \delta_K$.

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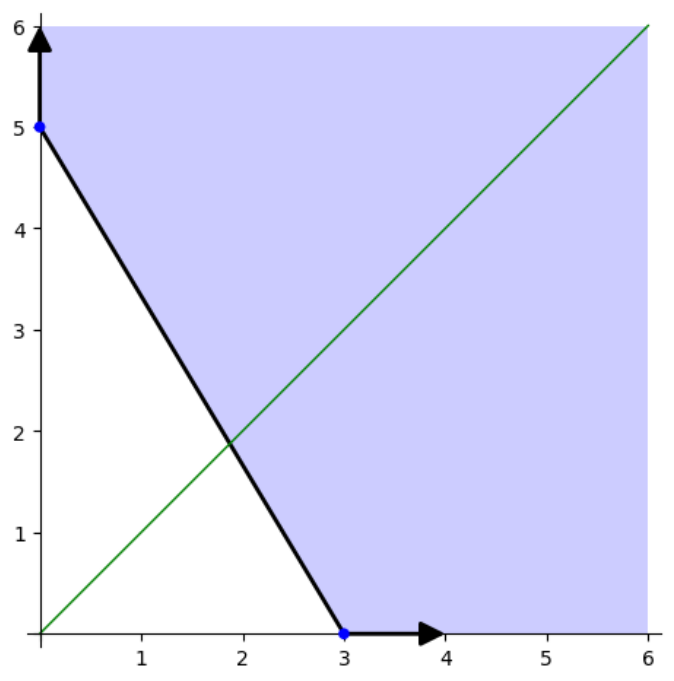

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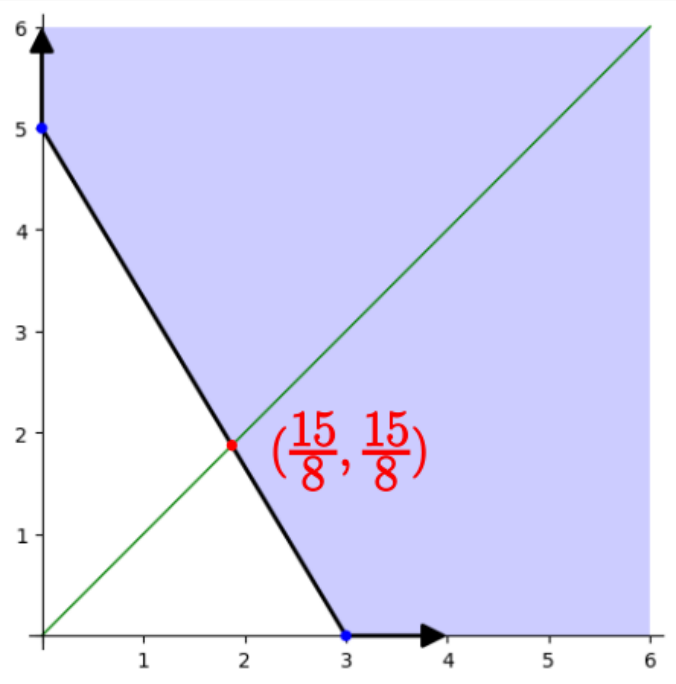

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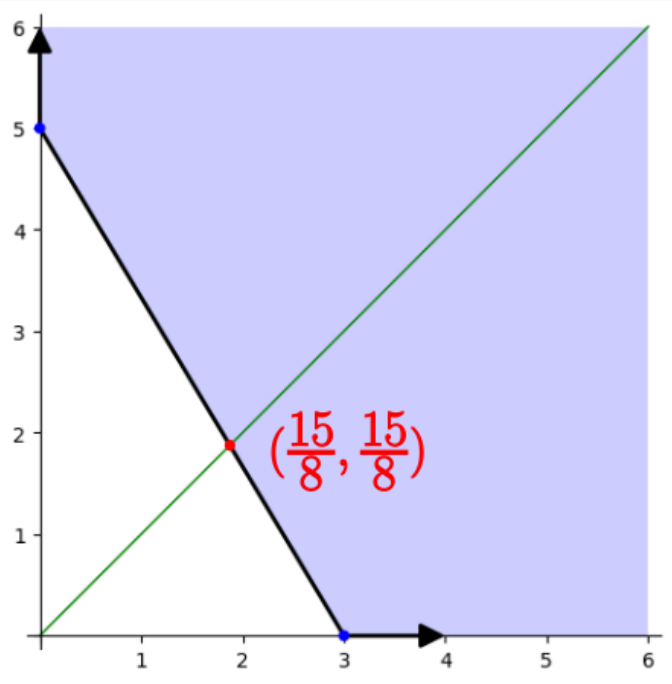

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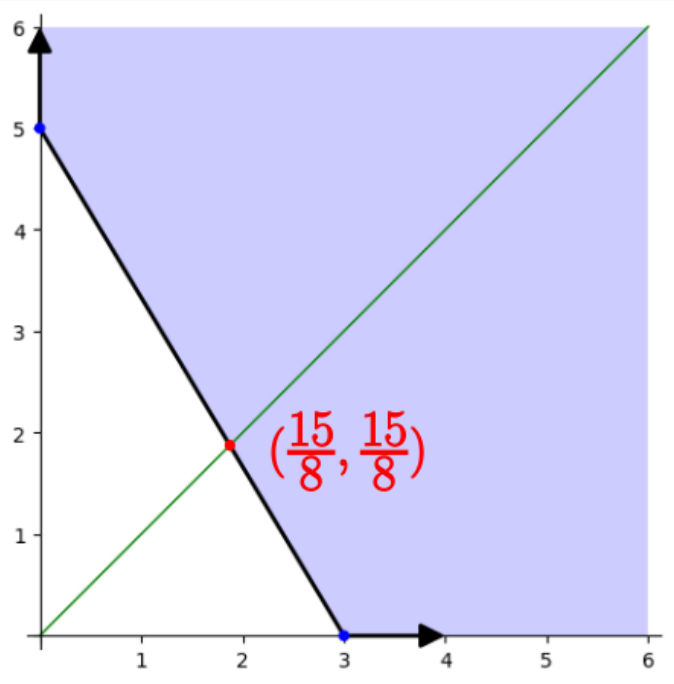

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Theorem [Varchenko, PSS, Collins]

If $K(X, Y)$ is normalized, then $\mathrm{RLCT}_0(K) = \frac{1}{\delta_K}$. If $K(X, Y)$ is not normalized, there exists an change of variables $\Psi : (X, Y) \mapsto (X, Y - Q(X))$, with $Q(X) \in \bar{\mathbb{Q}}[[X]]$ such that $\tilde{K}(X, Y) = K \circ \Psi(X, Y)$ is normalized and $\mathrm{RLCT}_0(\tilde{K}) = \mathrm{RLCT}_0(K) = \frac{1}{\delta_{\tilde{K}}}$.

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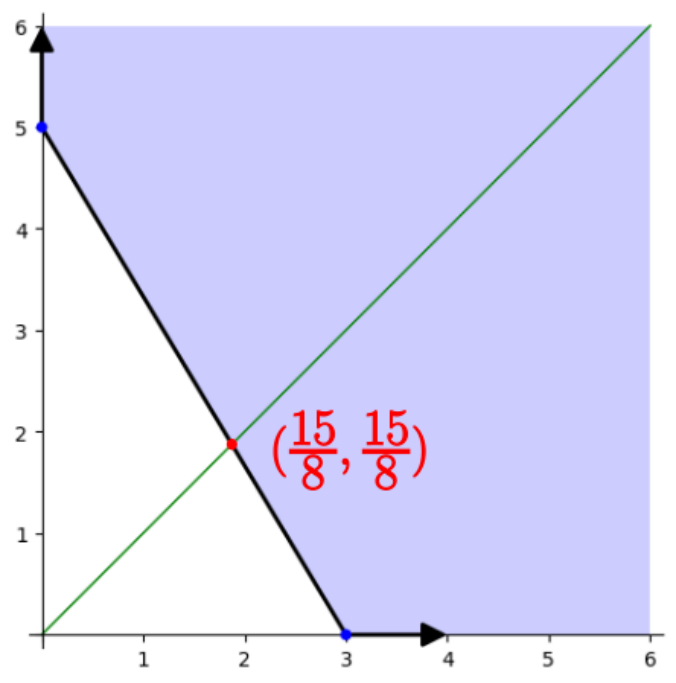

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Ψ can be computed with the Newton-Puiseux algorithm + Normalized check!

Puiseux Theorem

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Let $K(X, Y)$ be a polynomial in $\mathbb{Q}[X][Y]$. The algebraic closure of $\mathbb{Q}[X]$ is contained in the field of Puiseux series $\mathbb{C}\langle\langle X\rangle\rangle = \bigcup_n \mathbb{C}((X^{1/n}))$.

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  - $\beta_j(X) = -X + X^2 + \nu_j X^{\frac{5}{2}} + X^3 + \ldots$, where ν_j are roots of $T^2 - 3$, for $j = 1, 2$

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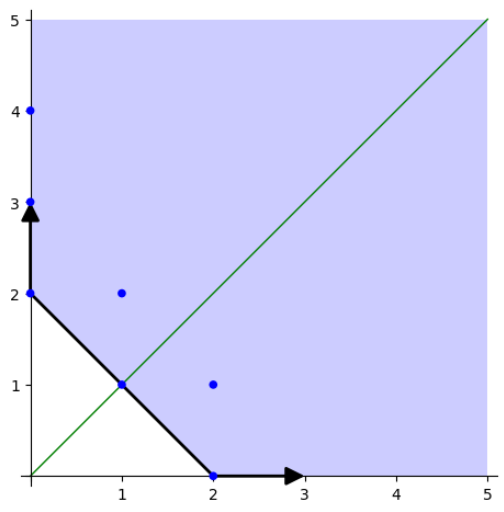

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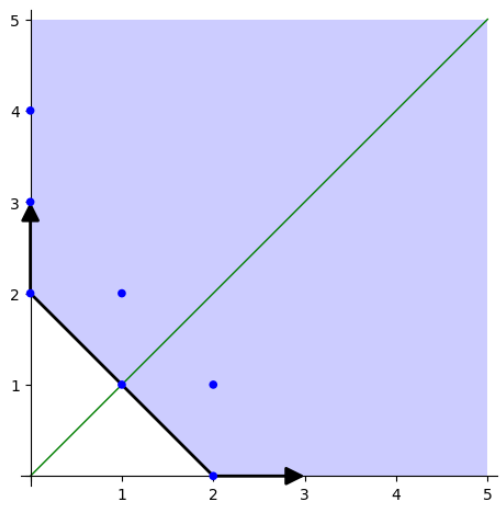

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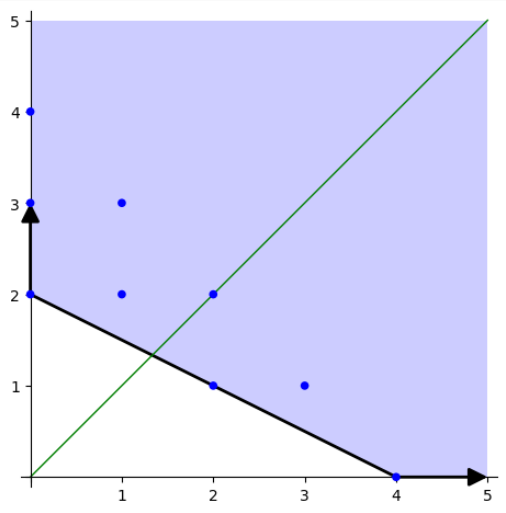

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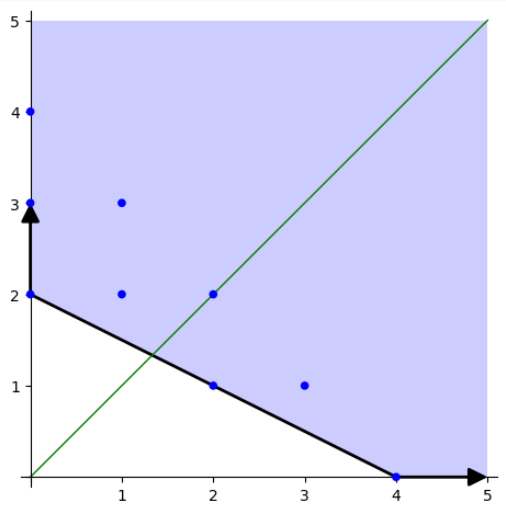

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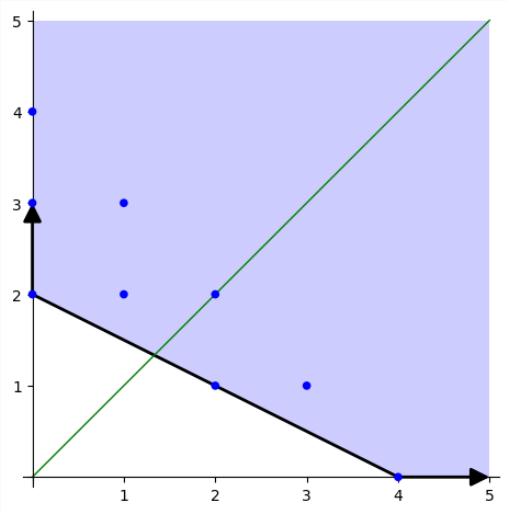

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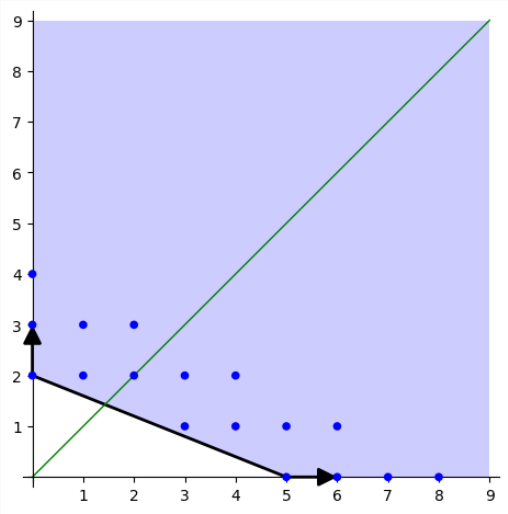

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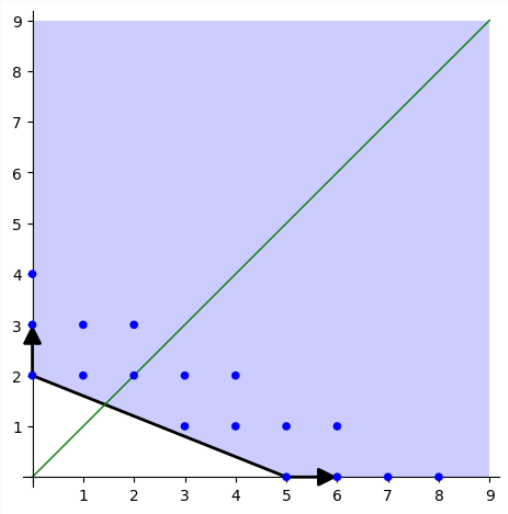

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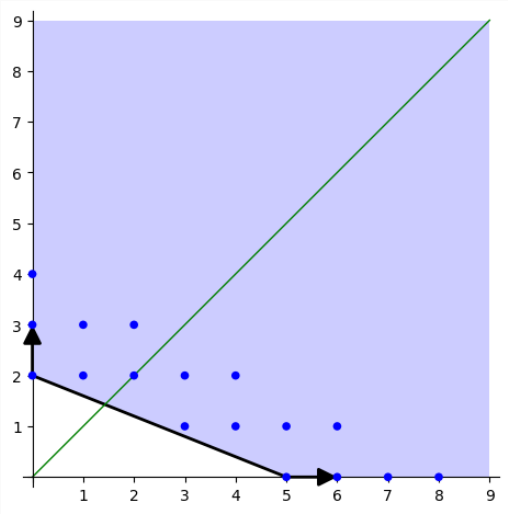

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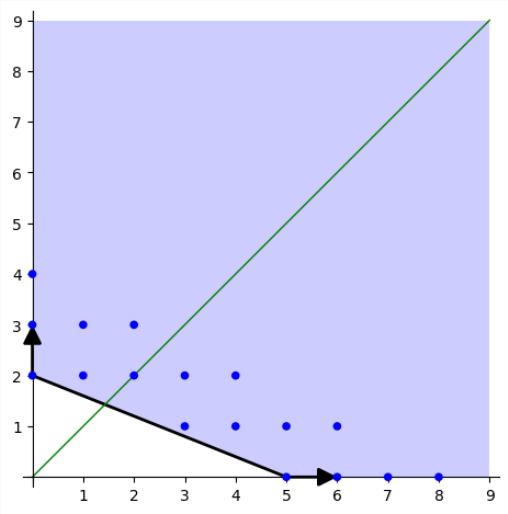

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- Get $K_1(X, Y) = Y^2 + (-2)X^2Y + X^4 + (-4)X^3Y + 6X^2Y^2 + (-4)XY^3 + Y^4 + XY^2 + Y^3$
- $\delta_{K_1} = 4/3$, $(K_1)_\Delta = Y^2 - 2X^2Y + X^4 = (Y - X^2)^2$, $m_1 = 2 > \delta_{K_1}$
- Apply the change of variables $K_2(X, Y) = K_1(X, Y + X^2)$
- Get $K_2(X, Y) = Y^2 - 3X^5 +$ (higher-order terms)
- $\delta_{K_2} = 10/7$, $(K_2)_\Delta = Y^2 - 3X^5$, $m_2 = 1 < \delta_{K_2} = 10/7$
- $\mathrm{RLCT}_0(K) = 7/10$

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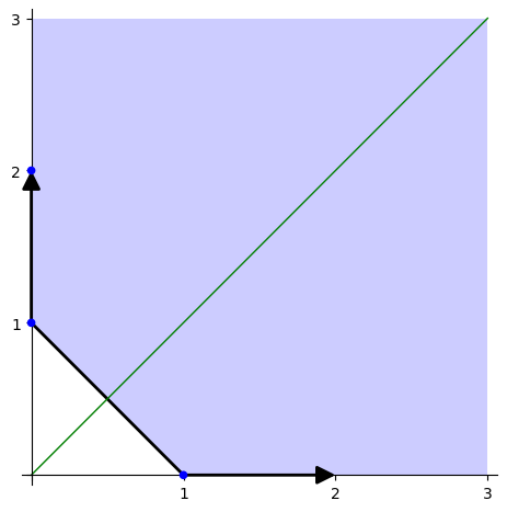

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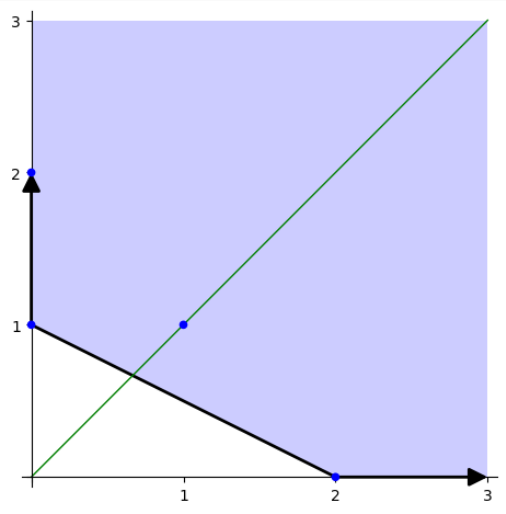

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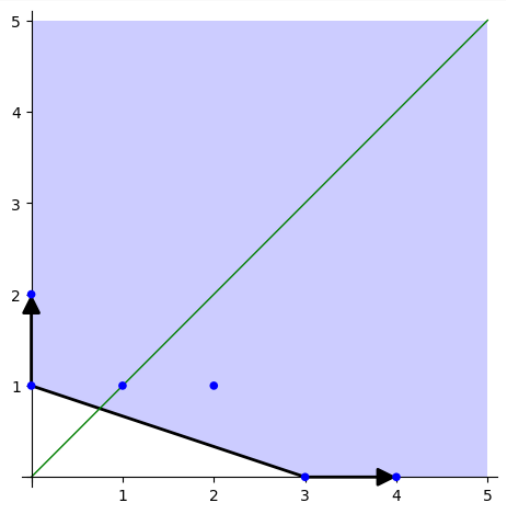

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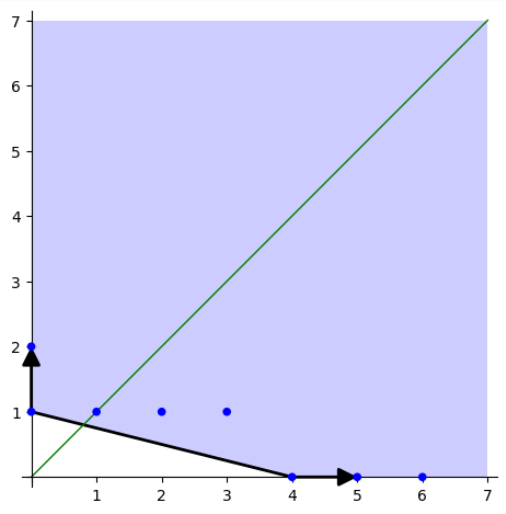

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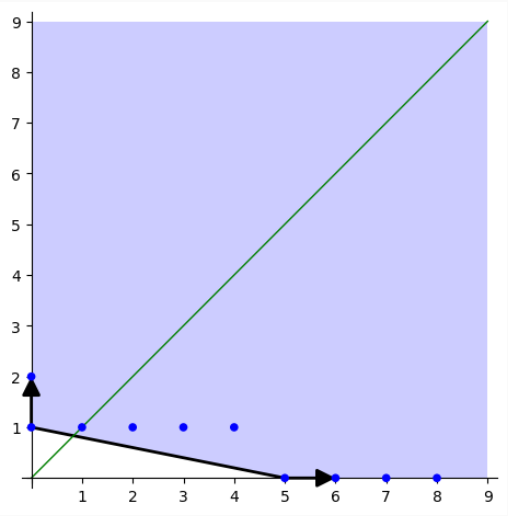

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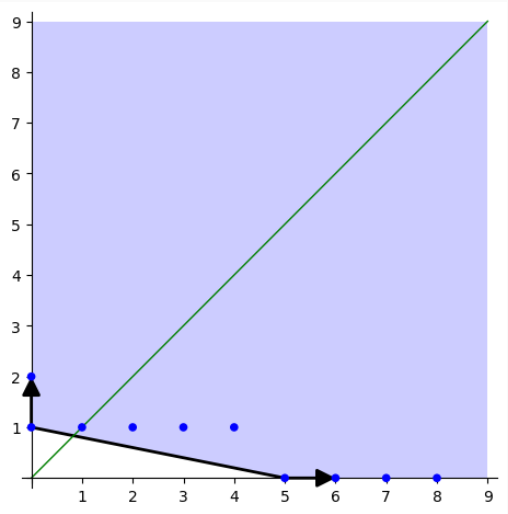

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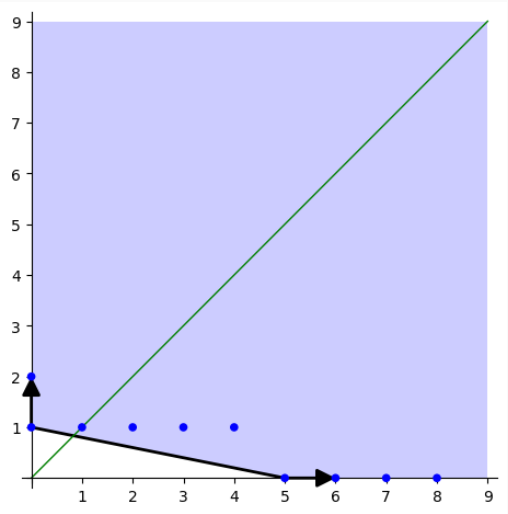

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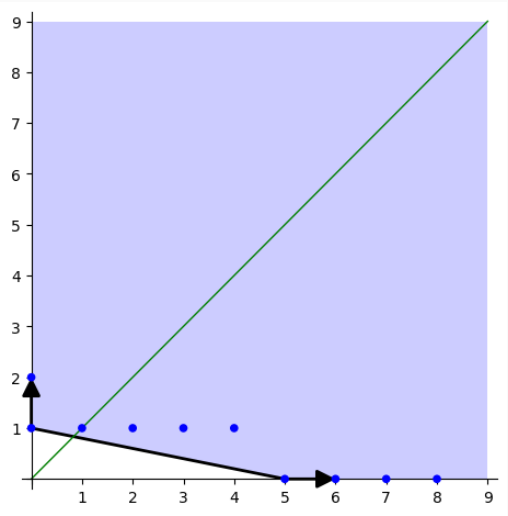

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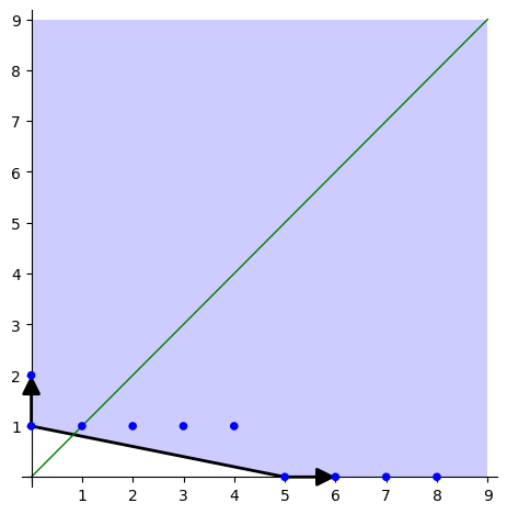

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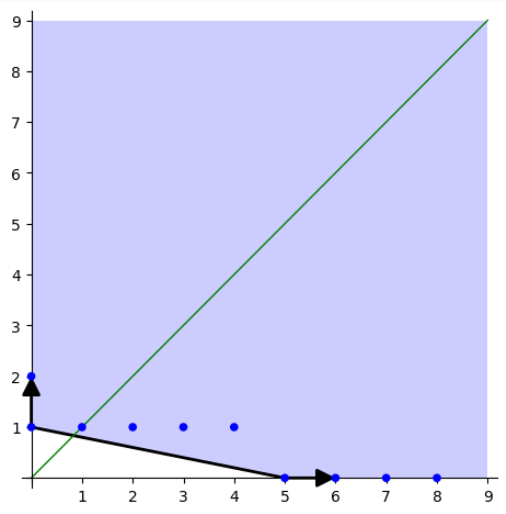

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This can be used as an upper bound on the number of iterations of the algorithm!

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We apply the algorithm to a family of **polynomial neural networks** (PNNs) with parameters $\theta = (\theta_1, \theta_2) \in \Theta \subset \mathbb{R}^2$, activation degree $r = 2$, and a single weight $W(\theta)$ repeated L times (regression task). By [Aoyagi]'s theorem, the Kullback–Leibler divergence $K_L(\theta)$ is *contact equivalent* to an explicit sum-of-squares polynomial $H_L(\theta) \in \mathbb{Q}[\theta_1, \theta_2]$, so $\lambda_L = \mathrm{RLCT}_0(H_L)$.

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The learning coefficient shrinks as depth grows.

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Thank You!