Approximate Computations in Commutative Algebra

Martin Kreuzer

Fachbereich Mathematik

Universität Dortmund

martin.kreuzer@uni-dortmund.de

An approximate lecture, given at the

Fifth Int. CoCoA School

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Tell me what you know.

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$\mathbb{X} = \{p_1, \ldots, p_s\}$ finite set of points in $\mathbb{R}^n$

The map $\mathrm{eval} : P \longrightarrow \mathbb{R}^s$ given by $f \mapsto (f(p_1), \ldots, f(p_s))$ is called the **evaluation map** associated to $\mathbb{X}$.

The ideal $I_{\mathbb{X}} = \ker(\mathrm{eval})$ is called the **vanishing ideal** of $\mathbb{X}$.

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The Gretchen Question:

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The Gretchen Question: What happens if the points of $\mathbb{X}$ are only empirical points, e.g. points whose coordinates are derived from measured data?

In the following we let $-\varepsilon < \mathbf{0}$ be a given **threshold number**.

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And here is the (hori-)**crux** of the matter: the polynomials which vanish ε-approximately at $\mathbb{X}$ **do not form an ideal**.

Example 1.1 If $|f(p)| = 0.001 < \varepsilon = 0.1$ then $|(1000\, f)(p)| = 1 > \varepsilon$.

Hence the question whether f vanishes at p or not depends on the size of f, i.e. we need a **metric** on P.

Definition 1.2 Let $f = a_1 t_1 + \cdots + a_s t_s \in P$, where $a_1, \ldots, a_s \in \mathbb{R} \setminus \{0\}$ and $t_1, \ldots, t_s \in \mathbb{T}^n$.

Then the number $\|f\| = \|(a_1, \ldots, a_s)\|$ is called the (Euclidean) **norm** (or the **size**) of f.

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A very small polynomial **always** vanishes ε-approximately at $\mathbb{X}$!

Hence it is reasonable to consider the condition that polynomials $f \in P$ with $\|f\| = 1$ vanish ε-approximately at p.

2 – Approximate Vanishing Ideals

Definition 2.1 An ideal $I \subseteq P$ is called an **ε-approximate vanishing ideal** of $\mathbb{X}$ if there exists a system of generators $\{f_1, \ldots, f_r\}$ of I such that $\|f_i\| = 1$ and f_i vanishes ε-approximately at $\mathbb{X}$ for $i = 1, \ldots, r$.

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It's kind of fun to do the impossible. (Walt Disney)

3 – The Singular Value Decomposition

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Theorem 3.1 *Let* $\mathcal{A} \in \mathrm{Mat}_{m,n}(\mathbb{R})$.

There are orthogonal matrices $\mathcal{U} \in \mathrm{Mat}_{m,m}(\mathbb{R})$ *and* $\mathcal{V} \in \mathrm{Mat}_{n,n}(\mathbb{R})$ *and a matrix* $\mathcal{S} \in \mathrm{Mat}_{m,n}(\mathbb{R})$ *of the form* $\mathcal{S} = \begin{pmatrix} \mathcal{D} & 0 \\ 0 & 0 \end{pmatrix}$ *such that*

$$\mathcal{A} = \mathcal{U} \cdot \mathcal{S} \cdot \mathcal{V}^{\mathrm{tr}} = \mathcal{U} \cdot \begin{pmatrix} \mathcal{D} & 0 \\ 0 & 0 \end{pmatrix} \cdot \mathcal{V}^{\mathrm{tr}}$$

where $\mathcal{D} = \mathrm{diag}(s_1, \ldots, s_r)$ *is a diagonal matrix.*

In this decomposition, it is possible to achieve:

1. $s_1 \geq s_2 \geq \cdots \geq s_r > 0$. The numbers $s_1, \ldots, s_r$ depend only on $\mathcal{A}$ and are called the **singular values** of $\mathcal{A}$.

2. The number r is the rank of $\mathcal{A}$.

3. The matrices $\mathcal{U}$ and $\mathcal{V}$ have the following interpretation:

$$
\begin{array}{ccc}
\text{first } r \text{ columns of } \mathcal{U} & \equiv & \text{ONB of the column space of } \mathcal{A} \\
\text{last } m - r \text{ columns of } \mathcal{U} & \equiv & \text{ONB of the kernel of } \mathcal{A}^{\text{tr}} \\
\text{first } r \text{ columns of } \mathcal{V} & \equiv & \text{ONB of the row space of } \mathcal{A} \\
 & \equiv & \text{ONB of the column space of } \mathcal{A}^{\text{tr}} \\
\text{last } n - r \text{ columns of } \mathcal{V} & \equiv & \text{ONB of the kernel of } \mathcal{A}
\end{array}
$$

Definition 3.2 Let $\mathcal{A} \in \mathrm{Mat}_{m,n}(\mathbb{R})$, and let $\varepsilon > 0$ be given. Let $k \in \{1, \ldots, r\}$ be chosen such that $s_k > \varepsilon \geq s_{k+1}$. Form the matrix $\widetilde{\mathcal{A}} = \mathcal{U}\,\widetilde{\mathcal{S}}\,\mathcal{V}^{\mathrm{tr}}$ by setting $s_{k+1} = \cdots = s_r = 0$ in $\mathcal{S}$. Then $\widetilde{\mathcal{A}}$ is called the **singular value truncation** of $\mathcal{A}$ at ε.

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Corollary 3.3 *Let $\widetilde{\mathcal{A}}$ be the singular value truncation of $\mathcal{A}$ at ε.*

1. $\|\mathcal{A} - \widetilde{\mathcal{A}}\| = s_{k+1} = \min\{\|\mathcal{A} - \mathcal{B}\| : \mathrm{rank}(\mathcal{B}) \leq k\}$
2. *The vector subspace* $\mathrm{apker}(\mathcal{A}, \varepsilon) = \ker(\widetilde{\mathcal{A}})$ *is the largest dimensional kernel of a matrix whose Euclidean distance from $\mathcal{A}$ is at most ε. It is called the* **ε-approximate kernel** *of $\mathcal{A}$.*
3. *The last $n - k$ columns $v_{k+1}, \ldots, v_n$ of $\mathcal{V}$ are an ONB of* $\mathrm{apker}(\mathcal{A}, \varepsilon)$. *They satisfy $\|\mathcal{A}v_i\| < \varepsilon$.*

4 – The BM-Algorithm

Let $\mathbb{X} = \{p_1, \ldots, p_s\} \subseteq \mathbb{R}^n$ and σ a degree compatible term ordering.

1. Let $G = \emptyset$, $\mathcal{O} = \{1\}$, $\mathcal{M} = (1, \ldots, 1)$, and $d = 0$.
2. Increase d by one. Let $L = [t_1, \ldots, t_\ell]$ be $\mathbb{T}^n_d \setminus \langle \mathrm{LT}_\sigma(G) \rangle$ ordered decreasingly w.r.t. σ. If $L = \emptyset$, return $(G, \mathcal{O})$ and stop.
3. Append $\mathrm{eval}(t_1), \ldots, \mathrm{eval}(t_\ell)$ as new first rows to $\mathcal{M}$ and get a matrix $\mathcal{A}$. Find a matrix $\mathcal{B}$ whose rows are a basis of $\ker(\mathcal{A}^{\mathrm{tr}})$.
4. Reduce $\mathcal{B}$ to row echelon form and get a matrix $\mathcal{C} = (c_{ij})$.
5. For the columns j of $\mathcal{C}$ containing a pivot element c_{ij}, append the polynomial corresponding to row i to G.
6. For the columns j of $\mathcal{C}$ containing no pivot element, append t_j to $\mathcal{O}$, append the row $\mathrm{eval}(t_j)$ to $\mathcal{M}$, and continue with (2).

5 – The ABM-Algorithm

Let $\mathbb{X} = \{p_1, \ldots, p_s\} \subseteq [-1, 1]^n$, let σ be a degree compatible term ordering, and let $\varepsilon > \varepsilon' > 0$.

1. Let $G = \emptyset$, $\mathcal{O} = \{1\}$, $\mathcal{M} = (1, \ldots, 1)$, and $d = 0$.
2. Increase d by one. Let $L = [t_1, \ldots, t_\ell]$ be $\mathbb{T}^n_d \setminus \langle \mathrm{LT}_\sigma(G) \rangle$ ordered decreasingly w.r.t. σ. If $L = \emptyset$, return $(G, \mathcal{O})$ and stop.
3. Append $\mathrm{eval}(t_1), \ldots, \mathrm{eval}(t_\ell)$ as new first rows to $\mathcal{M}$ and get a matrix $\mathcal{A}$. Using the SVD of $\mathcal{A}^{\mathrm{tr}}$, compute a matrix $\mathcal{B}$ whose rows are a basis of $\mathrm{apker}(\mathcal{A}^{\mathrm{tr}}, \varepsilon)$.
4. Reduce $\mathcal{B}$ to row echelon form. Normalize each row after every reduction step. If at some point a column contains no pivot element of absolute value $> \varepsilon'$ in the untreated rows, replace the corresponding elements by zero. The result is a matrix $\mathcal{C} = (c_{ij})$.

5. For the columns j of $\mathcal{C}$ containing a pivot element c_{ij}, append the polynomial corresponding to row i to G.

6. For the columns j of $\mathcal{C}$ containing no pivot element, append t_j to $\mathcal{O}$, append the row $\mathrm{eval}(t_j)$ to $\mathcal{M}$, and continue with (2).

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This is an algorithm which computes a pair $(G, \mathcal{O})$.

The list G is a unitary minimal σ-Gröbner basis of the ideal $I = \langle G \rangle \subset P$ and satisfies $\|\,\mathrm{eval}(g)\| < \delta$ for $\delta = \varepsilon\sqrt{\#G} + \varepsilon' s\sqrt{s}$ and all $g \in G$.

The list $\mathcal{O}$ contains an order ideal of monomials whose residue classes form an $\mathbb{R}$-vector space basis of P/I.

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We have $\dim_{\mathbb{R}}(P/I) \leq s$. **Thus I is a zero-dimensional ideal and a δ-approximate vanishing ideal of $\mathbb{X}$.**

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Let us follow the steps of ABM in a concrete case. We consider the set $\mathbb{X} = \{(0.01, 0.01),\ (0.49, 0),\ (0.51, 0),\ (0, 0.99)\}$ and use the threshold numbers $\varepsilon = 0.1$ and $\varepsilon' = 10^{-6}$.

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1. Let $G = \emptyset$, $\mathcal{O} = \{1\}$, $\mathcal{M} = (1, 1, 1, 1)$, and $d = 0$.
2. Consider $d = 1$ and $L = [x, y]$.
3. We form $\mathcal{A} = \begin{pmatrix} 0.01 & 0.49 & 0.51 & 0 \\ 0.01 & 0 & 0 & 0.99 \\ 1 & 1 & 1 & 1 \end{pmatrix}$. The SVD of $\mathcal{A}^{\mathrm{tr}}$ yields $s_1 = 2.13$, $s_2 = 0.91$ and $s_3 = 0.35$, so no singular value truncation is necessary. We compute $B = (0, 0, 0)$.

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2. Consider $d = 2$ and $L = [x^2, xy, y^2]$.

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6. Append x, y to $\mathcal{O}$ and get $\mathcal{O} = \{1, x, y\}$. Moreover, let $\mathcal{M} = \mathcal{A}$.

2. Consider $d = 2$ and $L = [x^2, xy, y^2]$.

3. We form the matrix $\mathcal{A} = \begin{pmatrix} 0.0001 & 0.2401 & 0.2601 & 0 \\ 0.0001 & 0 & 0 & 0 \\ 0.0001 & 0 & 0 & 0.9801 \\ 0.01 & 0.49 & 0.51 & 0 \\ 0.01 & 0 & 0 & 0.99 \\ 1 & 1 & 1 & 1 \end{pmatrix}$

   and compute SVD of $\mathcal{A}^{\mathrm{tr}}$. We get the singular values $s_1 = 2.22$, $s_2 = 1.21$, $s_3 = 0.40$, and $s_4 = 0.006$. Thus we have to truncate the singular value $s_4 < \varepsilon$. The SVD of $\widetilde{\mathcal{A}}^{\mathrm{tr}}$ yields that the space $\mathrm{apker}(\mathcal{A}^{\mathrm{tr}}, \varepsilon)$ is generated by the rows of

$$\mathcal{B} = \begin{pmatrix} 0.65 & -0.66 & 0.08 & -0.33 & -0.08 & 0.004 \\ 0.07 & -0.10 & -0.70 & -0.02 & 0.70 & -0.007 \\ 0.60 & 0.74 & -0.02 & -0.30 & 0.02 & 0.003 \end{pmatrix}$$

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4. Now we perform a **normalized** Gaußian reduction on $\mathcal{B}$ and get the matrix

$$\mathcal{C} = \begin{pmatrix} 0.65 & -0.66 & 0.08 & -0.33 & -0.08 & 0.004 \\ 0 & -0.027 & -0.707 & 0.014 & 0.707 & -0.007 \\ 0 & 0 & -0.707 & 0.014 & 0.707 & -0.007 \end{pmatrix}.$$

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5. Append the polynomials
$g_1 = 0.65x^2 - 0.66xy + 0.08y^2 - 0.33x - 0.08y + 0.004$,
$g_2 = -0.027xy - 0.707y^2 + 0.014x + 0.707y - 0.007$, and
$g_3 = -0.707y^2 + 0.014x + 0.707y - 0.007$ to G.

2. For $d = 3$, we find $L = [\ ]$. Hence the result is $G = \{g_1, g_2, g_3\}$ and $\mathcal{O} = \{1, x, y\}$.

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Therefore an approximate vanishing ideal of $\mathbb{X} = \{p_1, p_2, p_3, p_4\}$ is given by $\langle g_1, g_2, g_3 \rangle$ where $g_1 \approx x(x - y - \frac{1}{2})$, $g_2 \approx -0.03xy + g_3$, and $g_3 \approx (-1/\sqrt{2})(y^2 - y)$.

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The ideal $\langle g_1, g_3, g_3 \rangle$ is the **exact** vanishing ideal of **three** points! The two points $(0.49, 0)$ and $(0.51, 0)$ have been combined and count as **one approximate point**.

Corollary 6.1 (The BB Version of ABM)
In the setting of the ABM-Algorithm, replace step **2** *by the following step* **2'**.

2'. Increase d by one, and let L be the list of all terms of degree d, ordered decreasingly w.r.t. σ. Remove from L all terms which are contained in $\langle \mathrm{LT}_\sigma(g) \mid g \in G \rangle$, **but not the ones in the border of $\mathcal{O}$**. *If $L = \emptyset$, return the pair $(G, \mathcal{O})$ and stop. Otherwise, let $L = [t_1, \ldots, t_\ell]$.*

The resulting algorithm computes a pair $(G, \mathcal{O})$. The set $\{\mathrm{LC}_\sigma(g)^{-1} g \mid g \in G\}$ is the $\mathcal{O}$-border basis of a δ-approximate vanishing ideal $I = \langle G \rangle \subset P$ of $\mathbb{X}$ where $\delta < \varepsilon\sqrt{\#G} + \varepsilon' s\sqrt{s}$. The list $\mathcal{O}$ consists of all terms which are not contained in $\mathrm{LT}_\sigma(I)$.

The Last Remark

In the ABM-Algorithm we assumed $\mathbb{X} \subset [-1, 1]^n$. If the initial data points are not in this set, we have to perform **data scaling**.

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Mathematically, the ABM-Algorithm and the stated error estimates are also correct for arbitrary $\mathbb{X} \subseteq \mathbb{R}^n$. But the data scaling provides additional **numerical stability** for the solution.

We considered a real-world example consisting of 2541 points. For both computations, we used $\varepsilon = 0.0001$. The scaled computation took 2 sec., the unscaled one took 4 sec. The following pictures show the mean size of the evaluation vectors of the computed GB polynomials.

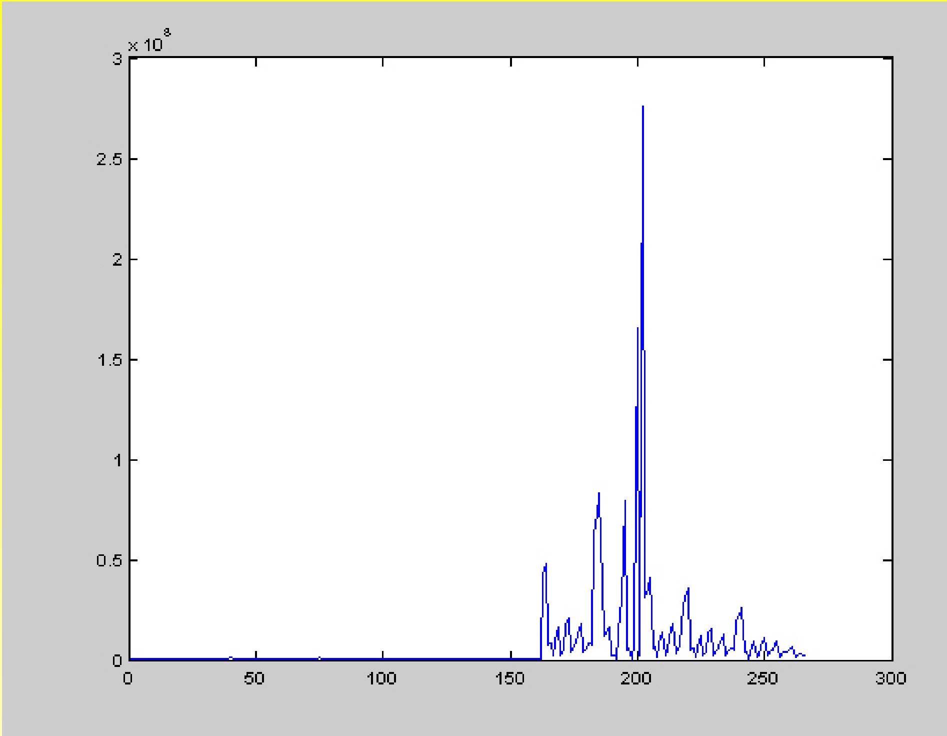

Figure 1: Without Data Scaling

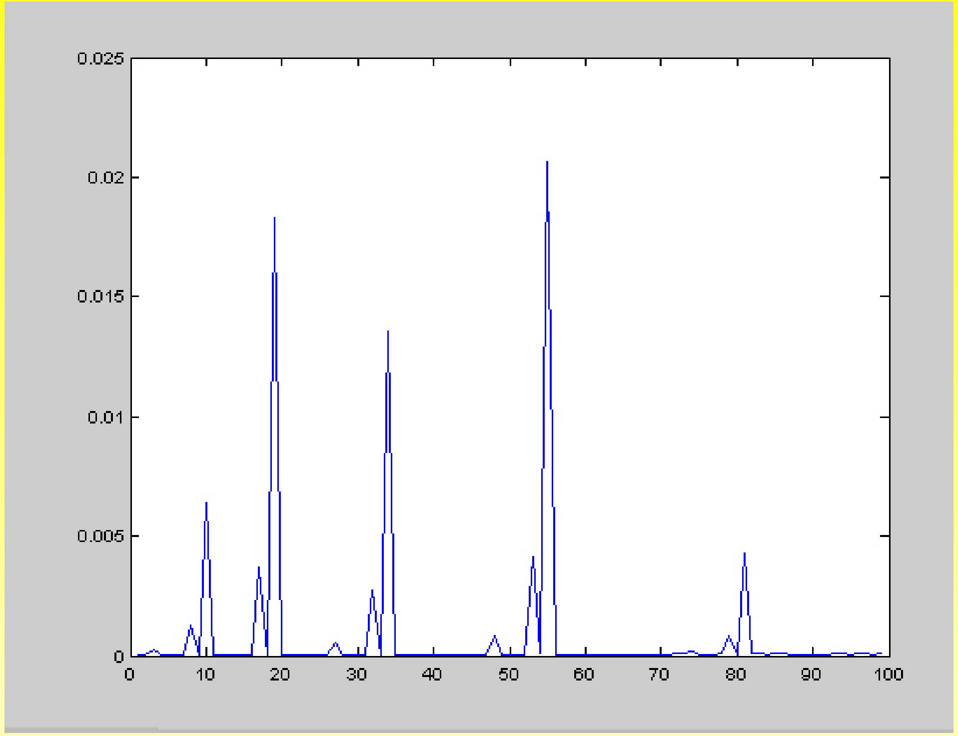

Figure 2: With Data Scaling

Without Data Scaling: 280 GB polynomials

GB mean evaluation error: $2.8 \cdot 10^8$

Without Data Scaling: 280 GB polynomials

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With Data Scaling: 100 GB polynomials

GB mean evaluation error: 0.025

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The Upshot:

Without Data Scaling: 280 GB polynomials

GB mean evaluation error: $2.8 \cdot 10^8$

With Data Scaling: 100 GB polynomials

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The Upshot: **Treat your approximate data right!**

Then they will treat you *approximately* **right!**

Without Data Scaling: 280 GB polynomials

GB mean evaluation error: $2.8 \cdot 10^8$

With Data Scaling: 100 GB polynomials

GB mean evaluation error: 0.025

The Upshot: Treat your approximate data right!

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Thank you for your attention!