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Efficient Calculation of Second Degree Polynomial Features on Sparse Matrices

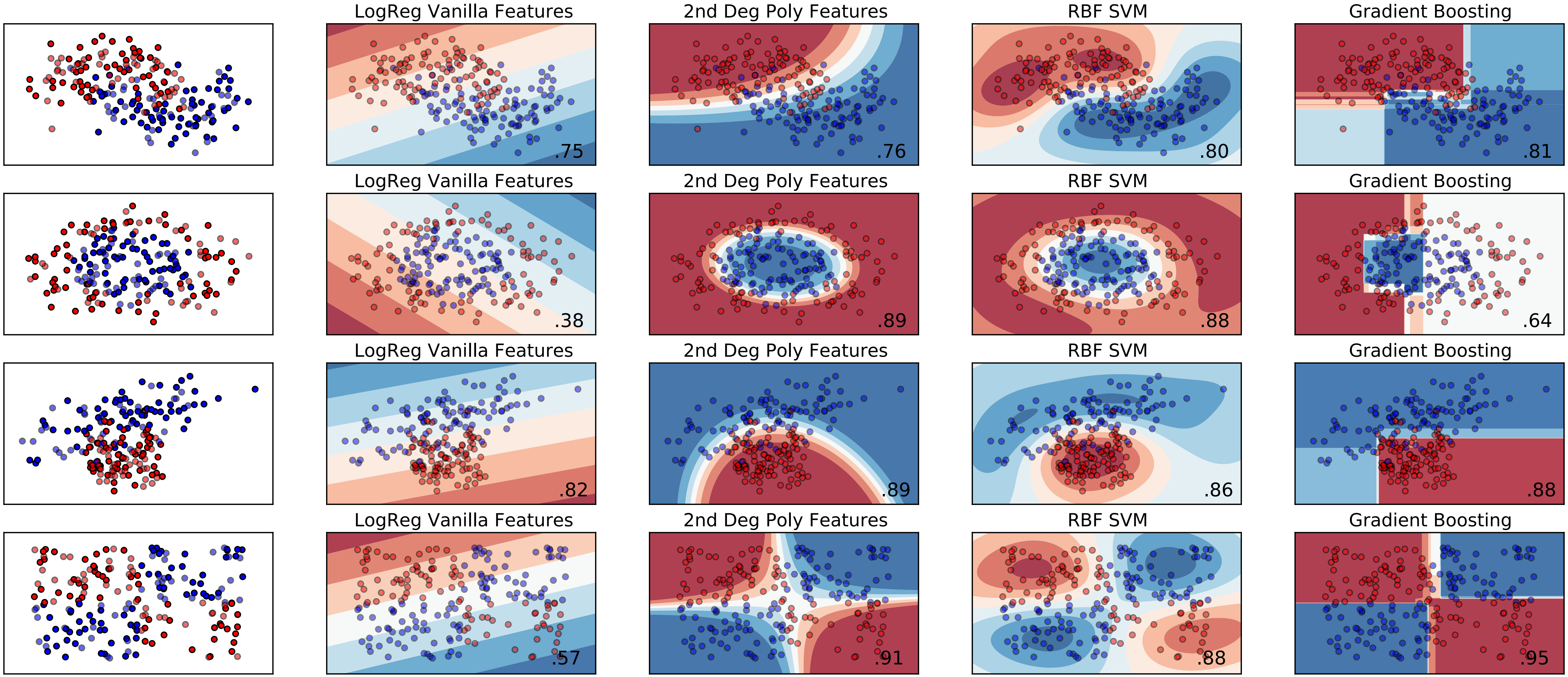
Handling Nonlinearity

- Work in kernel space, e.g. rbf kernel
- Nonlinear model, e.g. gradient boosting
- Apply an input transformation
  - e.g. x_i -> $\cos(x_i)$ for all components

Polynomial Features

- Products of combinations of features
    - $\{x_i \cdot x_j : i,j \in \{0,1,\ldots,D-1\} \wedge i \leq j\}$
- [a, b, c] has polynomial features [a^2, ab, ac, b^2, bc, c^2]
- D features, $(D^2+D)/2$ 2nd degree polynomial features

What they can do (graphically)



Calculation

- Naive Calculation
  - Walk through all pairs, take products
  - Zero whenever either inputs are zero
  - Unnecessary calculations when matrix is sparse
- Smarter Calculation
  - Take products of non-zero elements
  - Problem: knowing output column index given input indices

Column Output Location

$\{x_i \cdot x_j : i, j \in \{0, 1, ..., D-1\} \wedge i \leq j\}$

$\{(i, j) : i, j \in \{0, 1, ..., D-1\} \wedge i \leq j\} \rightarrow \{0, 1, ..., \frac{D^2+D}{2} - 1\}$

$$
\begin{array}{ccc}
 & & j \\
 & \vec{x} & \begin{array}{ccccc} x_0 & x_1 & x_2 & x_3 & x_4 \end{array} \\
i & \begin{array}{c} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \end{array} & \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ - & 5 & 6 & 7 & 8 \\ - & - & 9 & 10 & 11 \\ - & - & - & 12 & 13 \\ - & - & - & - & 14 \end{pmatrix}
\end{array}
$$

$$\text{polynomial-index}(i, j | D) = \frac{2Di - i^2 + 2j - 3i - 2}{2} + i + 1$$

Algorithm Comparison

Dense Polynomials(A)

N = row count of A
D = column count of A
B = Matrix of size $N \times \frac{D^2+D}{2}$
for row in A
    $k = 0$
    for $\imath = 0$ **to** D
        for $\jmath = i$ **to** D
            $B[i,k] = row[i] \cdot row[j]$
            $k = k + 1$

$O(ND^2)$, $\Theta(ND^2)$

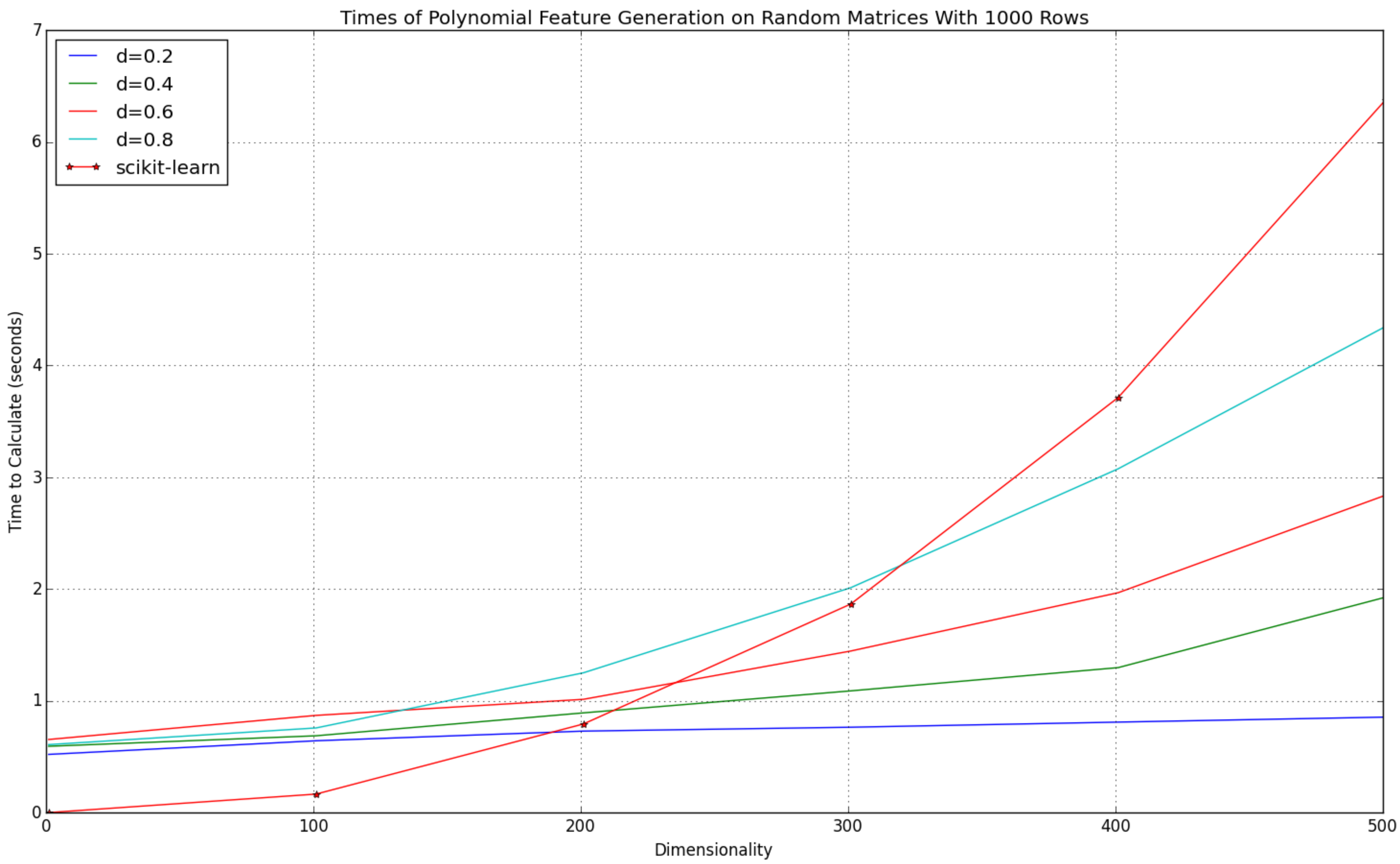
Sparse Polynomials(A)

$\mathrm{map}(a,b) = \frac{2Da - a^2 + 2b - 3a - 2}{2} + a + 1$
N = row count of A
D = column count of A
B = Compressed Sparse Row Matrix of size $N \times \frac{D^2+D}{2}$
for row in A
    N_{zc} = nonzero columns of row
    for $i = 0$ **to** $|N_{zc}|$
        for $j = i$ **to** $|N_{zc}|$
            $k = \mathrm{map}(i,j)$
            r = index of row
            $B[r,k] = row[i] \cdot row[j]$

$O(ND^2)$, $\Theta(Nd^2D^2)$
where d is density

Average complexities decrease quadratically w.r.t. density!

How fast is it?



Real Usage

dataset	instances	features	polynomial features	density	dense space	sparse space	dense time	sparse time
20 Newsgroups	11,314	130,107	8,463,980,778	0.12	scikit-learn: MemoryError	5333 MB	scikit-learn: MemoryError	109 s
Connect Four	67,557	126	8,127	0.11	4191 MB	735 MB	26 s	44 s

Code available on github.com/AWNystrom