Oblivious Sketching of High-Degree Polynomial Kernels

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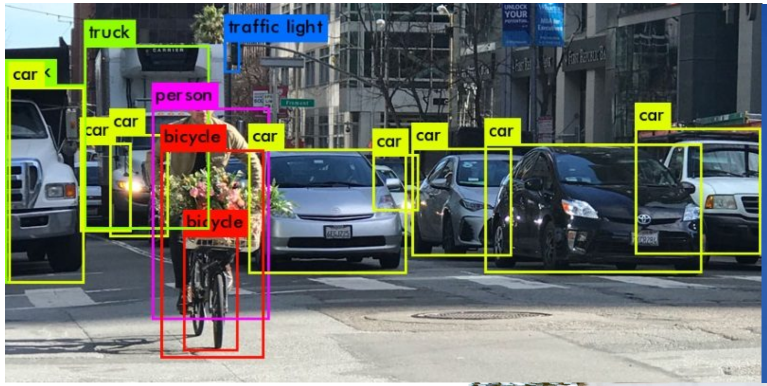
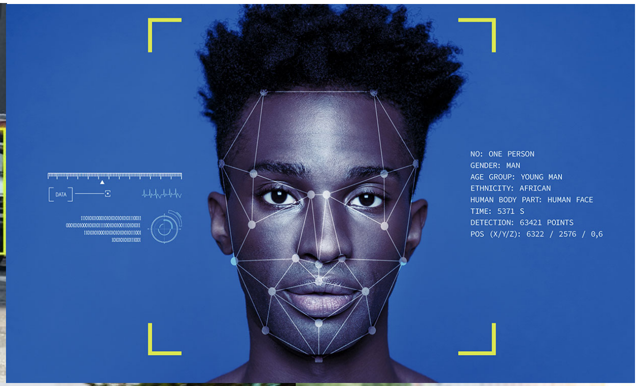
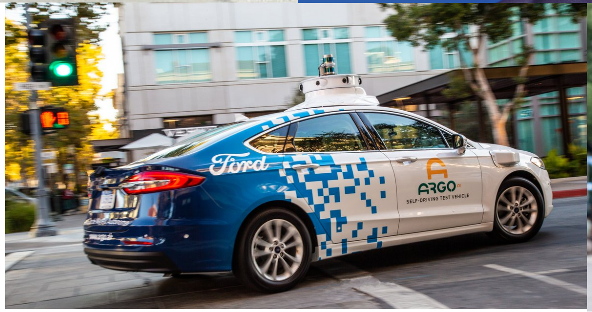
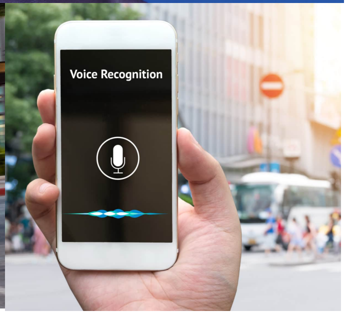
Kernel Methods

- Widely used in *kernel-based* learning, statistics, and control
- Classical machine learning tool with real-world applications





Real-World Applications of Kernel Methods

- **Hyperparameter tuning of deep neural networks:** e.g. Google Vizier
- **Multi-Armed Bandit Optimization** [Srinivas, Krause, Kakade, Seeger' 09]
- **Neural Tangent Kernel:** The evolution of a neural network during training can be described by kernel methods [Jacot, Gabriel, Hongler'18]

Kernel Methods

- Learn a nonlinear function $f: \mathcal{R}^d \rightarrow \mathcal{R}$ from noisy samples

$$\gamma_i = f(x_i) + \epsilon_i \text{ for } i = 1,2, \ldots n$$

  - ϵ_i are iid Gaussian noise with zero mean and variance λ
- **Kernel Ridge Regression** is a simple and yet powerful solution

Kernel Methods

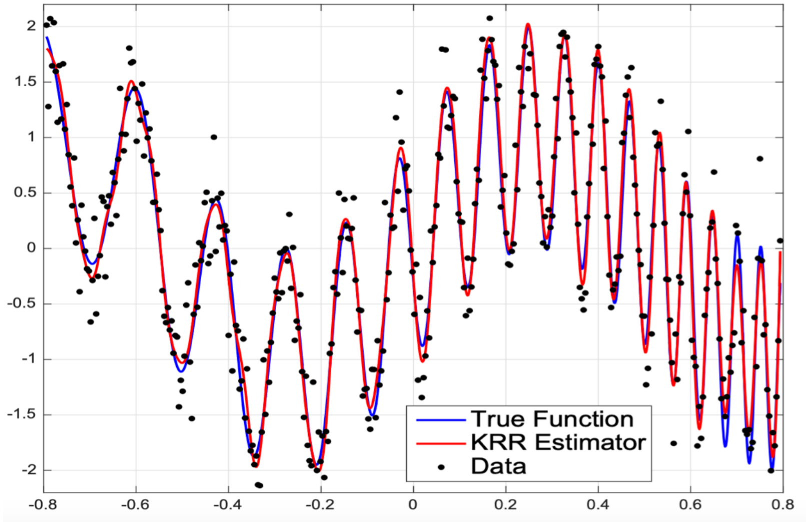
- Learn a nonlinear function $f: \mathcal{R}^d \to \mathcal{R}$ from noisy samples

$$y_i = f(x_i) + \epsilon_i \text{ for } i = 1,2, \ldots n$$

  - ϵ_i are iid Gaussian noise with zero mean and variance λ
- **Kernel Ridge Regression** is a simple and yet powerful solution
  - If $f(\cdot)$ is a GP with covariance $k: \mathcal{R}^d \times \mathcal{R}^d \to \mathcal{R}$, then the optimal estimator is,

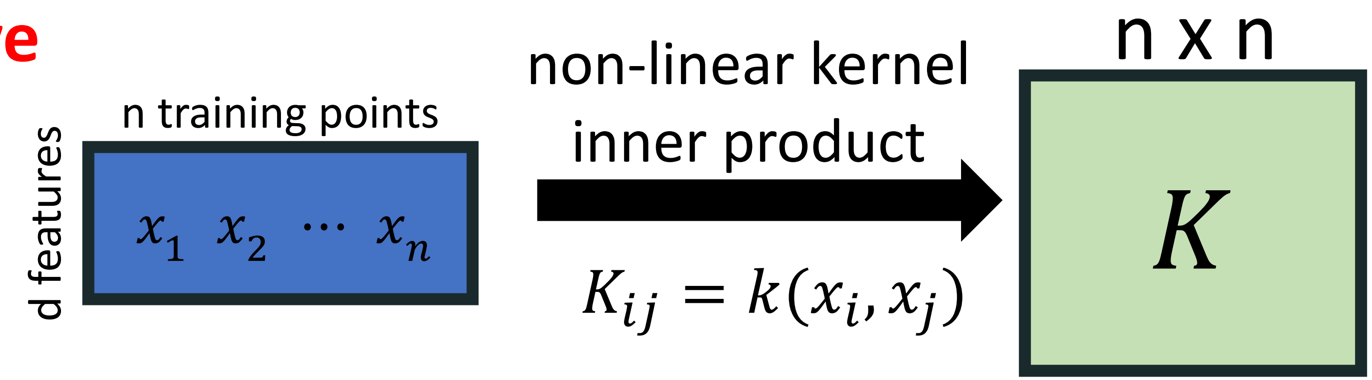
$$\tilde{f}(x) = \sum_{i=1}^{n} \alpha_i k(x, x_i)$$

$$\alpha = \text{argmin}_{\beta \in \mathbb{R}^n} \|\boldsymbol{K}\beta - y\|_2^2 + \lambda \beta^\top \boldsymbol{K} \beta$$



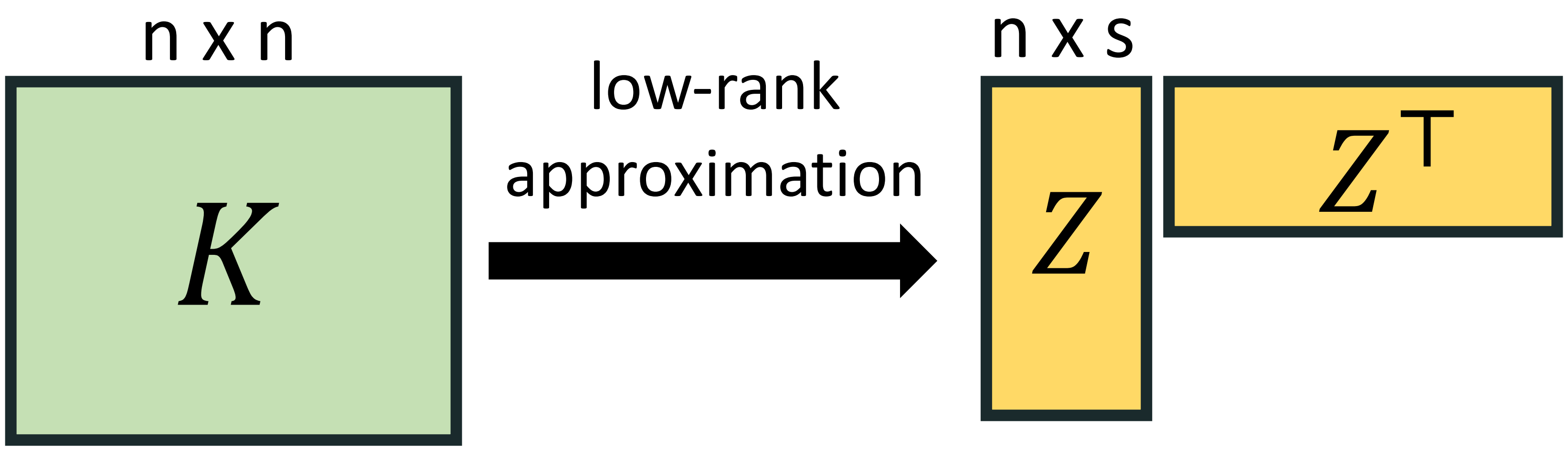
Kernel Method

- **Kernel methods are expensive**



- Computing all kernel entries takes $n \cdot nnz(X) + n^2$ time
- Even writing it down takes n^2 time and memory
- A single iteration of a linear system solver takes n^2 time
- For $n = 100\,000$, K has 10 billion entries. Takes 80 GB of storage

Classical Solution: **Dimensionality Reduction**



- Storing Z uses $O(ns)$ space and computing $ZZ^\top\alpha$ takes $O(ns)$ time.
- Orthogonalization, eigen-decomposition, and pseudo-inversion of $ZZ^\top$ all take just $O(ns^2)$ time.

Efficient Low-Rank Approximation?

- Direct eigen decomposition, or even approximation via Krylov subspace methods are out of question since they at least require fully forming K

Efficient Low-Rank Approximation?

- Direct eigen decomposition, or even approximation via Krylov subspace methods are out of question since they at least require fully forming K

- **Sketching:** a powerful approach to speeding up matrix problems
- Our approach: design a sketching solution for kernel low-rank approximation

Feature Space Mapping

- Any positive definite kernel $k\colon \mathcal{R}^d \times \mathcal{R}^d \to \mathcal{R}$ defines a lifting $\varphi\colon \mathcal{R}^d \to \mathcal{R}^D$ such that for all $x, y \in \mathcal{R}^d$

$$k(x, y) = \varphi(x)^\top \varphi(y)$$

- The kernel computes the inner product between the lifted data points

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- The kernel computes the inner product between the lifted data points

$$K = \boldsymbol{\phi}^\top \boldsymbol{\phi},$$

where $\boldsymbol{\phi}$ is a $D \times n$ matrix whose i^{th} column is the projection of x_i into the feature space $\varphi(x_i)$

Sketching the Feature Space

- **Sketch** the feature space

$$K = \boldsymbol{\phi}^\top \boldsymbol{\phi} \approx \boldsymbol{\phi}^\top \Pi^\top \Pi \boldsymbol{\phi}$$

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Sketching the Feature Space

- **Sketch** the feature space

$$K = \boldsymbol{\phi}^\top \boldsymbol{\phi} \approx \boldsymbol{\phi}^\top \Pi^\top \Pi \boldsymbol{\phi}$$

- Challenge: forming the feature matrix $\boldsymbol{\phi}$ explicitly is expensive as the feature space is typically high-dimensional (even infinite-dimensional)
- Goal: Design a sketch matrix $\Pi \in \mathcal{R}^{s \times D}$ such that $\Pi \cdot \varphi(x)$ is computable without needing to explicitly form $\varphi(x)$

Kernel Sketching techniques

- The most popular method for kernel sketching is the **Fourier Features Method** of Rahimi & Recht (Test of Time Award winner at NeurIPS'17)
- Works for shift invariant kernels, such as Gaussian kernel

$$\varphi(x)_\xi = e^{-2\pi i \xi^\top x} \text{ for } \xi \in \mathcal{R}^d$$

- Π: Sampling matrix that samples frequencies ξ from the pdf $\hat{k}(\xi)$

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Works only for shift invariant kernels and constant dimensional datasets

Polynomial Kernel

- In this work we focus on the important case of **Polynomial Kernel**

$$k(x, y) = (x^\top y)^q$$

- The lifting function for this kernel is $\varphi(x) = x^{\otimes q}$,

where $\varphi(x) \in \mathcal{R}^{d^q}$ is defined as $\varphi(x)_{i_1, i_2, \cdots i_q} = x_{i_1} x_{i_2} \cdots x_{i_q}$ for $i_1, i_2, \cdots i_q \in \{1,2, \cdots d\}$

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- Goal: design a linear sketch $\Pi \in \mathcal{R}^{s \times d^q}$ such that $\Pi x^{\otimes q}$ is efficiently computable without needing to form $x^{\otimes q}$ explicitly

Key Properties of Sketch

- **Approximate Matrix Product:** for every matrices $A, B \in \mathcal{R}^{d^q \times n}$ whp
$$\|A^\top \Pi^\top \Pi B - A^\top B\|_F \leq \epsilon \|A\|_F \|B\|_F$$
- **Oblivious Subspace Embedding:** for every $\lambda > 0$ and every matrix $A \in \mathcal{R}^{d^q \times n}$ whp
$$\frac{A^\top A + \lambda I}{1 + \epsilon} \preccurlyeq A^\top \Pi^\top \Pi A + \lambda I \preccurlyeq \frac{A^\top A + \lambda I}{1 - \epsilon}$$
  - Want: target dimension at most **statistical dimension** $\boldsymbol{tr}(A^\top A(A^\top A + \lambda I)^{-1})$

Prior Work: TensorSketch

- Originally introduced by Pagh and Pham [KDD 2013], [TOCT 2013]

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1. Satisfies **Approximate Matrix Product** with probability 9/10 if target dimension $s = \Omega\left(\frac{3^q}{\epsilon^2}\right)$
2. Satisfies **Oblivious Subspace Embedding** with probability 9/10 if target dimension $s = \Omega\left(\frac{3^q}{\epsilon^2} \cdot s_\lambda^2\right)$
3. Time to sketch the tensor $x^{\otimes q}$ is $\tilde{O}\big(\mathrm{q}s + \mathrm{q} \cdot nnz(x)\big)$

Statistical Dimension $s_\lambda := \boldsymbol{tr}(K(K + \lambda I)^{-1})$

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Main contribution:
improve the exponential dependence on **q** to polynomial

Statistical Dimension $s_\lambda := \boldsymbol{tr}\left(K(K + \lambda I)^{-1}\right)$

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3. Time to sketch the tensor $x^{\otimes q}$ is $\tilde{O}\left(\mathrm{q}s + \mathrm{q} \cdot nnz(x)\right)$

Contribution 2: improve the quadratic dependence on s_λ to linear

Statistical Dimension $s_\lambda := \boldsymbol{tr}\left(K(K+\lambda I)^{-1}\right)$

Prior Work: TensorSketch

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3. Time to sketch the tensor $x^{\otimes q}$ is $\tilde{O}(\mathrm{q}s + \mathrm{q} \cdot nnz(x))$

Contribution 3: improve the success probability to $1 - \frac{1}{\mathrm{poly}(n)}$

Statistical Dimension $s_\lambda := \boldsymbol{tr}(K(K + \lambda I)^{-1})$

Main Results

- **Theorem 1:** there exists a distribution on linear sketches $\Pi \in \mathcal{R}^{s \times d^q}$ such that:

1. If target dimension $s = \Omega\left(\frac{q}{\epsilon^2}\right)$ then Π has the **Approximate Matrix Product** property with probability 9/10
2. If target dimension $s = \Omega\left(\frac{q}{\epsilon^2} \cdot s_\lambda^2\right)$ then Π is an **Oblivious Subspace Embedding** with probability 9/10
3. For any $x \in \mathcal{R}^d$, $\Pi \cdot x^{\otimes q}$ is computable in time $\tilde{O}(\mathrm{q}s + \mathrm{q} \cdot nnz(x))$

Main Results

- **Theorem 2:** there exists a distribution on linear sketches $\Pi \in \mathcal{R}^{s \times d^q}$ such that:

1. If target dimension $s = \tilde{\Omega}\left(\frac{q^4}{\epsilon^2}\right)$ then Π has the **Approximate Matrix Product** property with **high probability**
2. If target dimension $s = \tilde{\Omega}\left(\frac{q^4}{\epsilon^2} \cdot s_\lambda\right)$ then Π is an **Oblivious Subspace Embedding** with **high probability**
3. For any vector $x \in \mathcal{R}^d$, the product $\Pi \cdot x^{\otimes q}$ is computable in time $\tilde{O}\left(qs + q^5 \epsilon^{-2} nnz(x)\right)$

Review: TensorSketch

$$\Pi x^q = \mathcal{F}^{-1}\left[(\mathcal{F}C_1 x) \circ (\mathcal{F}C_2 x) \circ \cdots \circ \left(\mathcal{F}C_q x\right)\right]$$

- $\mathcal{F}$ is the Fourier transform matrix and $C_1, C_2, \cdots C_q \in \mathcal{R}^{s \times d}$ are independent copies of CountSketch

Review: TensorSketch

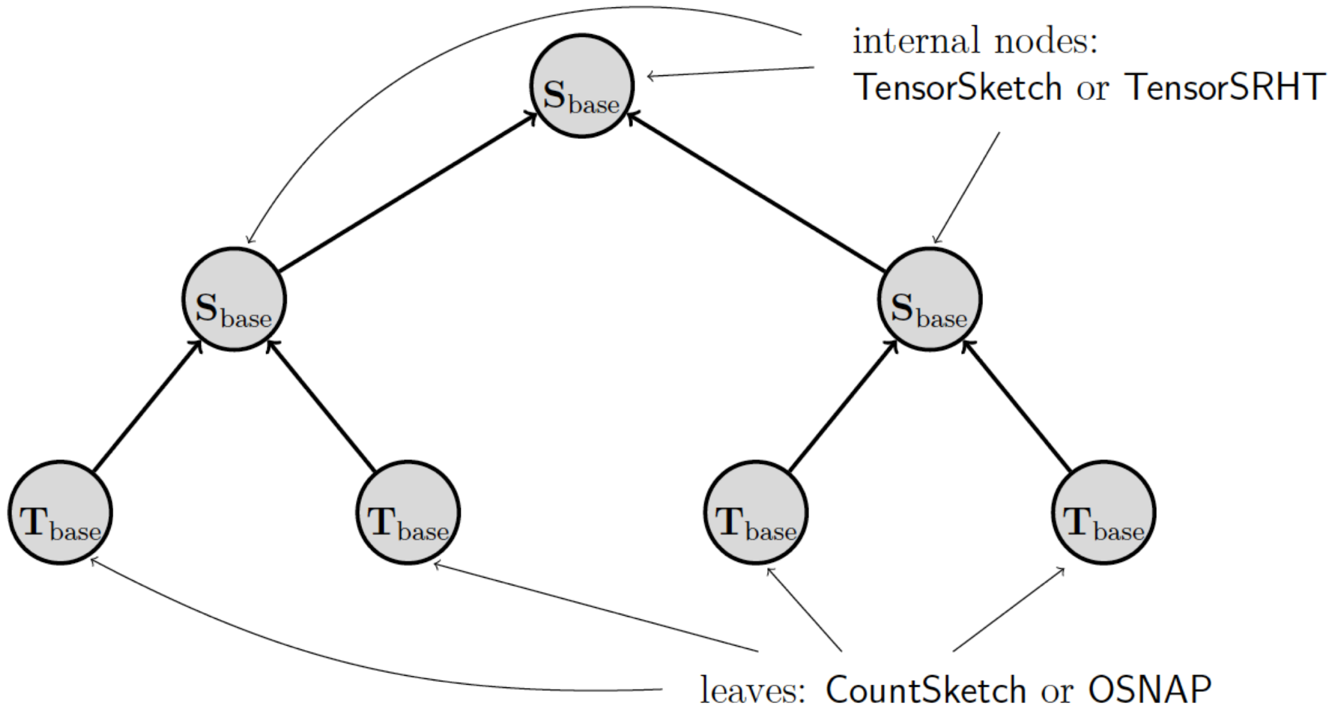
$$\Pi x^q = \mathcal{F}^{-1}\left[(\mathcal{F}C_1 x) \circ (\mathcal{F}C_2 x) \circ \cdots \circ \left(\mathcal{F}C_q x\right)\right]$$

- $\mathcal{F}$ is the Fourier transform matrix and $C_1, C_2, \cdots C_q \in \mathcal{R}^{s \times d}$ are independent copies of CountSketch
- The second moment of this estimator for $x = \{1\}^d$

$$\mathbb{E}\left[\left\|\Pi x^{\otimes q}\right\|_2^4\right] \geq \frac{\mathbf{3^q}}{2s^2}\left\|x^{\otimes q}\right\|_2^4$$

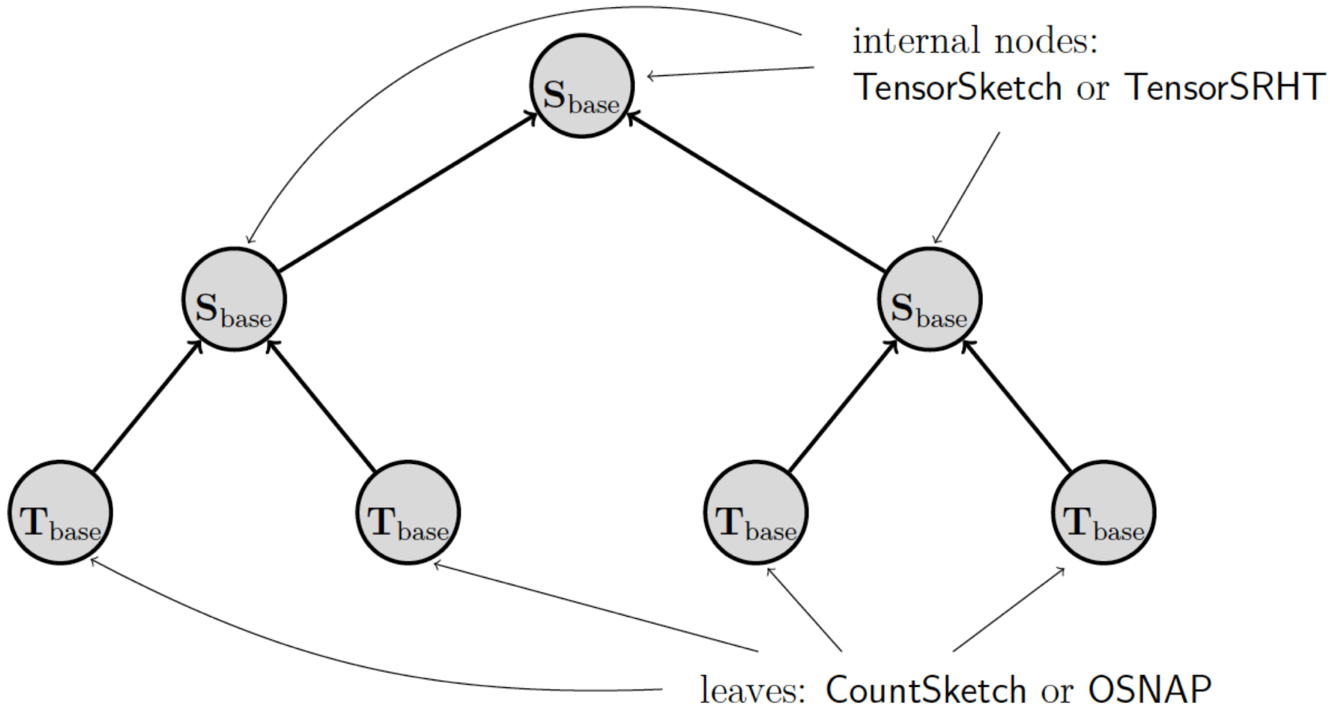
Our Sketch Construction

- Every node is an independent instance of some base sketch
- Leaves: sketch the input vector
- Internal nodes: sketch the tensor product of their children



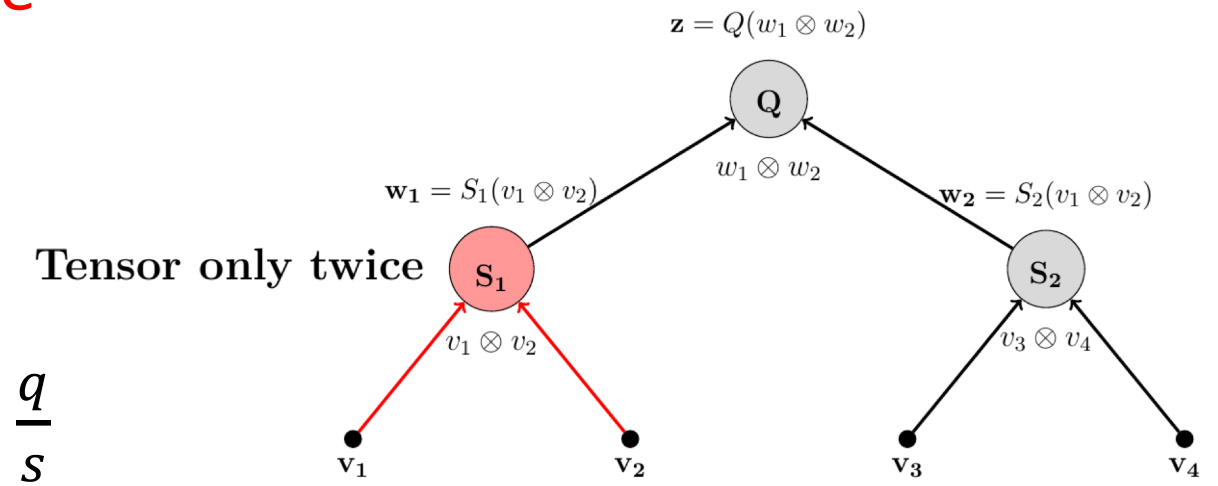
Our Sketch Construction

- Every leaf is a sketch that runs in input sparsity time
- Internal nodes support fast application time



Our Sketch Construction

- Intermediate nodes tensor only twice
- Loss in internal nodes is only $\frac{3^2}{s}$
- Number of such nodes is $O(q)$
- Hence $\frac{Var(\|\Pi x\|_2^2)}{\|x\|_2^4} \approx \left(1 + \frac{1}{s}\right)^q - 1 \approx \frac{q}{s}$
- In particular, there is no exponential dependence on q



s: target dimension of intermediate sketches

OSE for **Gaussian Kernel**

- The polynomial dependence of our sketch on the degree q leads to significant improvements on sketching the **Gaussian kernel** in high-d

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Prior work

- **Fast multipole method** of Greengard and Rokhlin: suffers from curse of dimensionality $(\log n)^d$
- **Fourier features** method of Rahimi & Recht: significantly suboptimal runtime of $\frac{n}{\lambda} \cdot nnz(X)$
- **Modified Fourier features** of Avron, Kapralov, Musco, Musco, Velingker, **Z**' 17: Optimal for constant dimensions d but does not apply to high dimensional data

OSE for **Gaussian Kernel**

- **Theorem 3:** for any dataset $x_1, x_2, \cdots x_n \in \mathbb{R}^d$ such that $\|x_i\|_2^2 \leq r$ if $K \in \mathbb{R}^{n\times n}$ is the Gaussian kernel matrix defined as $K_{i,j} = e^{-\|x_i - x_j\|_2^2}$ there exists an algorithm that computes $Z \in \mathbb{R}^{n\times s}$ such that:

1. If target dimension $s = \tilde{\Omega}\left(\frac{r^5}{\epsilon^2} \cdot s_\lambda\right)$ then $\mathrm{ZZ}^\top$ is an **Oblivious Subspace Embedding** for kernel K with **high probability**
2. The runtime to compute Z is $\tilde{O}\left(r^6\epsilon^{-2}ns_\lambda + r^6\epsilon^{-2}nnz(X)\right)$