Efficient k-Means on GPUs
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Abstract

k-Means is widely used in diverse fields of study. Quick execution allows practitioners to explore more data. Fast, data-parallel GPUs expose the cross-processing problem and the multi-pass problem as bottlenecks. We present a new centroid update algorithm for GPUs & fuse GPU kernels for a single data pass per iteration.

Problem 1: Cross-Processing between GPU and CPU

\textbf{Point Assignment} \quad \textbf{Transfer} \quad \textbf{Centroid Update}

Problem 2: Multiple Data Passes on same Processor

\textbf{Point Assignment} \quad \textbf{Centroid Update}

Goal: Single Data Pass

\textbf{Point Assignment} \quad \textbf{Centroid Update}

Open Source Repository

github.com/TU-Berlin-DIMA/CL-kmeans

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Take Home

Partitioning by both points and features reduces cache footprint of centroid update for up to 10$\times$ faster execution on GPUs.

A single data pass increases throughput by up to 2$\times$, but enlarges cache footprint.

20$\times$ better overall performance paves the way for high-bandwidth NVLink.

Execution Strategy Comparison

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{strategy_comparison.png}
\end{figure}

Point Assignment

Centroid Update

Cross-processing incurs transfer overhead. Single-pass reduces data accesses by half.

Thread-wise Centroid Update

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{thread_wise_update.png}
\end{figure}

Partitioning on data points requires each thread to store all data features in cache.

Thread-Group Centroid Update

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{thread_group_update.png}
\end{figure}

Partitioning on points and features unties cache footprint from number of features.

Thread-Group-Local Synchronization

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{thread_group_sync.png}
\end{figure}

Multi-Pass Strategy \textit{vs.} Single-Pass Strategy

Scale to Large Data Sets

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{data_scale.png}
\end{figure}

GPU clusters faster than CPU despite data transfer on each iteration.

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