Importance Sampling via Locality Sensitive Hashing.

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Motivating Problem: Stochastic Gradient Descent

\[ \theta^* = \arg \min_{\theta} F(\theta) = \arg \min_{\theta} \frac{1}{N} \sum_{i=1}^{N} f(x_i, \theta) \quad (1) \]

Standard GD

\[ \theta_t = \theta_{t-1} - \eta^t \frac{1}{N} \sum_{i=1}^{N} \nabla f(x_j, \theta_{t-1}) \quad (2) \]

SGD, pick a random \( x_i \), and

\[ \theta_t = \theta_{t-1} - \eta^t \nabla f(x_j, \theta_{t-1}) \quad (3) \]

SGD Preferred over GD in Large-Scale Optimization.

- Slow Convergence per epoch.
- Faster Epoch, \( O(N) \) times and hence overall faster convergence.
Better SGD?

Why SGD Works? (It is Unbiased Estimator)

$$\mathbb{E}(\nabla f(x_j, \theta_{t-1})) = \frac{1}{N} \sum_{i=1}^{N} \nabla f(x_i, \theta_{t-1}).$$

(4)

Are there better estimators? YES!!

- Pick $x_i$, with probability proportional to $w_i$
- Optimal Variance (Alain et. al. 2015): $w_i = ||\nabla f(x_i, \theta_{t-1})||_2$
- Many works on other Importance Weights (e.g. works by Rachel Ward)

The Chicken-and-Egg Loop

- Maintaining $w_i$, requires $O(N)$ work.
- For Least Squares, $w_i = ||\nabla f(x_i, \theta_t)||_2 = \left|2(\theta_t \cdot x_i - y_i)||x_i||_2\right|$, changes in every iteration.
Better SGD?

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The Chicken-and-Egg Loop
- Maintaining \( w_i \), requires \( O(N) \) work.
- For Least Squares, \( w_i = ||\nabla f(x_i, \theta_t)||_2 = |2(\theta_t \cdot x_i - y_i)||x_i||_2| \), changes in every iteration.

Can we Break this Chicken-and-Egg Loop? Can we get adaptive sampling in constant time \( O(1) \) per Iterations, similar to cost of
Detour: Probabilistic Hashing
Probabilistic Fingerprinting (Hashing)

**Hashing:** Function (**Randomized**) $h$ that maps a given data object (say $x \in \mathbb{R}^D$) to an integer key $h : \mathbb{R}^D \mapsto \{0, 1, 2, \ldots, N\}$. $h(x)$ serves as a discrete fingerprint.

**Locality Sensitive Property:**
- If $x = y$, $\text{Sim}(x, y)$ is high then $h(x) = h(y)$; $\Pr(h(x) = h(y))$ is high.
- If $x \neq y$, $\text{Sim}(x, y)$ is low then $h(x) \neq h(y)$; $\Pr(h(x) = h(y))$ is low.

Similar points are more likely to have the same hash value (hash collision) compared to dissimilar points.
Probabilistic Fingerprinting (Hashing)

**Hashing:** Function (Randomized) \( h \) that maps a given data object \( (x \in \mathbb{R}^D) \) to an integer key \( h : \mathbb{R}^D \mapsto \{0, 1, 2, \ldots, N\} \). \( h(x) \) serves as a discrete fingerprint.

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- if \( x = y \) \( \text{Sim}(x,y) \) is high then \( h(x) = h(y) \) \( \Pr(h(x) = h(y)) \) is high.
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Similar points are more likely to have the same hash value (hash collision) compared to dissimilar points.
Popular Hashing Scheme 1: SimHash (SRP)

\[ h_r(x) = \begin{cases} 
1 & \text{if } r^T x \geq 0 \\
0 & \text{otherwise} 
\end{cases} \quad r \in \mathbb{R}^D \sim N(0, I) \]

\[ Pr_r(h_r(x) = h_r(y)) = 1 - \frac{1}{\pi} \cos^{-1}(\theta), \quad \text{monotonic in } \theta \ (\text{Cosine Similarity}) \]

A classical result from Goemans-Williamson (95)
Popular Hashing Scheme 1: SimHash (SRP)

\[ \mathbf{r}^T \mathbf{x} > 0 \quad \mathbf{r}^T \mathbf{x} < 0 \]

\[ h_r(x) = \begin{cases} 1 & \text{if } \mathbf{r}^T \mathbf{x} \geq 0 \\ 0 & \text{otherwise} \end{cases} \]

\[ r \in \mathbb{R}^D \sim N(0, \mathcal{I}) \]

\[ Pr_r(h_r(x) = h_r(y)) = 1 - \frac{1}{\pi} \cos^{-1}(\theta), \quad \text{monotonic in } \theta \quad \text{(Cosine Similarity)} \]

A classical result from Goemans-Williamson (95)
Some Popular Measures that are Hashable

Many Popular Measures.
- Jaccard Similarity (MinHash)
- Cosine Similarity (Simhash and also MinHash if Data is Binary)
- Euclidian Distance
- Earth Mover Distance, etc.

Recently, Un-normalized Inner Products\(^1\)
  1. With bounded norm assumption.
  2. Allowing Asymmetry.

\(^1\)SL [NIPS 14 (Best Paper), UAI 15, WWW 15], APRS [PODS 16].
Sub-linear Near-Neighbor Search

Given a query \( q \in \mathbb{R}^D \) and a giant collection \( C \) of \( N \) vectors in \( \mathbb{R}^D \), search for \( p \in C \) s.t.,

\[
p = \arg \max_{x \in C} \sim(q, x)
\]

- \( \sim \) is the similarity, like Cosine Similarity, Resemblance, etc.
- Worst case \( O(N) \) for any query. \( N \) is huge.
- Querying is a very frequent operation.
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- Querying is a very frequent operation.

**Our goal is to find sub-linear query time algorithm.**

1. Approximate (or Inexact) answer suffices.
2. We are allowed to pre-process \( C \) once. (offline costly step)
Probabilities Hash Tables

**Given:** \( Pr_h[h(x) = h(y)] = f(sim(x, y)), \) f is monotonic.
Given: $Pr_h[h(x) = h(y)] = f(sim(x, y))$, $f$ is monotonic.
Probabilities Hash Tables

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<table>
<thead>
<tr>
<th>( h_1 )</th>
<th>( h_2 )</th>
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</tbody>
</table>
| ... | ... | ...
| 11 | 11 | ![Diagram](attachment:image.png) |

\( h_1, h_2 : R^D \to \{0, 1, 2, 3\} \)

Given query \( q \), if \( h_1(q) = 11 \) and \( h_2(q) = 01 \), then probe bucket with index 1101. It is a good bucket! (Locality Sensitive)
Given: $Pr_h[h(x) = h(y)] = f(sim(x, y))$, $f$ is monotonic.

Given query $q$, if $h_1(q) = 11$ and $h_2(q) = 01$, then probe bucket with index 1101. It is a good bucket!!
Probabilities Hash Tables

**Given:** $Pr_h[h(x) = h(y)] = f(sim(x, y))$, $f$ is monotonic.

- Given query $q$, if $h_1(q) = 11$ and $h_2(q) = 01$, then probe bucket with index $1101$. It is a good bucket !!
- (Locality Sensitive) $h_i(q) = h_i(x)$ noisy indicator of high similarity.
- Doing better than random !!

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The Classical LSH Algorithm

Table 1

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- We use $K$ concatenation.
## The Classical LSH Algorithm

### Table 1

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- We use \( K \) concatenation.
- Repeat the process \( L \) times. (\( L \) Independent Hash Tables)
The Classical LSH Algorithm

We use $K$ concatenation.

Repeat the process $L$ times. ($L$ Independent Hash Tables)

**Querying**: Probe one bucket from each of $L$ tables. Report union.
The Classical LSH Algorithm

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- **Querying**: Probe one bucket from each of $L$ tables. Report union.

Two knobs $K$ and $L$ to control.
Success of LSH

Similarity Search or Related (Reduce n)

- Similarity Search or related.
- Plenty of Applications.

\(^2\)Li et. al. NIPS 2011
Success of LSH

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Similarity Estimation and Embedding (Reduce dimensionality \(d\))
- Basically JL (Johnson-Lindenstrauss) or Random Projections does most of the job!!
- Similarity Estimation. (Usually not optimal in Fisher Information Sense)
- Non-Linear SVMs in Learning Linear Time\(^2\).


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Success of LSH

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**Result:** Won 2012 ACM Paris Kanellakis Theory and Practice Award.

Are there other Fundamental Problems?

\(^2\)Li et. al. NIPS 2011
Is LSH really a search algorithm?

- Given the query $x$, LSH samples $\theta_y$ from the dataset, with probability exactly $p_y = 1 - (1 - p(x, \theta_y)^K)^L$.
- LSH is considered a black box for near-neighbor search. It is not!!
- Adaptive Sampling is being converted into an algorithm for high similarity search.
**New View:** Hashing is an Efficient Adaptive Sampling in Disguise.
Partition Function in Log-Linear Models

\[ P(y|x, \theta) = \frac{e^{\theta_y \cdot x}}{Z_\theta} \]

- \( \theta_y \) is the weight vector
- \( x \) is the (current context) feature vector (word2vec).
- \( Z_\theta = \sum_{y \in Y} e^{\theta_y \cdot x} \) is the partition function

**Issues:**
- \( Z_\theta \) is expensive. \( |Y| \) is huge. (billion word2vec)
- Change in context \( x \) requires to recompute \( Z_\theta \).

**Question:** Can we reduce the amortized cost of estimating \( Z_\theta \)?
Importance Sampling (IS)

Summation by expectation: But sampling \( y_i \propto e^{\theta y \cdot x} \) is equally harder.

Importance Sampling

- Given a normalized proposal distribution \( g(y) \) where \( \sum_y g(y) = 1 \).
- We have an unbiased estimator
  \[
  \mathbb{E} \left[ \frac{f(y)}{g(y)} \right] = \sum_y g(y) \frac{f(y)}{g(y)} = \sum_y f(y) = Z_\theta
  \]
- Draw \( N \) samples \( y_i \sim g(y) \) for \( i = 1 \ldots N \). we can estimate
  \[
  Z_\theta = \frac{1}{N} \sum_{i=1}^{N} \frac{f(y_i)}{g(y_i)}.
  \]

Yet Another Chicken and Egg Loop:

- Does not really work if \( g(y) \) is not close to \( f(y) \).
- Getting \( g(y) \) which is efficient and close to \( f(y) \) is not known.
- No efficient choice in literature. Random sampling or other heuristics.
Detour: LSH as Samplers

\[(K, L)\] parameterized LSH algorithm is an efficient sampling:

- Given the query \(x\), LSH samples \(\theta_y\) from the dataset, with probability exactly \(p_y = 1 - (1 - p(x, \theta_y)^K)^L\).
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(K, L) parameterized LSH algorithm is an efficient sampling:
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Unnormalized Importance Sampling:
- It is not normalized \( \sum_y p_y \neq 1 \)
- Samples are correlated.

It turns out, we can still make them work!
Beyond IS: The Unbiased LSH Based Estimator

Procedure:
- For context $x$, report all the retrieved $y_i$s from the $(K, L)$ parameterized LSH Algorithm. (just one NN query)
- Report $\hat{Z}_\theta = \sum_i \frac{e^{\theta y_i \cdot x}}{1-(1-p(x,\theta y_i)^K)^L}$

Properties:
- $E[\hat{Z}_\theta] = Z_\theta$ (Unbiased)

$$Var[\hat{Z}_\theta] = \sum_i \frac{f(y_i)^2}{p_i} - \sum_{i=1}^{N} f(y_i)^2$$

$$+ \sum_{i \neq j} \frac{f(y_i)f(y_j)}{p_i p_j} Cov(1[y_i \in S] \cdot 1[y_j \in S])$$

- Correlations are mostly negative (favorable) with LSH.
MIPS Hashing is Ideal for Log-Linear Models

Theorem

For any two states $y_1$ and $y_2$:

$$P(y_1|x; \theta) \geq P(y_2|x; \theta) \iff p_1 \geq p_2$$

where

$$p_i = 1 - (1 - p(\theta_{y_i} \cdot x)^K)^L$$

$$P(y|x, \theta) \propto e^{\theta_y \cdot x}$$

Corollary

The modes of both the sample and the target distributions are identical.

Efficient as well as similar to target (Adaptive).
How does it work? (PTB and Text8 Datasets)

![Graph showing MAE vs #Samples for different methods.]

Running Time:

<table>
<thead>
<tr>
<th>Samples</th>
<th>Uniform</th>
<th>LSH</th>
<th>Exact Gumbel</th>
<th>MIPS Gumbel</th>
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Final Perplexity of Language Models

<table>
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<tr>
<th>Standard</th>
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Back to Adaptive SGD

Why SGD Works? (It is Unbiased Estimator)

$$\mathbb{E}(\nabla f(x_j, \theta_{t-1})) = \frac{1}{N} \sum_{i=1}^{N} \nabla f(x_i, \theta_{t-1}).$$ (5)

Are there better estimators? YES!!

- Pick $x_i$, with probability proportional to $w_i$
- Optimal Variance (Alain et. al. 2015): $w_i = ||\nabla f(x_i, \theta_{t-1})||_2$
- Many works on Other Importance Weights

Optimal Variance $w_i$

- $w_i = ||\nabla f(x_i, \theta_{t-1})||_2 = 2|\langle \theta_t, -1 \rangle \cdot (x_i||x_i||, y_i||x_i||)|$
- Large Inner Product, $\theta_t$ changes, $x_i$’s remains fixed :)
- We wont sample exactly in proportion to $w_i$, but with some $w'_i$, which is monotonic in $w_i$. 
The Complete Picture

One time Cost
- Preprocess $\langle x_i \| x_i \|, y_i \| x_i \| \rangle$ into Inner Product Hash Tables. (Data Reading Cost)

Per Iteration
- Query hash tables with $\langle \theta_{t-1}, -1 \rangle$ for sample $x_i$. (1-2 Hash Lookups)
- Estimate Gradient as $\frac{\nabla f(x_i, \theta_{t-1})}{N \times \text{SamplingProbability}}$
- Can show: Unbiased and better variance than SGD.
The Complete Picture

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- Estimate Gradient as $\frac{\nabla f(x_i, \theta_{t-1})}{N \times SamplingProbability}$
- Can show: Unbiased and better variance than SGD.

Per iterations cost is 1.5 times that of SGD, but superior variance.
How it works?

(a) Ada Time

(b) Plain Time

(c) Ada Epoch

(d) Plain Epoch
Conclusion

Hashing can change the equation!!