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Stochastic Gradient Descent for Large-scale Generalized CP Tensor Decomposition

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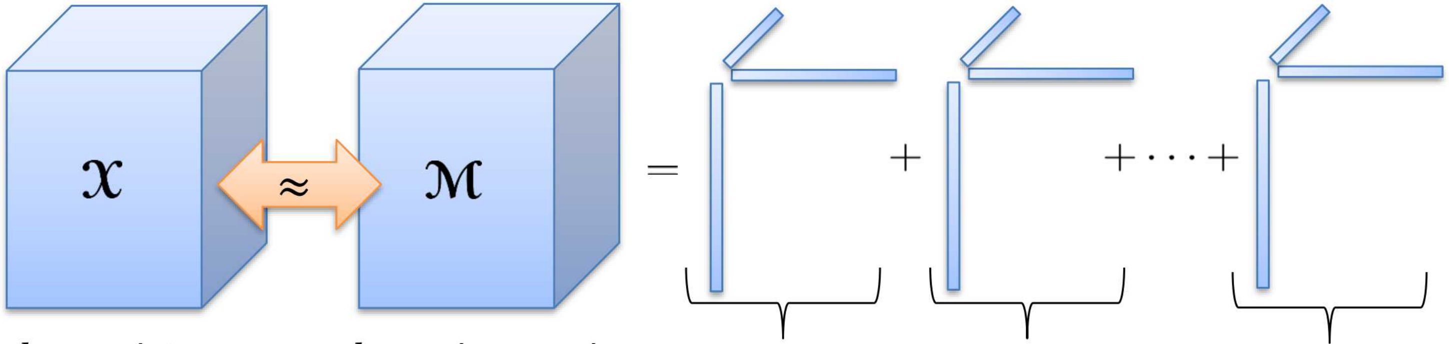
U.S. DEPARTMENT OF ENERGY

Generalized Canonical Polyadic (GCP) Tensor Decomposition



d-way data tensor of size n^d

d-way low-rank model tensor of size n^d and rank r

rank-one component $j = 1$

rank-one component $j = 2$

rank-one component $j = r$

$$\mathcal{X} \approx \mathcal{M} \quad \text{where} \quad \mathcal{M} = \sum_{j=1}^{r} \mathbf{A}_1(:,j) \circ \mathbf{A}_2(:,j) \circ \cdots \circ \mathbf{A}_d(:,j)$$

Low-rank: $\operatorname{rank}(\mathcal{M}) \leq r \ll n^d$

Factor matrices: $\mathbf{A}_k \in \mathbb{R}^{n \times r}$ for $k \in \{1, \ldots, d\}$

GCP

$$\min \; F(\mathcal{X}, \mathcal{M}) \equiv \sum_{i \in \Omega} f(x_i, m_i)$$

$$\text{s.t.} \; \operatorname{rank}(\mathcal{M}) \leq r$$

i = multi-index
Ω = all indices

- Standard CP [Hitchcock, 1927; Carrol & Chang, 1970; Harshman, 1970]

  $$f(x,m) = (x - m)^2$$

- Poisson CP [Welling & Webber, 2001; Chi & Kolda, 2009]

  $$f(x,m) = m - x \log m$$

- Logistic CP, etc. [Hong, Kolda, Duersch, 2018]

  $$f(x,m) = \log(m+1) - x \log(m)$$

Gradient-based Optimization for Fitting the GCP Model

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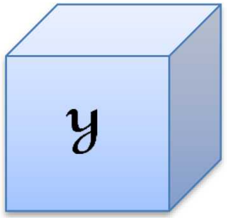
GCP

$$\min \; F(\mathcal{X}, \mathcal{M}) \equiv \sum_{i \in \Omega} f(x_i, m_i)$$

$$\text{s.t.} \; \text{rank}(\mathcal{M}) \leq r$$

Define: Elementwise partial gradient tensor, same size as data tensor = n^d



$$y_i = \begin{cases} \frac{\partial f}{\partial m}(x_i, m_i) & \text{if } i \in \Omega \\ 0 & \text{otherwise} \end{cases}$$

Define: Khatri-Rao product in all modes but one of size $n^{d-1} \times r$

$$\mathbf{Z}_k = \mathbf{A}_d \odot \cdots \odot \mathbf{A}_{k+1} \odot \mathbf{A}_{k-1} \odot \cdots \odot \mathbf{A}_1$$

Gradients computed via a sequence of MTTKRPs:

$$\mathbf{G}_k \equiv \frac{\partial F}{\partial \mathbf{A}_k} = \mathbf{Y}_{(k)} \mathbf{Z}_k$$

MTTKRP

gradient for mode k factor matrix of size $n \times r$

tensor unfolded in mode k into matrix of size $n \times n^{d-1}$

MTTKRPs can be computed efficiently…

- Bader & Kolda, SISC, 2007 – Dense and sparse
- Phan, Tichavsky, Cichocki, 2013 – Sequence
- Smith et al., IPDPS 2015 – Sparse
- Kaya & Ucar, SC 2015 – Sparse
- Li et al., IPDPS 2017 – Sparse
- Hayashi et al., 2017 – Dense
- Ballard, Knight, Rouse, 2017 – Dense

Hong, Kolda, Duersch, 2018

Stochastic Gradient Descent (SGD) for GCP

30-Second Tutorial on SGD

$$\min f(x)$$

Gradient Descent (GD)

α = learning rate

$$x^{(t+1)} = x^{(t)} - \alpha g^{(t)}$$

Stochastic Gradient Descent (SGD)

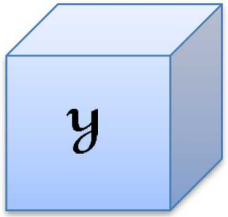
$$x^{(t+1)} = x^{(t)} - \alpha \tilde{g}^{(t)}$$

$$\mathbb{E}[\tilde{g}^{(t)}] = g^{(t)} \equiv \nabla f(x^{(t)})$$

Adam (Kingma & Ba, 2015)

Adaptive momentum SGD

Standard gradient

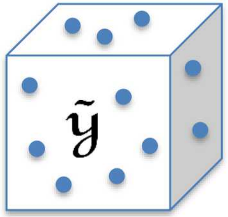


$$y_i = \begin{cases} \frac{\partial f}{\partial m}(x_i, m_i) & \text{if } i \in \Omega \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{G}_k = \mathbf{Y}_{(k)} \mathbf{Z}_k$$

Cost: $O(rn^d)$ flops

Stochastic gradient



Random sparse tensor: $\tilde{\mathcal{W}}$ $\quad s \equiv \text{nnz}(\tilde{\mathcal{W}}) \ll n^d$

$$\tilde{\mathcal{Y}} = \tilde{\mathcal{W}} * \mathcal{Y}$$

$$\tilde{y}_i = \begin{cases} \tilde{w}_i \cdot \frac{\partial f}{\partial m}(x_i, m_i) & \text{if } \tilde{w}_i \neq 0 \\ 0 & \text{if } \tilde{w}_i = 0 \end{cases}$$

$$\tilde{\mathbf{G}}_k = \tilde{\mathbf{Y}}_{(k)} \mathbf{Z}_k$$

Cost: $O(rds)$ flops

<u>Theorem</u>: $\mathbb{E}[\tilde{\mathcal{W}}] = \mathbf{1} \Rightarrow \mathbb{E}[\tilde{\mathbf{G}}_k] = \mathbf{G}_k$

($\mathbf{1}$: all ones tensor)

Stochastic Weight Matrix: Single Element

Goal: Random ***sparse*** tensor of size n^d such that every element has an expected value of 1

1. Choose random tensor entry ξ
2. Define random tensor with single nonzero as follows

$$\tilde{w}_i = \begin{cases} n^d & \text{if } i = \tilde{\xi} \\ 0 & \text{otherwise} \end{cases}$$

Theory

Claim: $\mathbb{E}[\tilde{\mathcal{W}}] = \mathbf{1}$

Proof:
$$\mathbb{E}(\tilde{w}_i) = p_i \cdot n^d + (1 - p_i) \cdot 0 = \frac{1}{n^d} \cdot n^d = 1$$

Shortcoming of sampling only single element…

- Higher variance in stochastic gradient
- Only one row of the unfolded tensor has a nonzero so stochastic gradient only nonzero for single row of each factor matrix
- Gradient = $O(rd)$ work versus Update = $O(rdn)$ work
- *Can afford more work per gradient calculation!*

Stochastic Weight Matrix: Multiple Elements

<u>Goal</u>: Random ***sparse*** tensor of size n^d such that every element has an expected value of 1

1. Choose $s \ll n^d$ random tensor entries (with replacement)
2. Define random tensor with up to s nonzeros as follows

$$\tilde{w}_i = \frac{\#\text{ times } i \text{ sampled}}{s} \cdot n^d$$

Theory

Claim: $\mathbb{E}[\tilde{\mathcal{W}}] = \mathbf{1}$

Proof: $$\mathbb{E}(\tilde{w}_i) = \frac{\mathbb{E}(\#\text{ times } i \text{ sampled})}{s} \cdot n^d = \frac{s \cdot \frac{1}{n^d}}{s} \cdot n^d = 1$$

Benefits of sampling multiple elements…

- Lower variance in stochastic gradient
- Gradient = $O(rds)$ work in line with Update = $O(rdn)$ work

Downside…

- If data tensor is sparse, few entries corresponding to nonzeros will be chosen

Stratified Sampling Decreases Variance

For very sparse tensors, the likelihood of getting a nonzero is exceedingly small….

Results by Needell, Srebro, and Ward (2013) argue for biasing the sampling toward functionals with higher Lipschitz smoothness constants

Consider Poisson loss…

$$f(m;x) = m - x \log m$$

$$f'(m;0) = 1 \quad \Rightarrow \quad L = 0$$

$$f'(m;1) = 1 - 1/m \quad \Rightarrow \quad L \text{ unbounded as } m \downarrow 0$$

Stochastic Weight Matrix: Stratified Sample

Goal: Random ***sparse*** tensor of size n^d such that every element has an expected value of 1

1. For each partition ℓ
   a) Choose $s_\ell \ll |\Omega_\ell|$ random tensor entries from Ω_ℓ (with replacement)
   b) For each $i \in \Omega_\ell$, the corresponding entry of the weight tensor is

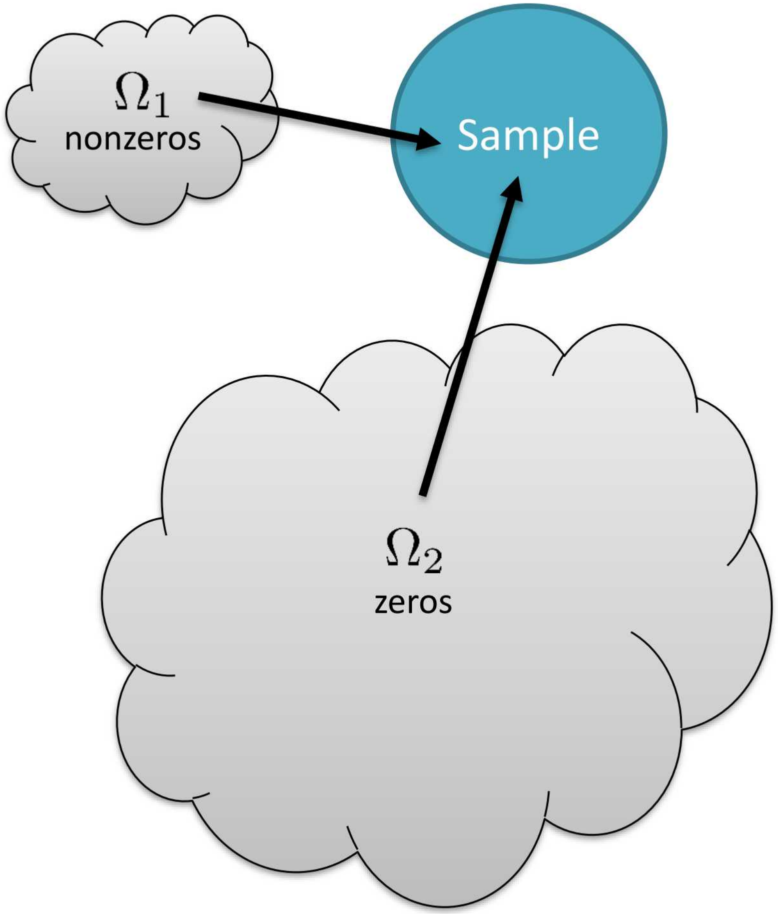
$$\tilde{w}_i = \#\text{ times } i \text{ sampled} \cdot \frac{|\Omega_\ell|}{s_\ell}$$

Theory

Claim: $\mathbb{E}[\tilde{\mathbf{W}}] = \mathbf{1}$

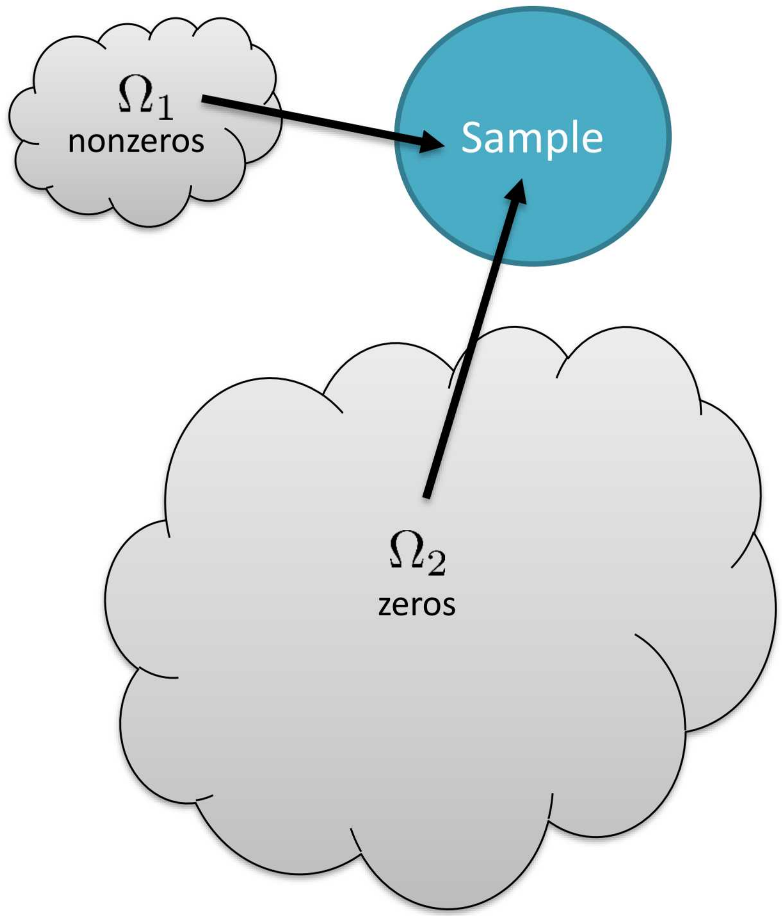
Proof: $\mathbb{E}(\tilde{w}_i) = \mathbb{E}[\#\text{ times } i \text{ sampled}] \cdot \frac{|\Omega_\ell|}{s_\ell}$

$$= s_\ell \cdot \frac{1}{|\Omega_\ell|} \cdot \frac{|\Omega_\ell|}{s_\ell} = 1$$

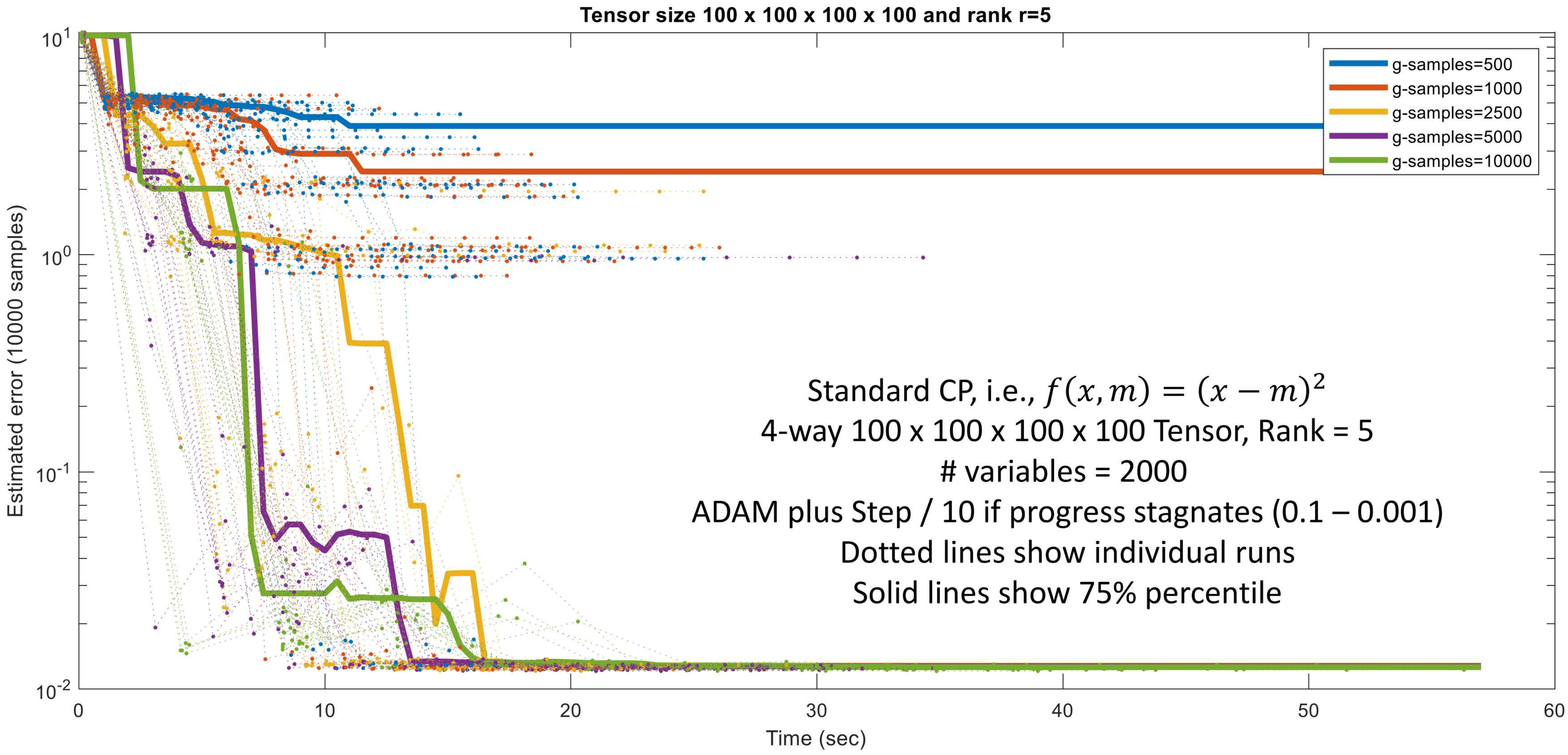


Rejection Sampling for Zeros in Sparse Tensor

- Most SGD-based tensor methods ignore zeros
  - Treating them as "unknown"
  - In contrast, we include them
- Zeros not stored explicitly
  - Generate candidate random index
  - Reject if in list of nonzeros
  - Can be expensive!



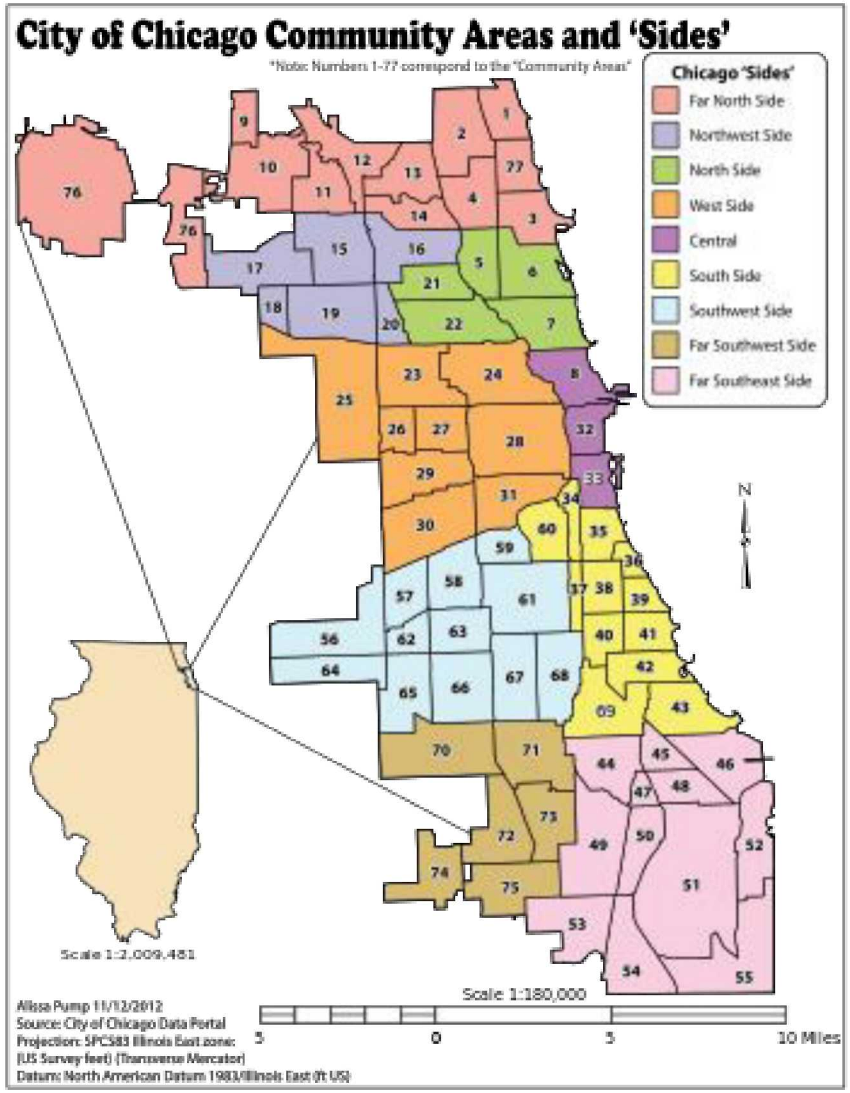
Dependence on Sample Size



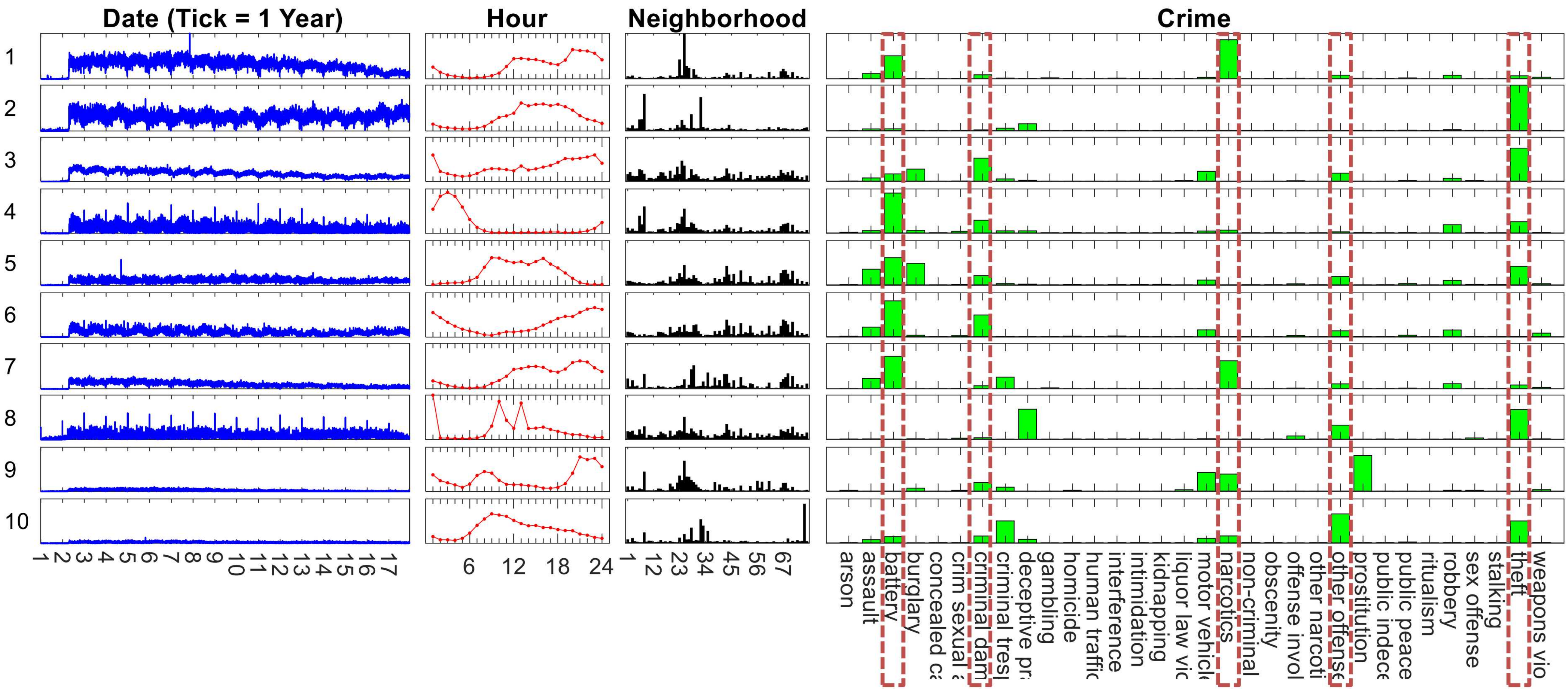
Chicago Crime Data

- 4-way count tensor
  - 6,186 Days
  - 24 Hours of the Day
  - 77 Community Areas
  - 32 Crime Types
- Non-zeros: 5,330,673
  - Storage: 0.21GB for sparse tensor
- Distribution of entries
  - 0: 98.54%
  - 1: 1.33%
  - $\geq$ 2: 0.12%
- Using binary version (every nonzero changed to 1)
- Obtained from FROSTT (http://frostt.io/tensors/chicago-crime/)
- Data originally from Chicago Data Portal (https://data.cityofchicago.org/Public-Safety/Crimes-2001-to-present/ijzp-q8t2)

GCP-Binary
Rank = 10
$s = 30{,}000$
$$f(x, m) = \log(m+1) - x\log(m)$$
1100 sec. (versus 65 sec. CP-ALS)

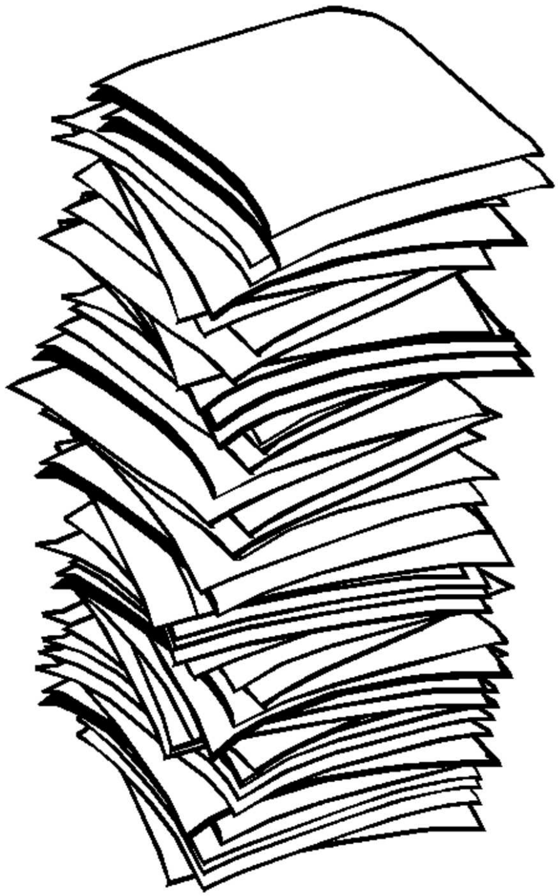


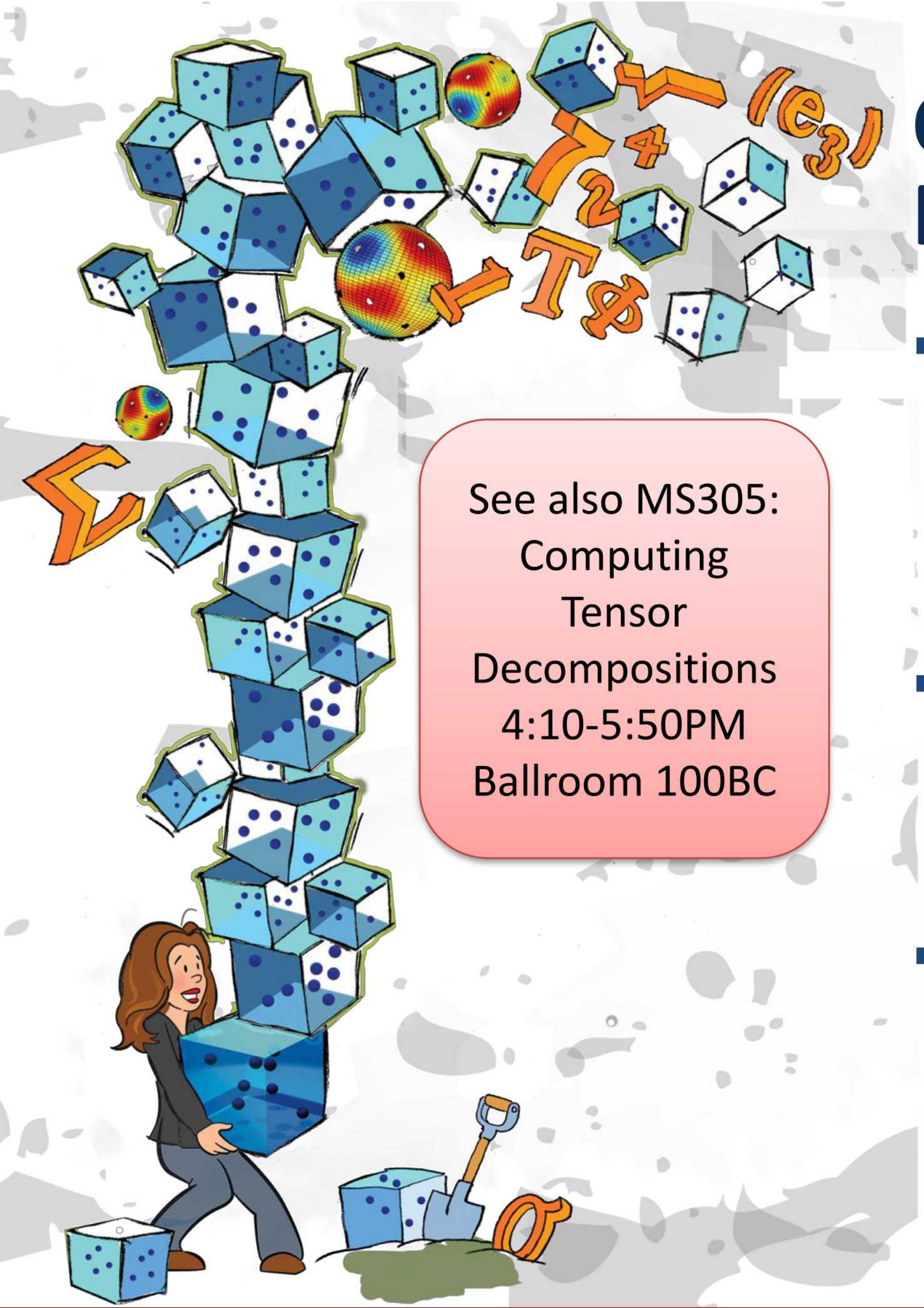
Application to Sparse Crime Binary Tensor



Related Work

- SGD for Matrix Decomposition
  - Gemulla et al., KDD'11 – Distributed SGD (DSGD) method: Partition matrix into blocks, run parallel SGD on independent blocks, cycling through the blocks in a way that ensures correctness. ***Only uses nonzero entries.***
  - Zhuang et al., RecSys'13 – Fast Parallel SGD (FPSGD) method: Matrix factorization in shared memory environment. No theoretical analysis. ***Only uses nonzero entries.***
- SGD for Tensor Decomposition
  - Mardini et al. (2015) – OnlineCP uses SGD for tensors that are streaming, one slice at a time
  - Maehara et al., AAAI-16 – Tensor can be written as sum or average of a finite(?) number of tensors. Proposes SGD plus several variations
  - Ge et al. [6] consider SGD for symmetric tensor decomposition
- Tensor Sketching
  - Acar et al. [1] show that, for dense tensors, it is heuristically possible to recover a full tensor decomposition with only a sketch of the data
  - Jain and Oh [11] and Bhojanapalli and Sanghavi [3] more formally prove under what conditions sketching works, albeit with a focus on orthogonal symmetric tensor decomposition





See also MS305: Computing Tensor Decompositions 4:10-5:50PM Ballroom 100BC

Conclusions, Future Work, References

- Conclusions
  - GCP not amenable to scaling because gradient "dense"
  - Developed GCP stochastic gradient
  - Use stratified sampling for sparse tensors
  - Recommend #samples = $O(rnd)$
- Future work
  - Release for MATLAB Tensor Toolbox
  - Parallel implementation (with Eric Phipps – GenTen)
  - Distributed implementation (with Karen Devine)
- References

  - D. Hong, T. G. Kolda, J. A. Duersch. **Generalized Canonical Polyadic Tensor Decomposition**. arXiv:1808.07452, 2018
  - T. G. Kolda, D. Hong, J. A. Duersch. **Stochastic Optimization for Large-Scale Tensor Decomposition**, in preparation