COMPSCI 590N
Lecture 9: Sparse Matrices and Probability 1

Roy J. Adams

College of Information and Computer Sciences
University of Massachusetts Amherst

Outline

Sparsity

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  - Multiple parallel event sequences can be arranged as a matrix. If the events are uncommon, then the matrix is sparse.
- If we know an matrix is sparse, we can take advantage of this structure to speed up computations on the matrix.

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- In general, how many multiplications must we perform?
- What if we know that only 10% of the entries in x are non-zero and we know where the are, how many multiplications do we need to perform?

Sparse Representations

There are two main strategies for storing sparse matrices:

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1. Formats that support **efficient modifications** include Dictionary of Keys (DOK), List of Lists (LIL), and Coordinate list (COO) formats.
2. Formats that support **efficient access and operations** include Compressed Sparse Row (CSR) and Compressed Sparse Column (CSC) formats.

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- What is the complexity of row or column slicing?

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- The CSC format is the same as CSR, but `data` is stored in column major order and `indices` stores the row of each entry.

Compressed Sparse Row Format: Example

$$\begin{bmatrix} 1 & 0 & 2 \\ 0 & 0 & 3 \\ 4 & 5 & 0 \end{bmatrix}$$

```
indptr:
  [0,2,3,5]
indices:
  [0,2,2,0,1]
data:
  [1,2,3,4,5]
```

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row = A[i,:]
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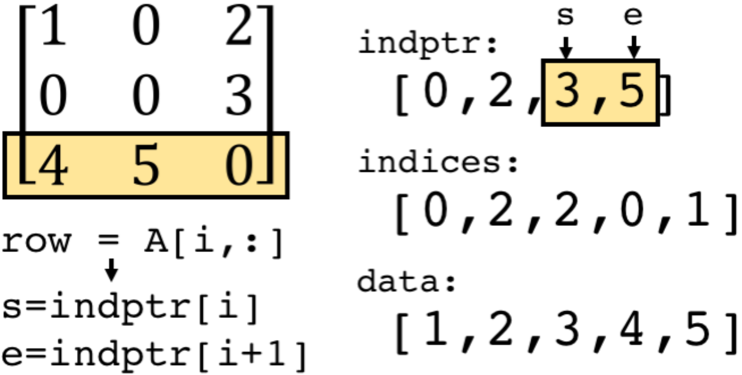

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```
row = A[i,:]
s=indptr[i]
e=indptr[i+1]
row=data[s:e]
```

```
indptr:    s   e
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indptr:

$[0,2,\boxed{\overset{s}{3},\overset{e}{5}}]$

indices:

$[0,2,2,0,1]$

data:

$[1,2,3,\boxed{4,5}]$

Scipy Sparse Matrices

The module `scipy.sparse` implements each of these sparse formats.

```
>>> import scipy.sparse as sps
>>> import numpy as np

>>> A = np.eye(5)
>>> identity = np.eye(5)
>>> sparse_identity = sps.csr_matrix(identity)

>>> sparse_identity.indptr
array([0, 1, 2, 3, 4, 5], dtype=int32)
>>> sparse_identity.indices
array([0, 1, 2, 3, 4], dtype=int32)
>>> sparse_identity.data
array([ 1.,  1.,  1.,  1.,  1.])
```

Interactive Demo

- What linear algebra operations are most sped up by using sparse matrices?

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Random Variables

A random variable, X, is a quantity that can take any value from a set of possible values, Ω, according to a set of probabilities.

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  - $\Omega = \{H, T\}$

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  - The number of people who log in to Netflix between 1pm and 2pm can be any non-negative integer.
  - The end of season goal differential for a soccer team can be any integer (positive or negative).

Probability Mass Functions

The probability of each possible outcome is defined by a Probability Mass Function.

Probability Mass Function

For a discrete random variable X with support Ω, a Probability Mass Function (PMF) $P : \Omega \to [0, 1]$ maps possible outcomes to probabilities. A PMF must satisfy two conditions:

1. Probability of any single outcome must be between zero and one (i.e. $P(x) \in [0, 1]$ for all $x \in \Omega$).

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1. Probability of any single outcome must be between zero and one (i.e. $P(x) \in [0, 1]$ for all $x \in \Omega$).
2. The probabilities of all possible outcomes must sum to one (i.e. $\sum_x P(x) = 1$).

Probability Mass Functions: Examples

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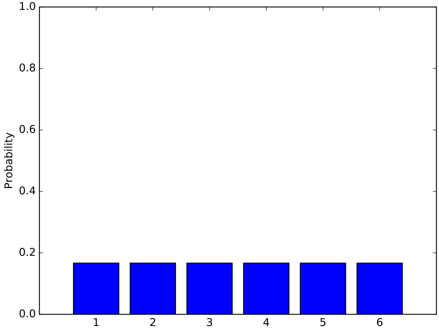

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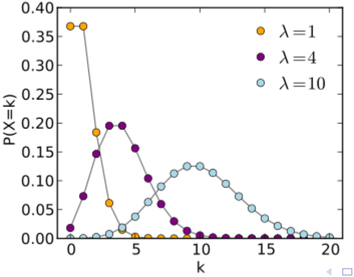

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- In this case the, the distribution has a single parameter λ that must be a positive real number.
- Much of statistics is concerned with inferring these parameters from data.

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  - The amount of time between hard drive failures in a server.

Probability Density Functions

The distribution over possible values of a continuous random variable is given by a **probability density function**.

Probability Density Function

For a continuous random variable X, the probability density function (PDF) $P(x)$ describes the relative likelihood of a continuous random variable taking a given value. A PDF must satisfy the following two conditions:

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The probability of X falling between a and b is given by the integral:

$$P(a < x < b) = \int_x p(x)dx$$

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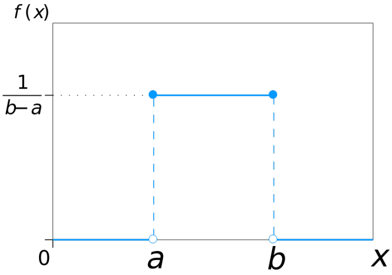

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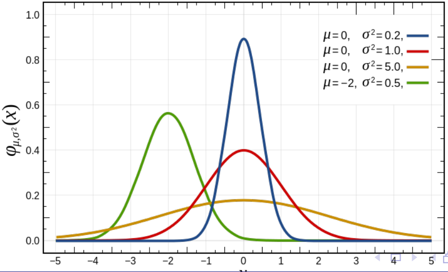
$$p(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



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- Normalizing the distribution (ensuring the PDF/PMF integrates to 1) requires a difficult to compute sum or integral.
- Probabilities near zero or near one can cause numerical errors.

Calculating PDFs: The Gamma Function

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The Gamma function and related Incomplete Gamma and Incomplete Beta functions are necessary/useful for working with the following common distributions (among others).

- Gamma, Z, t, χ^2, F, binomial, Poisson

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Importantly, the user can choose g and pre-calculate the constants c_i.

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$$P(X = x; n, p) = \binom{n}{x} p^x (1-p)^{n-x}$$

Calculating PMFs: Using Recursion

Evaluating the binomial PMF involves evaluating factorials (a special case of the Gamma function); however, if multiple values are desired, we can take advantage of the following recurrence relation:

$$
\begin{aligned}
P(X = x) &= \binom{n}{x} p^x (1-p)^{n-x} \\
&= \frac{n-x}{x+1} \frac{p}{1-p} \left[\binom{n}{x-1} p^{x-1} (1-p)^{n-(x-1)} \right] \\
&= P(X = x-1) \frac{n-x}{x+1} \frac{p}{1-p}
\end{aligned}
$$

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- The complexity of calculating the first k values of the binomial PMF is $\mathcal{O}(k)$ in both cases; however, we are replacing a special function with arithmetic operations only.

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- Many distributions require exponentiation of intermediate values.
- One common solution is to work in **log-space**.

Working in log-space and the Log-Sum-Exp trick

The multinomial distribution is the standard distribution for finite sets. Consider the following multinomial distribution over K discrete values parameterized by a length K vector of weights α.

$$P(X = i; \alpha) = \frac{e^{\alpha_i}}{\sum_i e^{\alpha_i}}, \ i = 1, ..., K$$

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Rather than evaluate this function directly, risking over/underflow, we can evaluate the log PMF,

$$\log P(X = i; \alpha) = \alpha_i - \log \sum_i e^{\alpha_i}$$

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$$P(X = i; \alpha) = \frac{e^{\alpha_i}}{\sum_i e^{\alpha_i}}, \; i = 1, ..., K$$

Rather than evaluate this function directly, risking over/underflow, we can evaluate the log PMF,

$$\log P(X = i; \alpha) = \alpha_i - \log \sum_i e^{\alpha_i}$$

Why does this not completely solve our problem?

Working in log-space and the Log-Sum-Exp trick

Calculating the second term $\log \sum_i e^{\alpha_i}$ (also known as the cumulant function) still requires exponentiating α. Instead, let $\alpha^* = \max_i \alpha_i$. Then, we can use the following trick,

$$
\begin{aligned}
\log \sum_i e^{\alpha_i} &= \log \frac{e^{\alpha^*}}{e^{\alpha^*}} \sum_i e^{\alpha_i} \\
&= \log \sum_i e^{\alpha_i - \alpha^*} + \log e^{\alpha^*} \\
&= \log \sum_i e^{\alpha_i - \alpha^*} + \alpha^*
\end{aligned}
$$

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- There can be no overflow and, while individual terms in the sum may underflow, this results only in round-off error in the final sum.
- Log-sum-exp is implemented in `scipy.misc.logsumexp`.