The Kauffman NK Model

A Stochastic Combinatorial Optimization Model for Complex Systems

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Outline of the Talk

- Introduction
- Mathematical Description
- NK Model as a Stochastic Network
- Computational Strategies using Stochastic Networks
- Dependency Graph and Bounds on Order Statistics
- Analysis for underlying Normal Distribution
- Analysis for underlying Uniform Distribution
- Concentration of Measure

Introduction

We want to model systems composed of several interacting components, where each component can be in one of many possible states.

Objective : Maximize a measure of performance of the system based on contributions from each component, depending on the state of the component and its ‘interaction’ with its neighbors.

Background

In 1987, Kauffman and Levin introduced

The NK model

- N counts the number of components in the system
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The NK model was originally proposed to study the evolution of genomes.

- system $\equiv$ genome
- components $\equiv$ genes
- states $\equiv$ gene mutations
- performance measure $\equiv$ fitness

Applications I

- In Biology
  - maturation of immune response
  - evolution of protein or RNA sequences
  - molecular quasi-species
- For example, an antibody (system) is a collection of amino acid sites (components) with each site containing one of twenty amino acids (states), then the affinity (performance measure) of an antibody for a particular antigen depends on how the chosen amino acids interact with each other.

Applications II

- In Physics and Management Science
  - spin glasses
  - effectiveness of a project team
  - process of organizational change

- For example, a spin glass is defined as a system consisting of contiguous atoms (components). For each atom, it is possible to select a spin up or spin down (states). The total energy (performance measure) depends on how the selected spins interact. The objective is to choose spins so that the energy is minimized.

Mathematical Description

System – A vector with N components, each of which can be in one of p possible states.
$\mathbf{x} = (x_0, ..., x_{N-1})$, with $x_i \in \{0, 1, 2, \ldots, p-1\}$ and the numbers $0, 1, 2, ..., p-1$ used as labels for the states.

Mathematical Description

System – A vector with N components, each of which can be in one of 2 possible states.
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Performance Measure –

$$\Phi(\mathbf{x}) = \frac{1}{N} \sum_{i=0}^{N-1} \phi_i(\mathbf{x})$$

$\phi_i(\mathbf{x})$ is the performance contribution from each component i.

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ϕ_i, the contribution of component i to the overall performance of the system depends on

- its own state, and
- the states of K 'neighboring' components.

Performance Measure

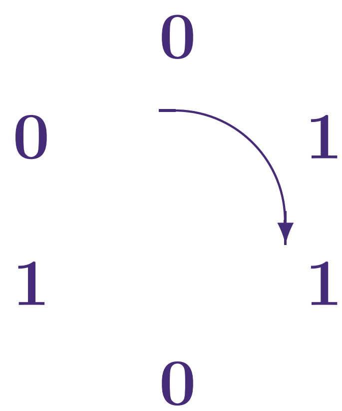
$N = 6$ and $K = 3$

System $(\mathbf{0}\ ,\ \mathbf{1}\ ,\ \mathbf{1}\ ,\ \mathbf{0}\ ,\ \mathbf{1}\ ,\ \mathbf{0})$

Performance Measure

$N = 6$ and $K = 3$

$$\mathbf{0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0}$$



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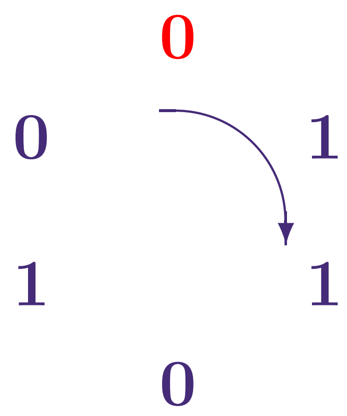

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$$\begin{matrix} & 0 & \\ 0 & & \color{red}{1} \\ 1 & & 1 \\ & 0 & \end{matrix}$$

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Overlap

Question – Given N, K, $0 \leq K \leq N-1$, and $\phi_i : \{0,1\}^{K+1} \rightarrow \mathbb{R}$, $i = 0, 1, \ldots, N-1$

How can we find a system with the best possible performance ?

$$\max\{\Phi(\mathbf{x}) \mid \mathbf{x} \in \{0,1\}^N\}$$

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Central Question

Given N, K, $0 \leq K \leq N-1$, and
$\phi_i : \{0,1\}^{K+1} \to \mathbb{R}$, $i = 0, 1, \ldots, N-1$

What can we say about the Global Optima, the system that maximizes the value of the performance measure?

$$\max\{\Phi(\mathbf{x}) \mid \mathbf{x} \in \{0,1\}^N\}$$

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- NP-complete problem.
- In applications it is difficult, if not impossible, to determine the values taken by ϕ_i.

So, this combinatorial optimization problem is formulated and studied probabilistically.

Probability and Optimization I

Generate values of $\phi_i(.)$ stochastically.
For real-life scenarios in which the functions ϕ_i are not deterministically known, a universally adopted approach is to generate for each $\phi_i(.)$ a random number based on a probability distribution F.

This is analogous to replacing a “weight” in a combinatorial optimization model with a random variable, to better model uncertainty.

This is an idea inherent in Stochastic Programming.

Probability and Optimization II

“Average behavior” – Intractable combinatorial optimization problems are often studied probabilistically by introducing some notion of a random instance.

For example, in stochastic Traveling Salesman Problem (TSP), the distances (“weights”) between the vertices of a graph are replaced by $i.i.d$ uniform random variables. Replace $\phi_i(.)$ with random variables.

This is an idea inherent in Probabilistic Combinatorial Optimization.

Probabilistic Question

Given N, K, with $0 \le K \le N-1$, and $N2^{K+1}$ random variables $\phi_i(\mathbf{y})$ for $\mathbf{y} \in \{0,1\}^{K+1}$, $i = 0, 1, \ldots, N-1$, independently and identically distributed as F.

Study the distribution of the global optima –

$$\boldsymbol{X_{N,K} = \max\{\Phi(\mathbf{x}) \mid \mathbf{x} \in \{0,1\}^N\}}$$

where $\Phi(\mathbf{x}) = \frac{1}{N}\sum_{i=0}^{N-1} \phi_i(x_i, \ldots, x_{i+K})$.

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Previous Research

Research Question– How do the varying values of N and K affect the performance of the systems?

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- Mostly study of local optima w.r.t. a Hamming distance based neighborhood structure.
- Mostly simulation-based results and applications.
- Solow et. al (2000) showed the global decision problem is NP-complete.

Previous Research

- Evans and Steinsaltz (2002)
  - convert to an infinite-dimensional variational problem
  - explicit bounds only when $K=1$ and F is exponential distribution
- Durrett and Limic (2003)
  - use the theory of substochastic Harris chains
  - explicit bounds only when $K=1$ and F is negative exponential distribution
- Numerous other papers (both Applications and Theory).

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Study $X_{N,K} = \max\{\Phi(\mathbf{x}) \mid \mathbf{x} \in \{0,1\}^N\}$

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- Find explicit bounds on the expectation of $X_{N,K}$ when K is function of N, for fundamental underlying distributions like uniform and normal.

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We use tools from Combinatorics and Graph Theory, Networks, Probability and Statistics, and Geometry.

NK model as a Stochastic Network

Network $\boldsymbol{D_{N,K}}$ $2^{K+1} \times (N+1)$ array of vertices,

$v^i_{\mathbf{t}}$, $\mathbf{t} \in \{0,1\}^{K+1}$, $0 \leq i \leq N$

each vertex, $v^i_{\mathbf{t}}$, corresponds to component i and $\mathbf{t}$, the state vector for the component and its K neighbors.

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$$v^i_{\mathbf{t}} \to v^j_{\hat{\mathbf{t}}} \quad \Leftrightarrow \quad j = i+1 \text{ and } \hat{t}_i = t_{i+1},\ i = 1, \ldots, K$$

$$\text{and } \hat{t}_{K+1} \in \{0,1\}$$

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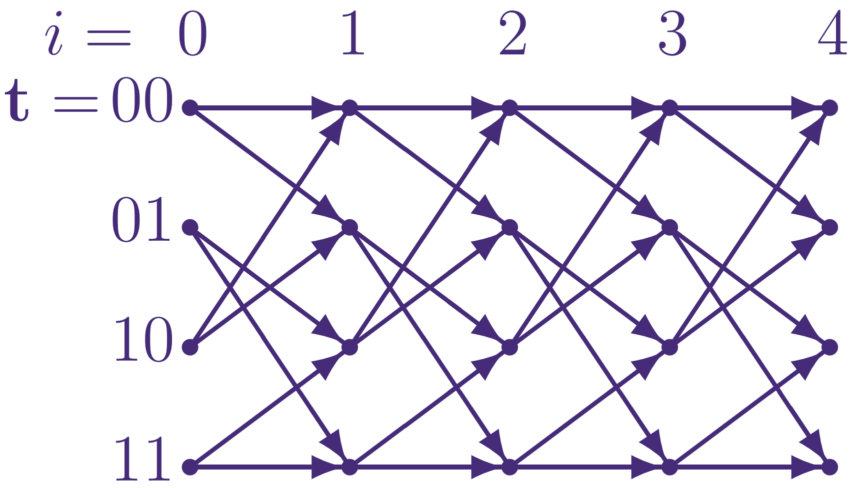
Each $v^i_{\mathbf{t}}$ has a weight generated by the performance contribution (and random variable) $\phi_i(\mathbf{t})$.

Network $D_{N,K}$

$\mathbf{N} = \mathbf{4}$ and $\mathbf{K} = \mathbf{1}$



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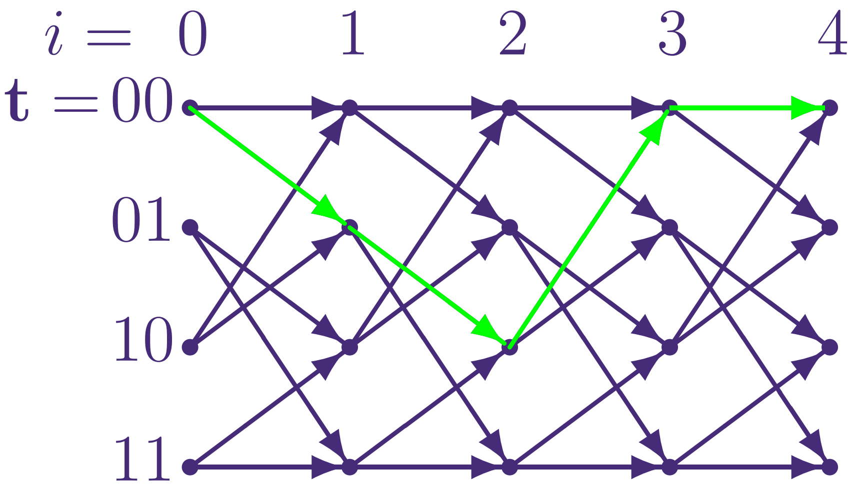

Green path corresponds to the system $\{0, 0, 1, 0\}$ and the weight of the path is the performance measure of this system.

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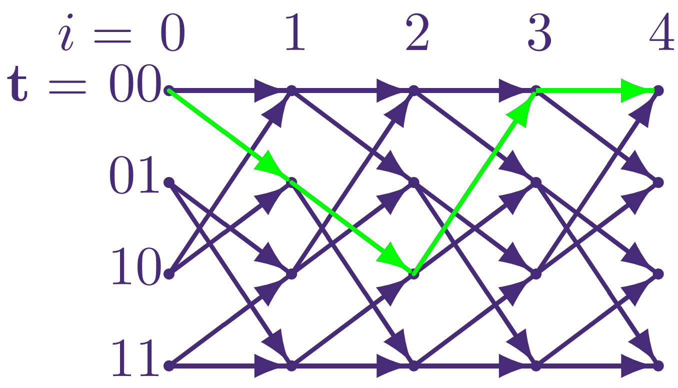

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Each directed path from from $v_{\mathbf{t}}^{0}$ to $v_{\mathbf{t}}^{N}$

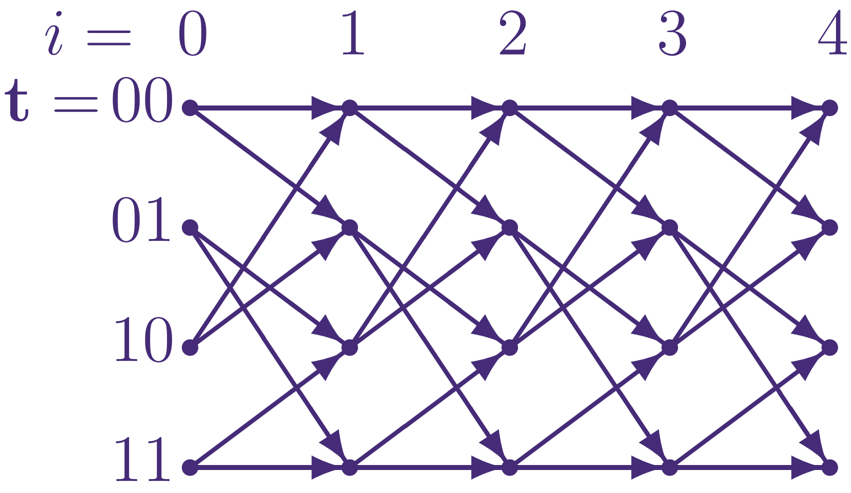
and its associated weight

$\updownarrow$

Each system and its performance

SubNetwork $D^{\mathbf{t}}_{N,K}$

$D^{\mathbf{t}}_{N,K} \equiv$ subnetwork of $D_{N,K}$ defined by all the directed paths between $v^0_{\mathbf{t}}$ and $v^N_{\mathbf{t}}$



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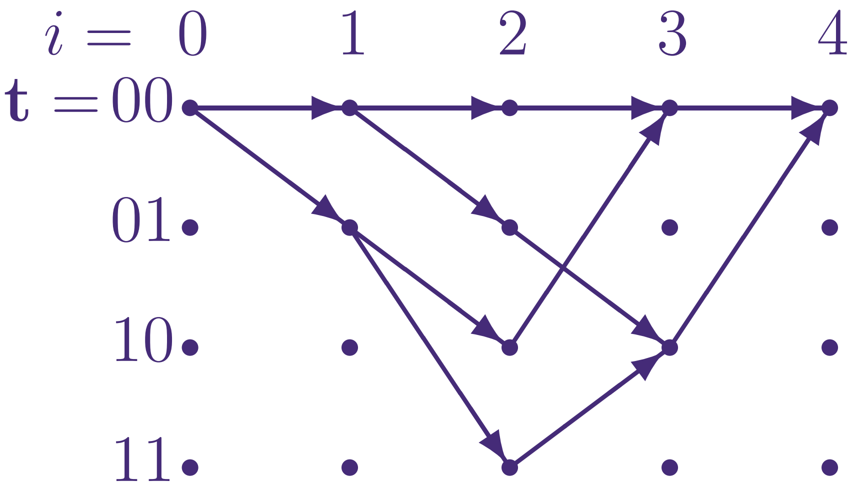

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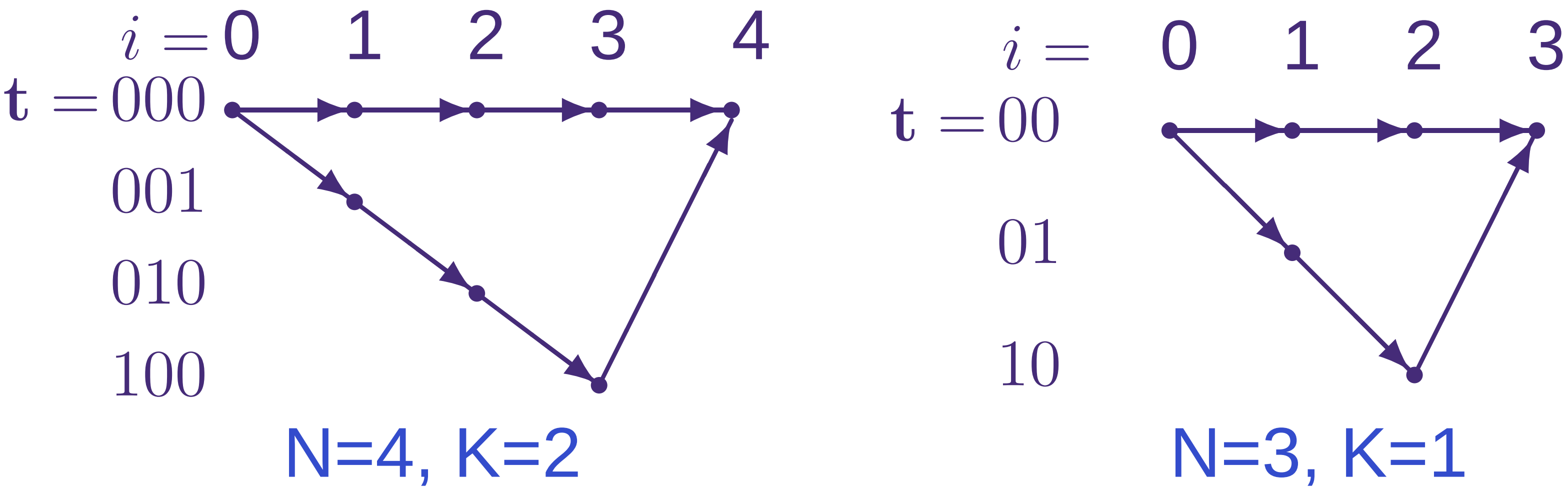
$$X_{N,K} = \frac{1}{N}\max\{2^{N}\ \textit{identically distributed}\ \ \Phi(\mathbf{x})\ \}$$

– Order Statistics

– Project Duration in PERT networks

Computational Strategy for K close to N

Observation – The value of $N-K$ determines the general structure of subnetwork $D^{\mathbf{t}}_{N,K}$, while N determines its size.



Subnetwork $D^{\mathbf{0}}_{N,K}$ for $N-K=2$

Computational Strategy for K close to N

This leads to –

For each K, $1 \le K \le N-3$,

$$l_{N,K} \quad = \quad X + \max\{two\ identically\ distributed\ l_{N-1,K}\}\ ,$$

where the boundary conditions are

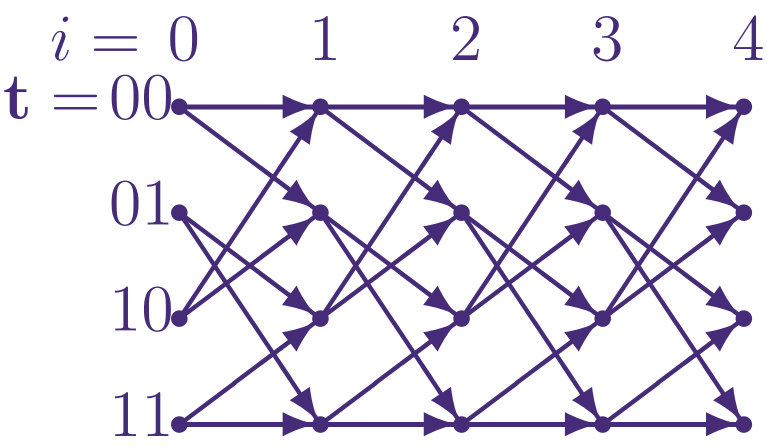
$$l_{K+2,K} \quad = \quad X + \max\{two\ \ i.i.d.\ \ l_{K+1,K}\}\ , \qquad X \sim F$$

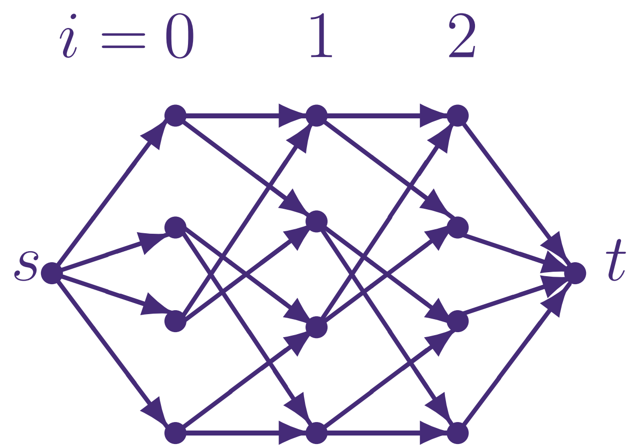
$$l_{K+1,K} \quad = \quad \sum_{i=1}^{N} X_i\ , \qquad \{X_i\}\ i.i.d.\ F$$

Each recursive step reduces the value of N and brings it closer to the (fixed) value of K, until $N = K + 1$.

$D'_{N,K}$ – Computational Strategy for small K

$D'_{N,K} \equiv$ Network formed from $D_{N,K}$ by deleting the vertices in the $K+1$ columns from $N-K$ to N and adding a source and a sink





$N=4\ ,\ K=1$ $D_{N,K}$ $D'_{N,K}$

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$$X_{N,K} \geq \frac{1}{N}\left[l'_{N,K} + \sum_{i=N-K}^{N-1} X_i\right], \quad X_i \; i.i.d. \; F$$

$l'_{N,K} \equiv$ maximum weight of a directed path in $D'_{N,K}$

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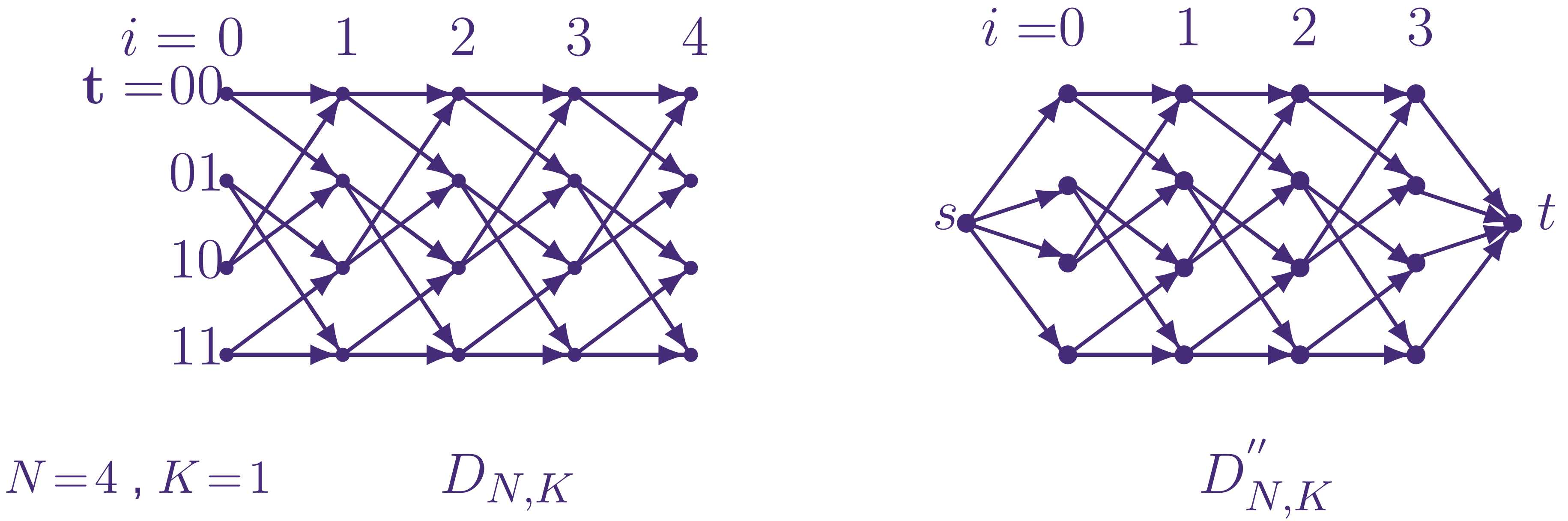

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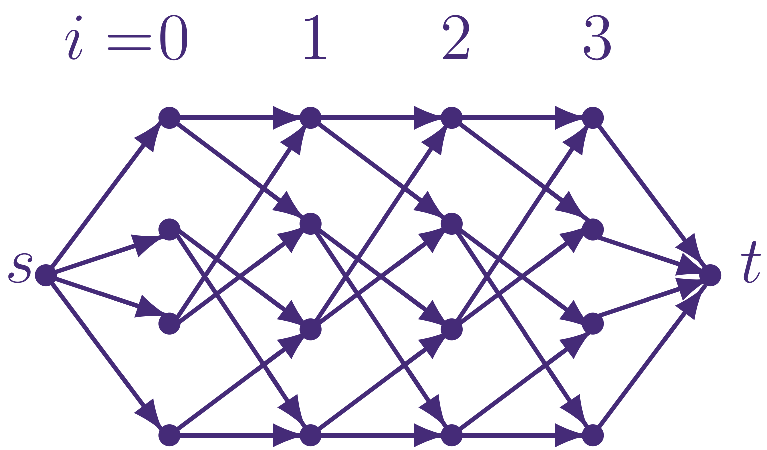
$$X_{N,K} \leq \frac{1}{N} \left[l''_{N,K} \right]$$

$l''_{N,K} \equiv$ maximum weight of a directed path in $D''_{N,K}$

$D'_{N,K}$ and $D''_{N,K}$



$N = 4$, $K = 1$ $D''_{N,K}$ $D'_{N,K}$

$D'_{N,K}$ has $N - K$ columns and $D''_{N,K}$ has N columns.

For fixed K, the bounds in terms of $l'_{N,K}$ and $l''_{N,K}$ will be asymptotically tight.

Dependency Graph

$$X_{N,K} = \frac{1}{N}\max\{2^N \textit{ identically distributed } \Phi(\mathbf{x})\}$$

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Dependence between $\Phi(\mathbf{x})$ and $\Phi(\mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \{0,1\}^N$

$$\Phi(\mathbf{x}) = \frac{1}{N}\sum_{i=0}^{N-1} \phi_i(x_i, \ldots, x_{i+K})$$

$$\Phi(\mathbf{y}) = \frac{1}{N}\sum_{i=0}^{N-1} \phi_i(y_i, \ldots, y_{i+K})$$

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$G_{N,K} \equiv$ dependency graph for given N, K

vertices $\equiv$ $\mathbf{x} \in \{0,1\}^N$

$\mathbf{x} \leftrightarrow \mathbf{y} \Leftrightarrow \Phi(\mathbf{x})$ and $\Phi(\mathbf{y})$ are dependent

Dependency Graph, contd.

- $G_{N,K}$ has 2^N vertices, one for each system.
- An edge between two vertices means there is dependence between the performance measures of the corresponding systems.

Dependency Graph, contd.

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- Want to partition the vertex set of $G_{N,K}$,
  $V(G_{N,K}) = V_1 \sqcup V_2 \sqcup \ldots \sqcup V_t$, such that

  - there are no edges within each class V_i

  - sizes of any two classes differ by at most 1

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t-equitable coloring of $G_{N,K}$

Theorem : $\Delta(G_{N,K}) \leq N2^{N-K-2}$ for all K, with equality for $\frac{N}{2} \leq K \leq N-2$.

$\Delta(G) \equiv$ maximum degree, the most number of vertices that are adjacent to a vertex in G

Dependency Graph, contd.

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How is this useful?

Bounds on Order Statistics

Notation : $Y_{[n]} = \max\{Y_1, \ldots, Y_n\}$

$F_N \equiv$ distribution of $\sum_{i=1}^{N} X_i$, for $X_i \; i.i.d. \; F$

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$$\begin{aligned}
\mathbf{X_{N,K}} &= \frac{1}{N}\max\{2^N \textit{ identically distributed } \Phi(\mathbf{x})\,\} \\
&= \frac{1}{N}\max\{2^N \textit{ identically distributed } \sum_{i=1}^{N}\phi_i\,\}\,,\ \{\phi_i\}\ i.\ i.\ d.\ F \\
&= \frac{1}{N}\max\{2^N \textit{ identically distributed } \Phi(\mathbf{x})\,\}\,,\ \Phi(\mathbf{x}) \sim F_N \\
&= \frac{1}{N}\,Y_{[2^N]}\,,\ Y_i \sim F_N\ ;\{Y_i\,|\,i=1,\ldots,2^N\} = \{\Phi(\mathbf{x})\,|\,x \in \{0,1\}^N\}
\end{aligned}$$

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Theorem : For all N, K, with underlying distribution F, if $G_{N,K}$ has t-equitable coloring then

$$\mathbf{E}[Y_{[2^N/t]}] \leq \mathbf{E}[X_{N,K}] \leq \mathbf{E}[Y_{[2^N/t]}] + \sqrt{t \ \mathbf{Var}[Y_{[2^N/t]}]}$$

where $Y_1, \ldots, Y_k$ i.i.d. F_N.

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where $Y_1, \ldots, Y_k$ **i.i.d.** F_N.

$Proofs$ use tools from Order Statistics and the Equitable Coloring of Graphs.

Order Statistics with Dependencies

A *dependency graph* for random variables $X_1, \ldots, X_n$, $G(X_1, \ldots, X_n)$, has vertex set $[n]$ and an edge set such that for each $i \in [n]$, X_i is mutually independent of all other X_j such that $\{i, j\}$ is not an edge.

$$Y_{[n]} = \max\{Y_1, \ldots, Y_n\}$$

Theorem : Let $X_1, \ldots, X_n$ be identically distributed random variables with distribution F. If $G(X_1, \ldots, X_n)$ has a t-equitable coloring, then

$$\mathbf{E}[Y_{[n/t]}] \leq \mathbf{E}[X_{[n]}] \leq \mathbf{E}[Y_{[n/t]}] + \sqrt{(t-1)\,\mathbf{Var}[Y_{[n/t]}]}$$

where $Y_1, \ldots, Y_k$ $i.i.d.$ F .

Order Statistics with Dependencies

Theorem : Let $X_1, \ldots, X_n$ be identically distributed (dependent) random variables with distribution F. If $G(X_1, \ldots, X_n)$ has a t-equitable coloring, then

$$\mathbf{E}[Y_{[n/t]}] \leq \mathbf{E}[X_{[n]}] \leq \mathbf{E}[Y_{[n/t]}] + \sqrt{(t-1)\,\mathbf{Var}[Y_{[n/t]}]}$$

where $Y_1, \ldots, Y_k$ ***i.i.d.*** F .

Convert the problem of bounding order statistics of dependent random variables into that of independent random variables while incorporating quantitative information about the mutual dependencies between the original random variables

Bounds when $F = \mathbf{n}(0,1)$

Theorem :For all $N \geq 2$, $K = N - 1$,

$$\sqrt{2\log 2} - \frac{o(1)}{\sqrt{N}} \;\leq\; \mathbf{E}[X_{N,K}] \;\leq\; \sqrt{(1+\frac{1}{N})2\log 2} - \frac{o(1)}{\sqrt{N}}$$

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Theorem :For all $N \geq 2$, $K = N - \alpha$, $\alpha \in \mathbb{Z}^+$, $\alpha \geq 2$, $c = \alpha - 2$

$$\sqrt{(1-\frac{c}{N})2\log 2 - \frac{2\log N}{N}} - \frac{o(1)}{\sqrt{N}} \leq \mathbf{E}[X_{N,K}] \leq \sqrt{(1+\frac{1}{N})2\log 2} - \frac{o(1)}{\sqrt{N}}$$

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Theorem : For all $N \geq 2$, $K = \beta N$, $\beta \in (0,1)$

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Tight bounds on $\mathbf{E}[X_{N,K}]$ valid for all N and for K close to N

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Leading Coefficients in both upper and lower bounds are equal to $\sqrt{2\log 2}$

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$Proofs$ use the previous Theorems and the properties of Normal Distribution & its order statistics

Bounds when $F = \mathbf{u}(0, 1)$

- "Sum of Normals is Normal"!
- Sum of Uniforms does not have a nice distribution.

Need to find an alternate description of the Distribution of sum of Uniforms !

Bounds when $F = \mathbf{U}(0,1)$

When $\{X_j\}$ $i.i.d.$ $\mathbf{U}(0,1)$,

$\mathbf{Pr}\left\{\sum_{j=1}^{N} X_j \le x\right\}$ is equal to the volume of

$$P(x) = \left\{\mathbf{y} \in \mathbb{R}^N \mid \sum_{j=1}^{N} y_j \le x \text{ and } 0 \le y_j \le 1\right\}$$

a subset of the N-dimensional hypercube $[0,1]^N$.

Bounds when $F = \mathbf{u}(0, 1)$

We prove lemmas about $Vol(P(x))$ that help to decompose the expectation integral.

Bounds when $F = \mathbf{u}(0,1)$

We prove lemmas about $Vol(P(x))$ that help to decompose the expectation integral.

For Example,
a lower bound on x that forces the volume of $P(x)$ to approach 1, the volume of the $[0,1]^N$ cube, very rapidly.

Lemma :

If $\boldsymbol{x > (1 - \frac{1}{2e})N}$, then $\boldsymbol{Vol(P(x)) \geq 1 - \frac{1}{\sqrt{2\pi N}\, 2^N}}$
for all $N \geq 2$.

Bounds when $F = \mathbf{u}(0,1)$

We prove lemmas about $Vol(P(x))$ that help to decompose the expectation integral.

For Example,
if the volume outside $P(x)$ is asymptotically small then x must be sufficiently large.

Lemma :
If $\boldsymbol{Vol(P(x)) > 1 - \frac{N}{2^N}}$, then $\boldsymbol{x > \left(1 - \frac{1}{4}(2N)^{1/N}\right)N}$ for all $N \geq 2$.

Bounds when $F = \mathbf{u}(0,1)$

Theorem : For all $N \geq 2$, $K = N-1$,

$$\left(1-\tfrac{1}{4}(2N)^{1/N}\right)\left(1-\left(1-\tfrac{N}{2^N}\right)^{2^N}\right) \leq \mathbf{E}[X_{N,K}] \leq 1-\frac{1}{2e}\left(1-\frac{1}{\sqrt{2\pi N}\,2^N}\right)^{2^N}$$

$$\lim_{N\to\infty} \mathbf{Var}[X_{N,K}] \leq \frac{7}{16}-\frac{1}{e}\left(1-\frac{1}{2e}\right) \approx 0.1373$$

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Theorem : For all $N \geq 2$, $K = N - 1$,

$$\left(1 - \tfrac{1}{4}(2N)^{1/N}\right)\left(1 - \left(1 - \tfrac{N}{2^N}\right)^{2^N}\right) \leq \mathbf{E}[X_{N,K}] \leq 1 - \tfrac{1}{2e}\left(1 - \frac{1}{\sqrt{2\pi N}\,2^N}\right)^{2^N}$$

$$\lim_{N\to\infty} \mathbf{Var}[X_{N,K}] \leq \tfrac{7}{16} - \tfrac{1}{e}\left(1 - \tfrac{1}{2e}\right) \approx 0.1373$$

Theorem : For all $N \geq 2$, $K = N - \alpha$, $\alpha \in \mathbb{Z}^+$, $\alpha \geq 2$, $c = \alpha - 2$

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Tight bounds on $\mathbf{E}[X_{N,K}]$ valid for all N and for K close to N

Bounds when $F = \mathbf{U}(0,1)$

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Leading Coefficients : $1-\frac{1}{4} = 0.75$ and $1-\frac{1}{2e} \approx 0.816$

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$Proofs$ use the previous Theorems and the geometric lemmas .

Concentration of $X_{N,K}$ around $\mathbf{E}[X_{N,K}]$

Probability of $X_{N,K}$ being far from $\mathbf{E}[X_{N,K}]$ is exponentially decaying.

Theorem : If F is a bounded distribution such that $X \sim F \Rightarrow |X| \leq c$, then

$$\mathbf{P}[\,|\,X_{N,K} - \mathbf{E}[X_{N,K}]\,|\geq t\,] \leq 2\exp\left(-\frac{2Nt^2}{c^2 2^{2N-K-1}}\right)$$

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Proof using Independent Bounded Differences Inequality, a variant of Azuma's Martingale inequality.

The Kauffman NK Model

- Background and Applications
- Mathematical Description
- NK Model as a Stochastic Network
- Computational Strategies using Stochastic Networks
- Dependency Graph and Bounds on Order Statistics
- Analysis for underlying Normal Distribution
- Analysis for underlying Uniform Distribution
- Concentration of Measure

Thank You !