Stochastic Models in Quantum Systems

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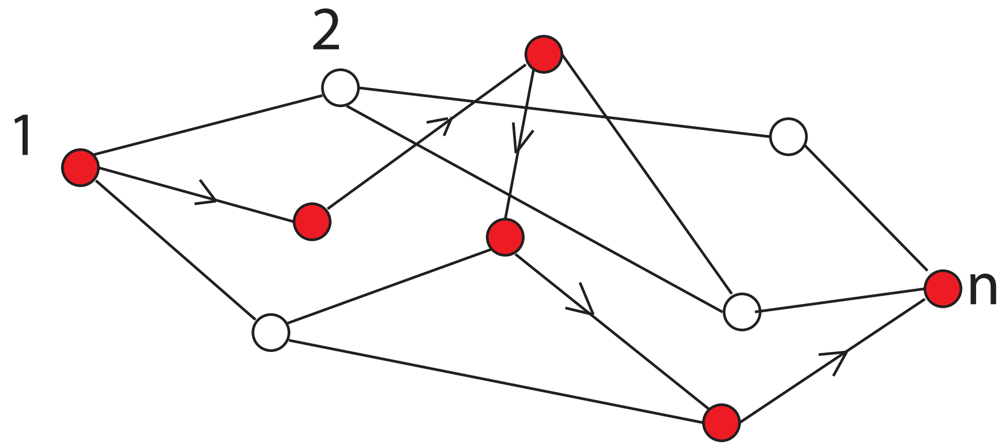
This is NOT an experimental talk and I recognize that I will be asking some of you to think about old things in a new way!

The purpose of this talk is to describe a way of calculating the best way of increasing the probability of transferring the state of a Markov process to a desired end state. The details of what this means will be given below but for now, here is some further motivation.

Suppose one has a system with states r,s,t and that with no external influence the system will jump from one of these to another with a certain transition rate a(r,s), a(s,t), etc. Suppose further that it is possible to provide control (e.g., an electromagnetic pulse) that alters these rates: a(r,s) goes to a(r,s) +u b(r,s), etc. Suppose further that there is a performance criterion that rewards the the system, depending only on the final state. How do we select the the control in such a way as to maximizes the the expected value of the performance? Many of talks at this conference have this flavor.

Finding the path with the greatest yield: Each link represents possible population transfer. It is traversed with some probability. The nodes have populations.

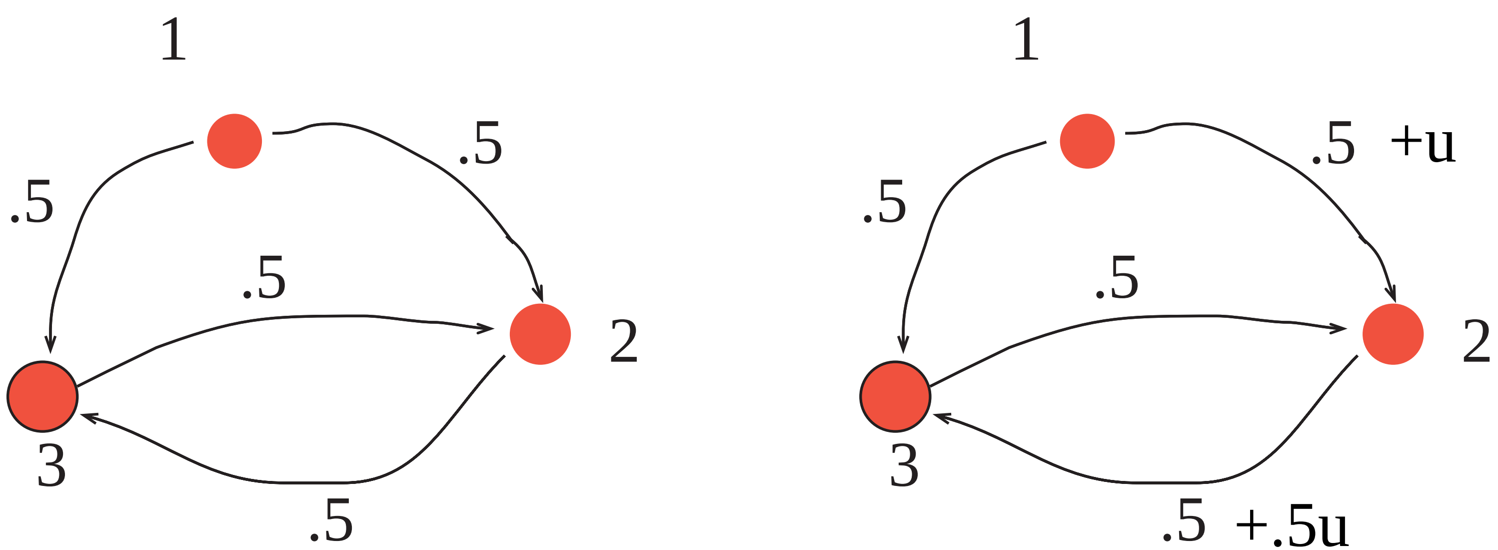


$$\begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \cdots \\ \dot{p}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \cdots \\ p_n \end{bmatrix}$$

Here $a_{ij} = a_{ij}(u_1, u_2, ..u_k)$

If you stick with me I will describe:

1. A particular, but completely general, sample path description for continuous time Markov chains with some controllable transition rates. Think control of atomic states. (But it also service systems, buffer management, routing, …)
2. The corresponding evolution of the probability law.
3. A differential equation for the minimum return function.
4. Some solved examples to show how it works. (These will not directly involve attosecond pulses, however.)



Related to examples with a suitable pedigree in physics!

The quantum theory of radiation involves spontaneous emission (think A) and stimulated emission (think $\rho(\omega)B$).

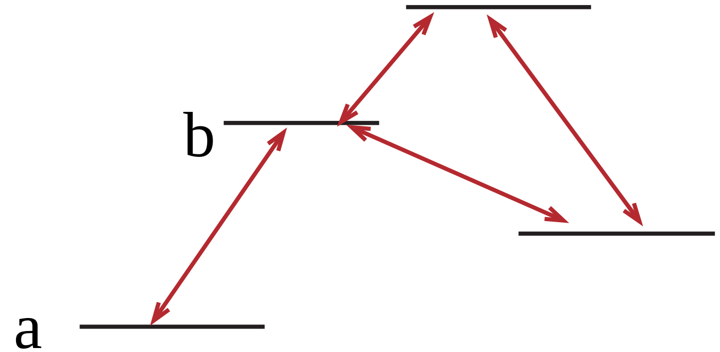
$$\begin{bmatrix} \dot{p}_a \\ \dot{p}_b \end{bmatrix} = \begin{bmatrix} -A-\rho B & \rho B \\ A+\rho B & -\rho B \end{bmatrix} \begin{bmatrix} p_a \\ p_b \end{bmatrix}$$

Reconsider

$$\dot{z} = u(t)e^{-At}Be^{At}z$$

now with u coming from a frequency dependent radiation field. Observe that what ever $\sin \omega t$ does $\sin(\omega t + \pi/\omega)$ undoes. This is stimulated emission.

Think: Bohr orbits associated with the hydrogen atom and their various energy levels.



If it was good enough for Einstein and Bohr it can’t be all bad!

A Motivational Example

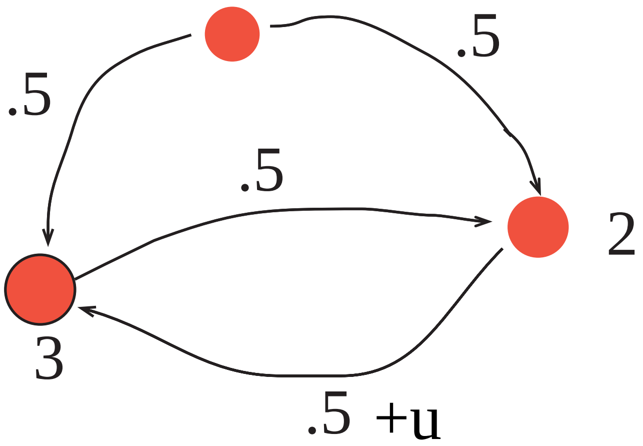
Consider the three state system with $z \in \{1, 0, -1\}$ the transition probability description is

$$\begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \dot{p}_3 \end{bmatrix} = \begin{bmatrix} -a-u & a/2 & 0 \\ a+u & -a & v \\ 0 & a/2 & -a-v \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

Minimize

$$\mathcal{E} \int z^2 + u^2 + v^2 dt$$

Path term plus final state term



The general model involves a controllable evolution equation for the various populations:

$$\dot{p}(t) = A(u(t))p(t)$$

A definition of the performance measure

$$\eta = \int_0^T c^T p + \phi(u)\, dt + \psi(x(T))$$

and a constraint describing the possible values of the control actions.

$$u(t) \in \mathcal{U}$$

Caveat: The constraint on u must be expressed in terms of the values it takes on–not e.g.,bandwidth.

Typical of the answers we get

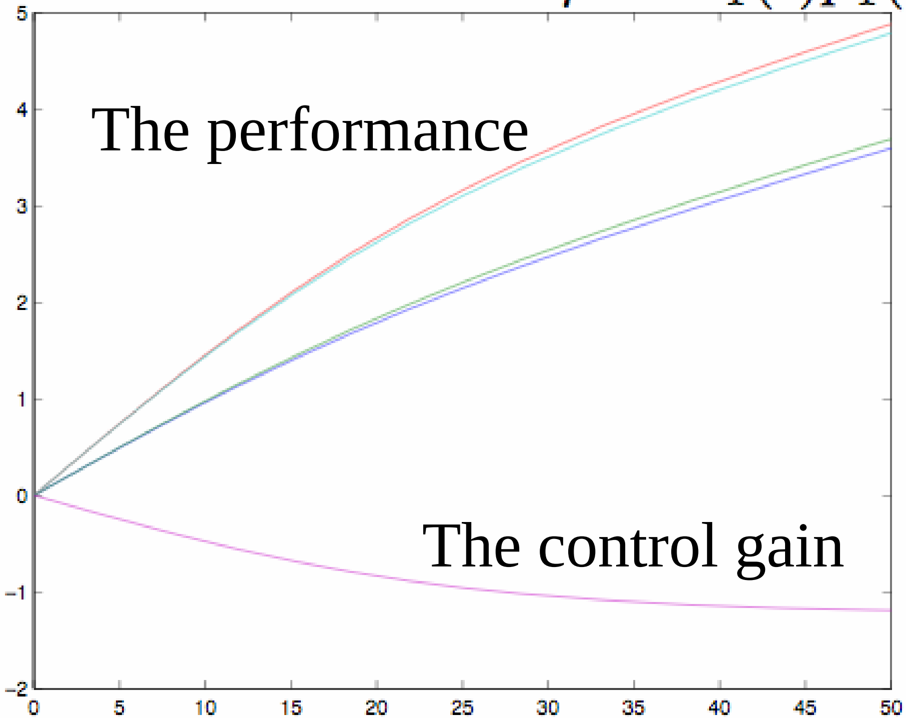
$$u^*(t) = (k_2 - k_3)x_2$$

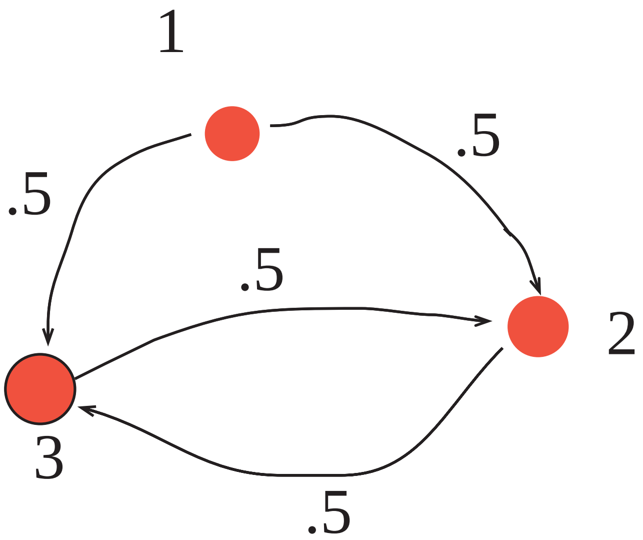
$$\dot{k}_1 = -k_1 + .5k_2 + .5k_3 + 1$$

$$\dot{k}_2 = .5k_1 - .5k_2 - .25(k_2 - k_3)^2$$

$$\dot{k}_3 = .5(k_2 - .k_3)$$

$$\eta^* = k_1(t)p_1(0) + k_2(t)p_2(0) + k_3(t)(t)p_3(0)$$





Accumulated cost vs. time and the feedback control gain vs. time (lower curve).

The next four slides are background to describe a particular kind of stochastic differential appropriate for finite state Markov processes. This also plays a role in defining the difference between closed loop and open loop control in the present context.

Basic Solution Concept

Let N be a Poisson counter of rate $\lambda(t)$. That is $N(t)$ is a stochastic process, $N(0) = 0$, monotone increasing, taking on values in the nonnegative integers such that the time between jumps is exponential with

$$\mathcal{E}N(t) = N(\tau) + \int_{\tau}^{t} \lambda(\sigma)d\sigma$$

We interpret differential equations of the form

$$dx+ = f(x)dt + \sum g_i(x)dN_i$$

as Itô equations. If $f = 0$ it can happen that x takes on values in a finite set.

Differentiation rule:

$$d\psi(x) = \langle \frac{\partial \psi}{\partial x}, f(x) \rangle dt + \sum \left(\psi(x + g_i(x)) - \psi(x)\right) dN_i$$

For example, for $dx = -xtd + dN$

$$dx^2 = -2x^2 dt + ((x+1)^2 - x^2) dN$$

Expectation rule: If $\mathcal{E}N_i(t) = \lambda_i t$ then

$$\frac{d}{dt}\mathcal{E}x = \mathcal{E}f(x) + \sum \mathcal{E}g_i(x)\lambda_i$$

For the example

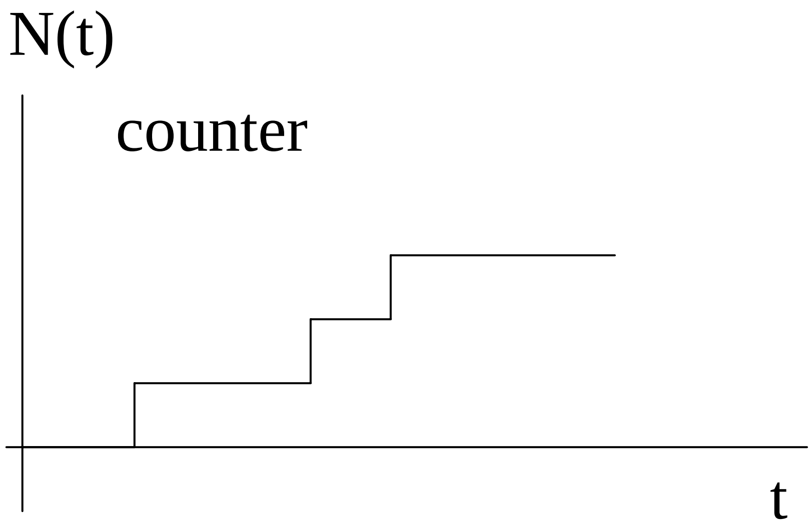
$$\frac{d}{dt}\mathcal{E}x = -\mathcal{E}x + \lambda$$

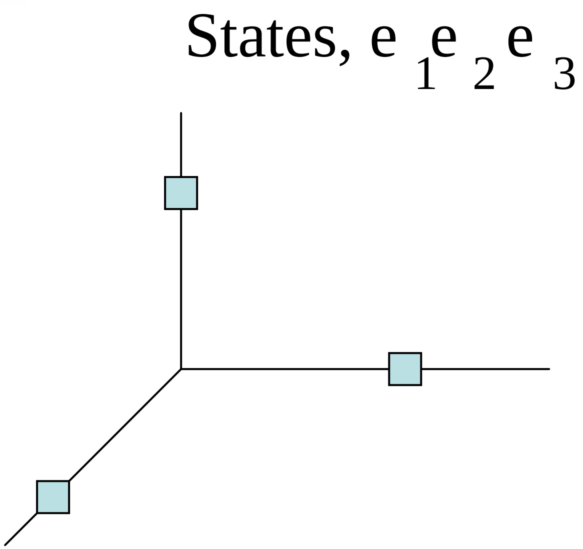
$$\frac{d}{dt}\mathcal{E}x^2 = -2\mathcal{E}x^2 + (2\mathcal{E}x + 1)\lambda$$

Setting up the special case used here

Based on a sample path representation of Markov process in terms of Poisson counters with states, 0,1,2,…

$$\mathcal{E}N(t) = \int_0^t \lambda(\sigma)d\sigma$$





The State Space and the Ito Rule

Let $x(t) \in \{e_1, e_2, ..., e_n\}$ where

This set called X below

$$e_i = \begin{bmatrix} 0 \\ ... \\ 1 \\ 0 \\ ... \end{bmatrix}$$

let G_j be such that for the equation

$$dx = \sum G_i x dN_i$$

x evolves in $\{e_1, e_2, ..., e_n\}$. Recall that with the Ito calculus the solution of a Poisson counter driven equation is defined such that x is continuous from the left and the jump is calculated as if x were frozen until after the jump.

We consider finite state Markov process with states $e_1, e_2, ..., e_n$. The evolution is via

$$dx = \sum G_i x dN_i$$

It must be that G_i has a special form such as that suggested by

$$G_i = \begin{bmatrix} 0 & 0 & 0 & ... & 0 \\ 0 & -1 & 0 & ... & 1 \\ 0 & 0 & 0 & ... & 0 \\ 0 & 0 & 0 & ... & 0 \\ 0 & 1 & 0 & ... & -1 \end{bmatrix}$$

Let N be a Poisson counter of rate $\lambda(t)$. That is $N(t)$ is a stochastic process, $N(0) = 0$, monotone increasing, taking on values in the nonnegative integers such that the time between jumps is exponential with

$$\mathcal{E}N(t) = N(\tau) + \int_{\tau}^{t} \lambda(\sigma)d\sigma$$

We interpret differential equations of the form

$$dx + \sum_{j=1}^{m} G_j x dN_j$$

as Itô equations and so they define equations in X. Note also that

$$p = \mathcal{E}x(t)$$

The rates of some of the counters are under our control as in

$$\lambda_i = \hat{\lambda}_i + u_i \lambda_i$$

The affine dependence of the rates on u is an assumption but not as restrictive as you might think.

In this way

$$\sum G_i \lambda_i = A + \sum_{i=1}^{m} u_i B_i$$

Leads to

$$\dot{p} = \left(A + \sum u_i B_i \right) p$$

The Evolution of the Minimum Return Function $\mathcal{E}k^T x(0)$

$$\frac{d}{dt}\mathcal{E}k^T x = \mathcal{E}\dot{k}^T x + k^T \sum G_j x \frac{dN_j}{dt} + c^T x + u^T u$$

Recall $x(t) \in \{e_1, e_2, ..., e_n\}$ so

$$(u + f^T x)^T (u + f^T x) = u^T u + 2u^T f^T x + (f^T x)^2 =$$

$$u^T u + 2u^T x + \langle \sum f_1^2, x_i \rangle = u^T u + 2u^T f^T x + f^{\cdot 2} x$$

where we use the notation

$$f^{\cdot 2} = \begin{bmatrix} f_i^2 \\ f_2^2 \\ \cdots \\ f_n^2 \end{bmatrix}$$

Linear and quadratic functions of x are interchangeable on X!

Now bring in the $\dot{k}^T x + \sum k^T B_i x$ terms and write

$$\mathcal{E} k^T(t) x \Big|_0^T = \int ||u + \frac{1}{2} k^T B^T x||^2 dt$$

provided that

$$\dot{k} = -A^T k - c + \frac{1}{4}(B^T k)^{\cdot 2}$$

This uses the special choice of state representation to express the linear term as a quadratic and also the choice of $\dot{k}$ to complete the square.

Returning to the more general situation,

$$dx = \sum G_i x dN_i$$

Then

$$dk^T x = \dot{k}^T x dt + \sum k^T G_i x dN_i$$

So

$$k^T x\Big|_0^T = \int_0^T \dot{k}^T x dt + \sum k^T G_i x dN_i$$

Use this to write

$$\eta = -\mathcal{E} k^T(t) x(t)\Big|_0^T + \int_0^T \left(c^T x + u^2 + \dot{k}^T x\right) dt + \int \sum k^T G_i x dN_i$$

Theorem 1: Let G_i, and N_i be as described with the rates of the N_i being $\lambda_{i0} + \sum \mu_{ij} u_j$. The λ_{i0} and μ_{ij} may be time varying but are assumed to be bounded. Assume that x satisfies the Itô equation

$$dx = \sum_{i=1}^{m} G_i x dN_i \;\; ; \;\; , x(t) \in \{e_1, e_2, ..., e_n\}$$

Define A and B_i as

$$A = \sum G_i \lambda_{i0} \;\; ; \; B_i = \sum_{j=1}^{m} \mu_{ij} G_j$$

and let $\mathcal{U}$ be the constraint set defined above.

There exists a unique solution of the equation

$$\dot{k} = -A^T k - c + \min_{u(x)\in\mathcal{U}} \left(\sum_{i=1}^{m} u_i k^T B_i x + \phi(u_i) \right) \; ; \; x(t_f) = \psi_f$$

on the interval $[0, T]$ and the control law

$$u(x) = \arg \min_{u(x)\in\mathcal{A}} \left(\sum_{i=1}^{m} u_i k^T B_i x + \phi(u_i) \right)$$

minimizes

$$\eta = \mathcal{E} \int_0^T c^T(t) x(t) + \phi(u) \, d\sigma + \mathcal{E}\psi(x(T))\rangle$$

If there is no running cost on u then typically the equation for k might take the form

$$\dot{k} = -A^T k - c + \mathrm{sgn}(\mathrm{B}^\mathrm{T}\mathrm{k})_\mathrm{i} \; ; \; \mathrm{x}(\mathrm{t_f}) = \psi_\mathrm{f}$$

If the matrices A and B_i and also the cost c are time invariant, it may be easier to conceptualize this not as

$$\dot{k} = -A^T k - c + \frac{1}{4}\sum (B_i^T k)^{.2} \; ; \; k(T) = 0$$

but rather to let time run backwards and write

$$\dot{k} = A^T k + c - \frac{1}{4}\sum (B_i^T k)^{.2} \; ; \; k(0) = 0$$

This plays the role played by the Riccati equation in other settings but this is typically not a Riccati equation.

There are three kinds of more technical conditions to go further, involving, irreducibility, controllability and non negativiety.

Recall

Optimal Control of a Markov chain whose rates can manipulated

$$\frac{d}{dt}\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} = \left(\begin{bmatrix} -1 & .5 & 0 \\ .5 & -.5 & .5 \\ .5 & 0 & -.5 \end{bmatrix} + u \begin{bmatrix} 0 & 0 & 0 \\ 0 & -.5 & 0 \\ 0 & .5 & 0 \end{bmatrix} \right) \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

$$\eta = \mathcal{E} \int_0^t c^T x + u^2 d\tau$$

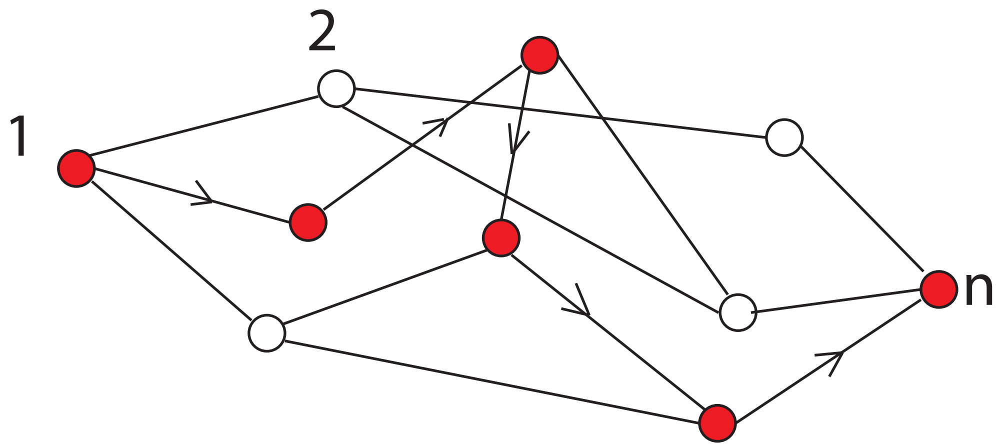
Cost Functional k(t) has a Affine Large t Behavior

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Why might you might care?   Well, the solution of the equation for k provides a rule for selecting the feedback signal that provides the maximal state transfer (possibly with constraints or penalty on the path and/or control). The user does not need to (and, in fact, can not) define the intermediate states; the optimal control does this. In this sense it does the design for you. It would seem to have the most potential for use on systems that have many intermediate states and many possible paths.

Conclusions: I did what I said I would do

Finding the path with the greatest yield: Each link represents possible population transfer. It is traversed with some probability. The nodes have populations.



$$\begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \cdots \\ \dot{p}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \cdots \\ p_n \end{bmatrix}$$

Here $a_{ij} = a_{ij}(u_1, u_2, ..u_k)$