# Part VI

Bayesian Solution of Ordinary Differential Equations

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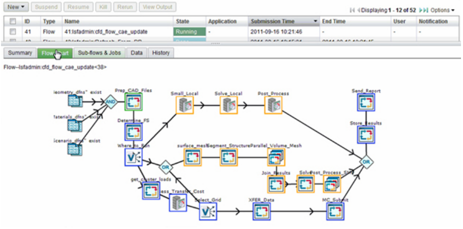
# Twelfth Job: Introduction to Graphical Models

Numerical analysis for the "drag and drop" era of computational pipelines:




[Fig: IBM High Performance Computation]

The sophistication and scale of modern computer models creates an urgent need to better understand the propagation and accumulation of numerical error within arbitrary - often large - pipelines of computation, so that "numerical risk" to end-users can be controlled.

$\Longrightarrow$ Need to consider graphical representations of computation.

# Recall Our Motivation: Computational Pipelines

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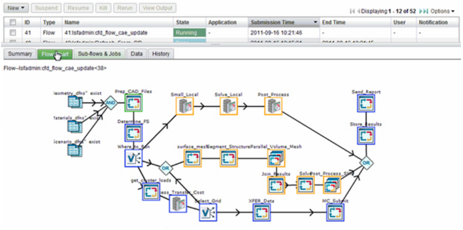


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$\Longrightarrow$ Need to consider graphical representations of computation.

A probabilistic graphical model comprises of:

- A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, with vertex set $\mathcal{V} = \{v_1, \dots, v_p\}$ and edge set $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$.
- Semantics that associate the graph to statements about conditional (in)dependence of random variables $\{X_v\}_{v \in \mathcal{V}}$.

Recall: $X$ is C.I. of $Y$ given $Z \leftrightarrow X \perp\!\!\!\perp Y | Z \leftrightarrow p_{X,Y|Z}(x, y) = p_{X|Z}(x) p_{Y|Z}(y)$

Example: In a Gaussian graphical model:

- The random variables $\{X_v\}_{v \in \mathcal{V}}$ are jointly Gaussian.
- The edges are undirected (i.e. $(i, j) \in \mathcal{E}$ iff $(j, i) \in \mathcal{E}$).
- Two vertices $v_1$ and $v_2$ are **not** connected by an edge iff $X_{v_1} \perp\!\!\!\perp X_{v_2} | X_{\mathcal{V} \setminus \{v_1, v_2\}}$.

Fact: The edge structure of a Gaussian graphical model characterises the sparsity structure of the associated precision matrix.

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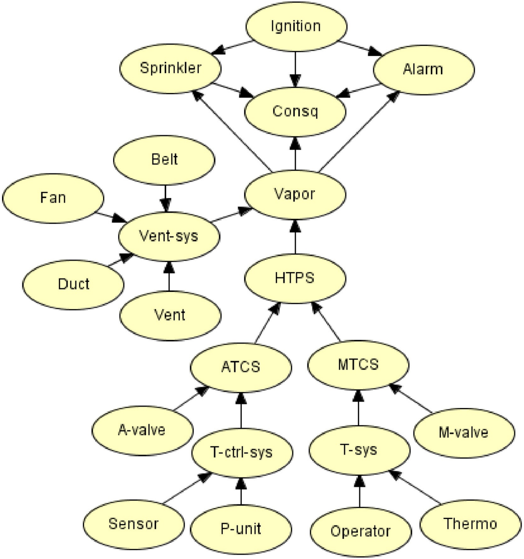
# Exercise: Is Vent-sys d-separated from HTPS?



## Local Markov Property

For a Bayesian network;

$$X_v \perp\!\!\!\perp X_{\mathrm{Nd}(v)\setminus\mathrm{Pa}(v)} | X_{\mathrm{Pa}(v)}$$

where, according to the graph $\mathcal{G}$,

- $\mathrm{Nd}(v)$ are the non-descendants of $v \in \mathcal{V}$
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Message: "Only immediate parents matter".

Practically important, as it allows local verification of the global Markov property.

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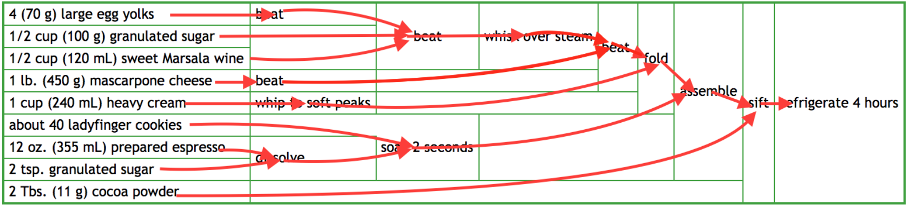
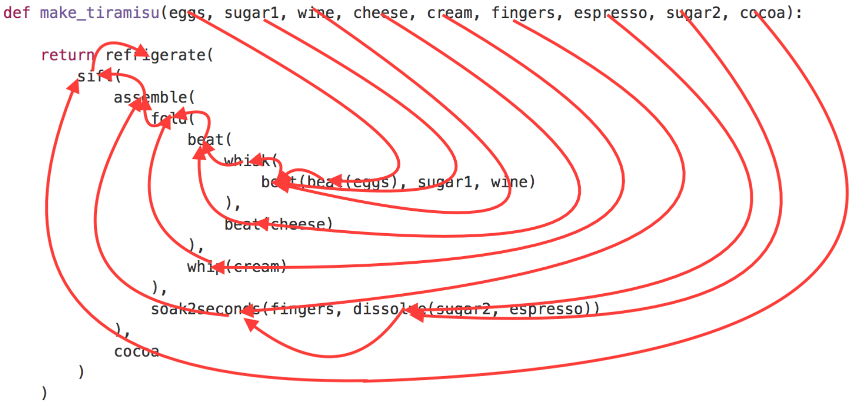
# Computational Work-Flows

Is there a connection to computation?




[Image from Li Haoyi's blog]

In particular, is there a connection to functional programming?

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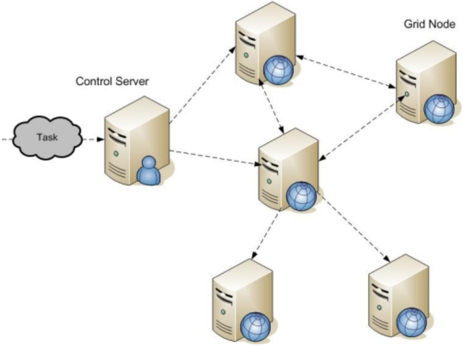
Or a connection to grid or cloud computing?



# Thirteenth Job: Pipelines of Computation

# Example: Split Integration

Consider estimation of the integral

$$\int_0^1 x(t)\mathrm{d}t$$

with a Bayesian probabilistic numerical method (Bayesian quadrature), based on the information $\{x(t_1), \ldots, x(t_{2m})\}$, where $t_1 = 0$, $t_m = 0.5$, $t_{2m} = 1$.

Under what circumstances can this computation be partitioned into two independent sub-computations?

$$\int_0^1 u(x)\mathrm{d}x = \int_0^{0.5} u(x)\mathrm{d}x + \int_{0.5}^1 u(x)\mathrm{d}x$$

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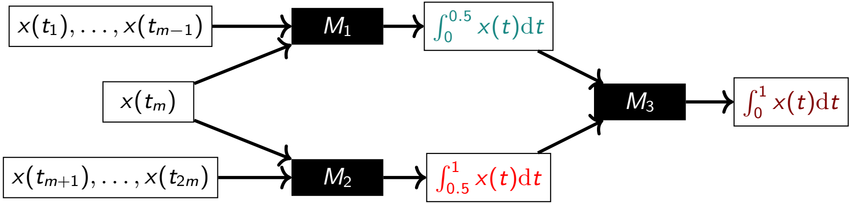


- Nodes are of two kinds: *Information* nodes □, and *method* nodes ■.
- The graph is bipartite, so that edges connect a method node to an information node or vice-versa. That is, edges are of the form □ → ■ or ■ → □.
- There are in general $n$ method nodes, each with a unique label in $\{1, \ldots, n\}$.
- The method node labelled $i$ has $m(i)$ parents and one child. Its in-edges are assigned a unique label in $\{1, \ldots, m(i)\}$.
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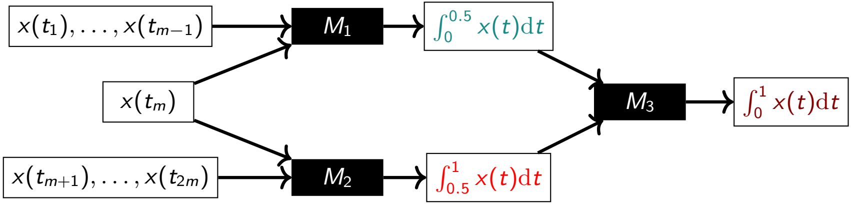


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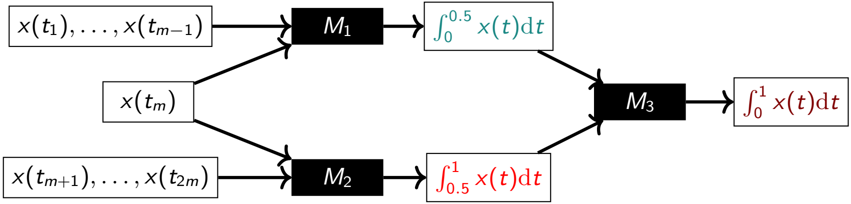


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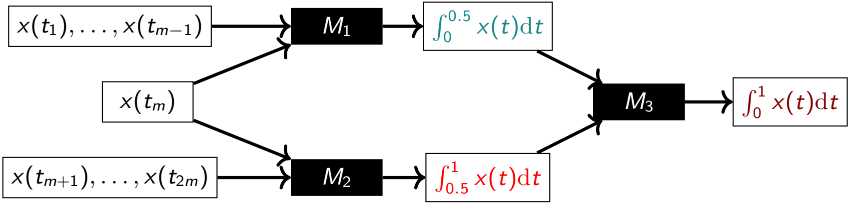


- Nodes are of two kinds: *Information* nodes $\square$, and *method* nodes $\blacksquare$.
- The graph is bipartite, so that edges connect a method node to an information node or vice-versa. That is, edges are of the form $\square \to \blacksquare$ or $\blacksquare \to \square$.
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- The method node labelled $i$ has $m(i)$ parents and one child. Its in-edges are assigned a unique label in $\{1, \ldots, m(i)\}$.
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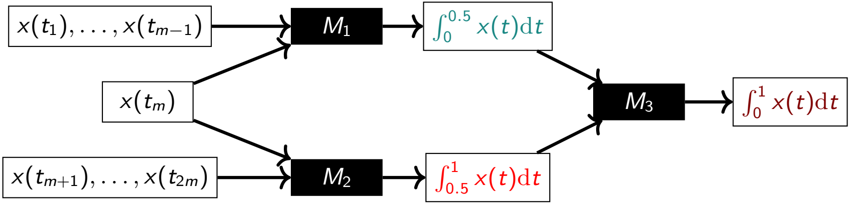


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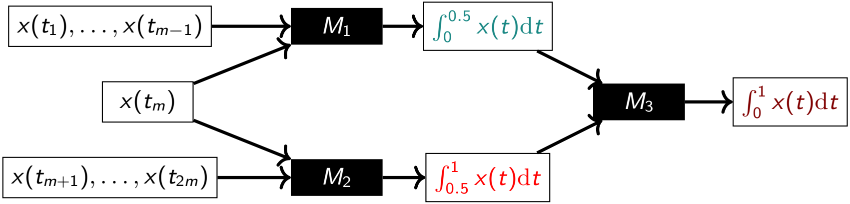


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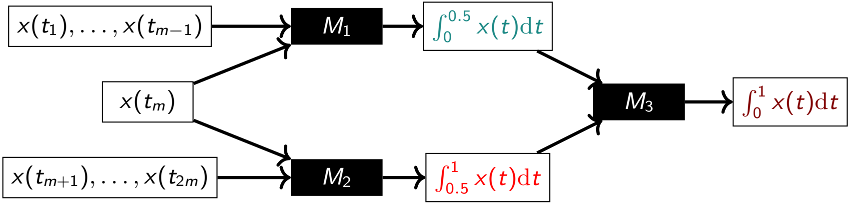


Let

- $M_1$ be Bayesian quadrature for $\int_0^{0.5} x(t)\mathrm{d}t$.
- $M_2$ be Bayesian quadrature for $\int_{0.5}^{1} x(t)\mathrm{d}t$.
- $M_3$ be the trivial probabilistic numerical method that adds its two inputs..

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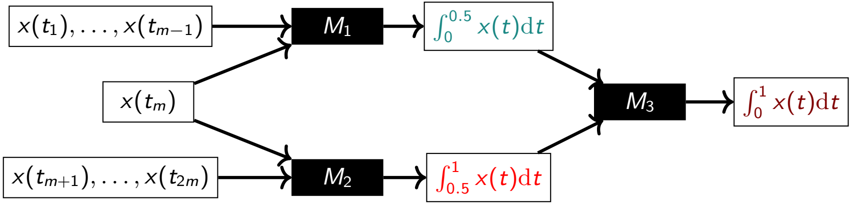
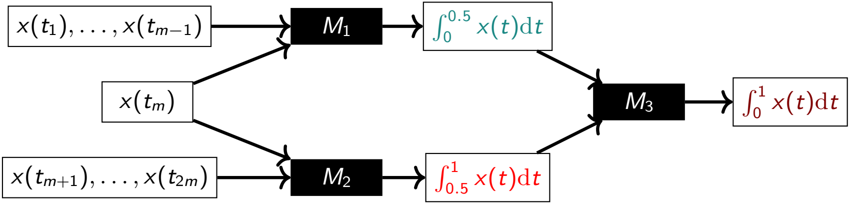



Q: When is the output of the pipeline Bayesian?

I.e. When does the output of the pipeline coincide with standard Bayesian quadrature performed on the full information $\{x(t_1), \ldots, x(t_{2m})\}$?

# Dependency Graphs

The abstract structure of the graph allows us to give a rigorous answer:




Pipeline

If we restrict attention to Bayesian probabilistic numerical methods, then $M_1$, $M_2$ and $M_3$ are uniquely determined by the prior distribution $P_x$ for the integrand.

So we can delete the method nodes to obtain the dependency graph of a pipeline.

Starting to look like a Bayesian network...

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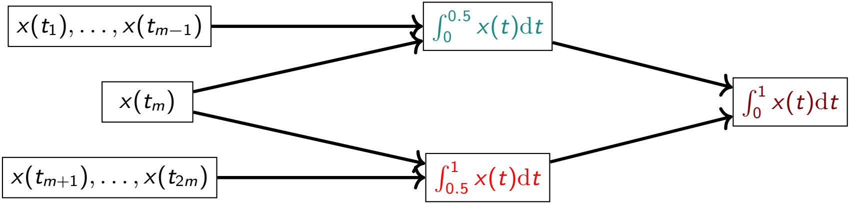


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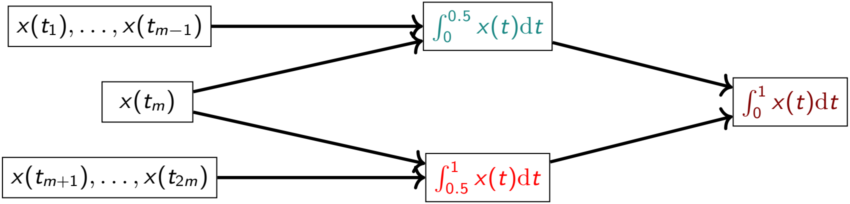


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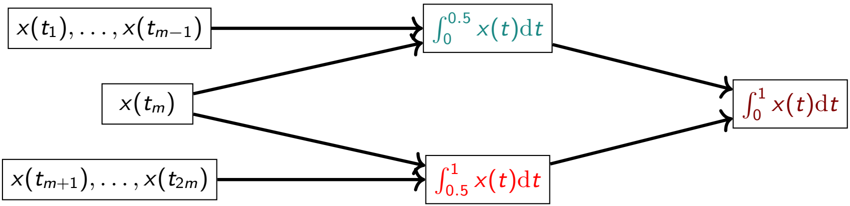


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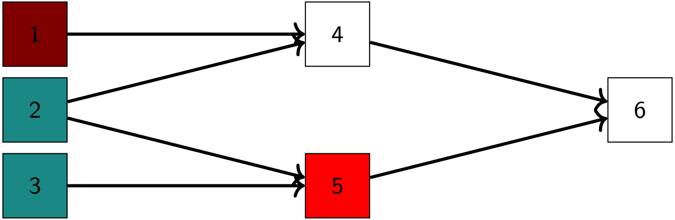
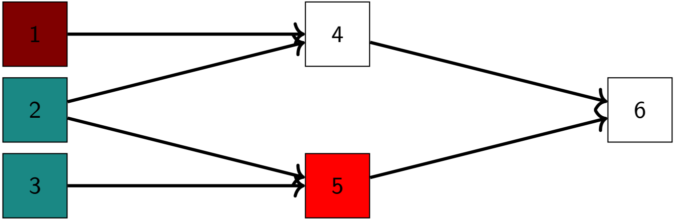



Associate each node $i$ with a random variable $X_i$.

e.g. $X_1 = \{x(t_1), \ldots, x(t_{m-1})\}$, $X_4 = \int_0^{0.5} x(t) \mathrm{d}t$.

A prior $P_x$ is coherent for the dependency graph if each $X_i \perp\!\!\!\perp X_{\mathrm{Nd}(i) \setminus \mathrm{Pa}(i)} \mid X_{\mathrm{Pa}(i)}$.

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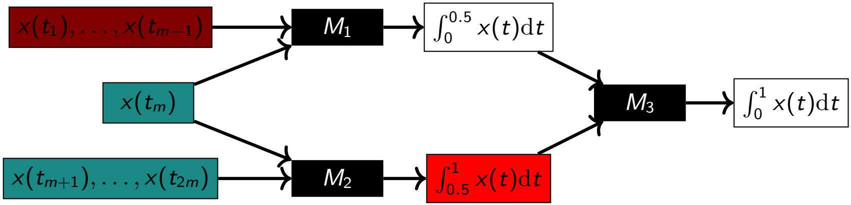
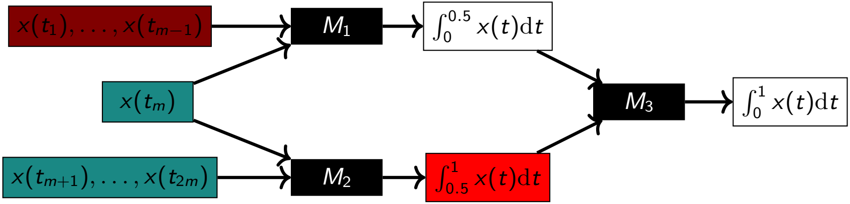
# Split Integration: Coherence




Thus in this instance we would ask whether $\int_{0.5}^{1} x(t)\mathrm{d}t$ is independent of $x(t_1), \ldots, x(t_{m-1})$ given $x(t_m), \ldots, x(t_{2m})$?

This is not true in general, but sometimes holds - e.g. a Wiener process prior $P_x$.

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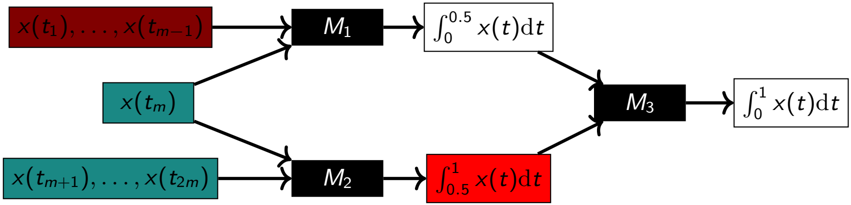


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The process illustrated here can be made formal:

A pipeline is Bayesian for estimation of its output if:

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# Conclusion

In Part VI it has been argued that:

- Computational work-flow can be related to graphical models used in statistical applications.
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# Minimal Take-Home Message

"All uncertainty is of one kind" $\sim$ Phil Dawid.

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