Fast Functional Integrals with Applications to Stochastic Dynamical Systems

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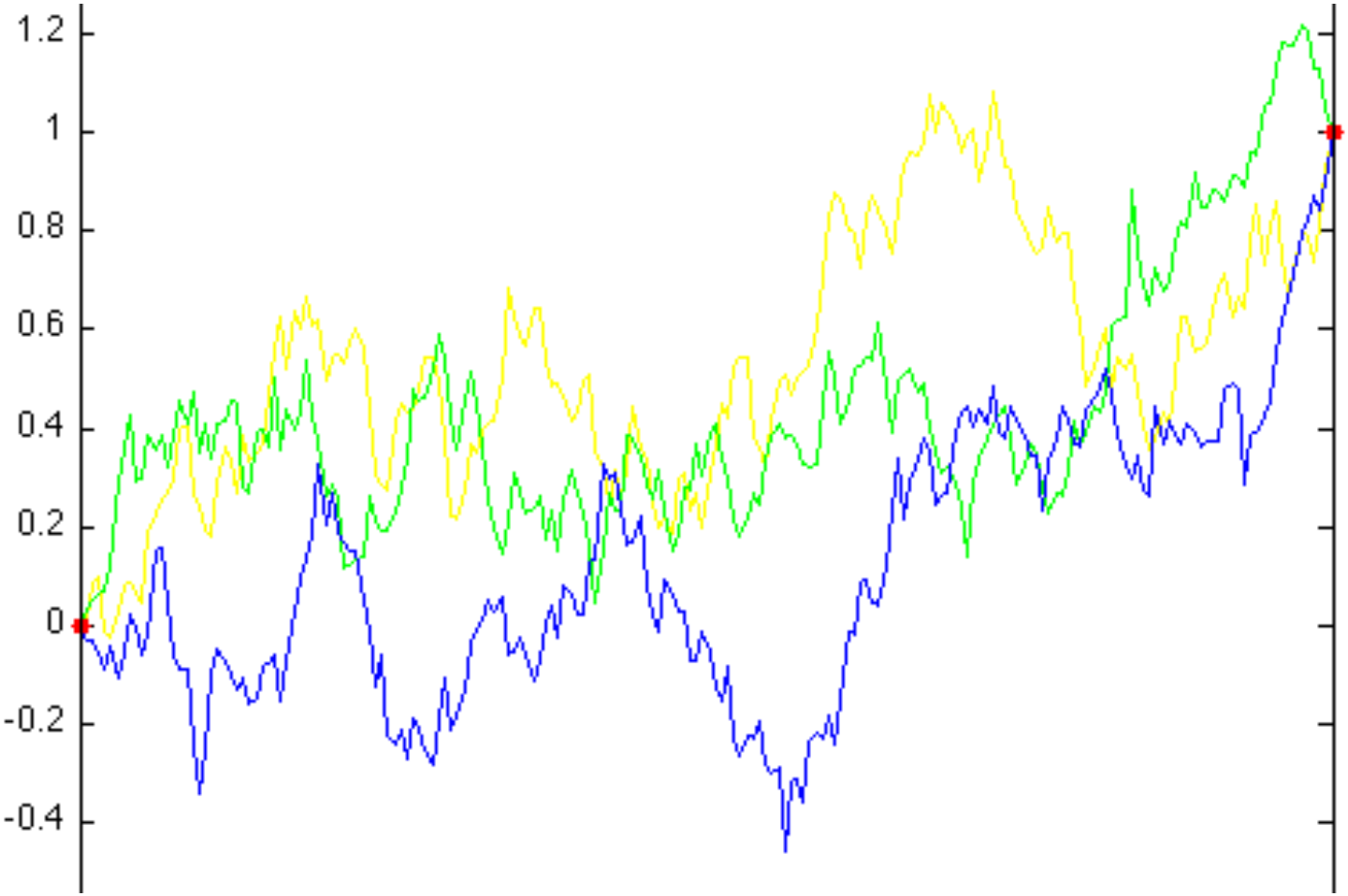
Overview

- Summary of functional integrals
- New application: parameter estimation for dynamical systems
- New method of calculating functional integrals
- Results for an infectious disease model (SIR) – equivalent results as Monte Carlo but much faster

Functional ("path") integrals

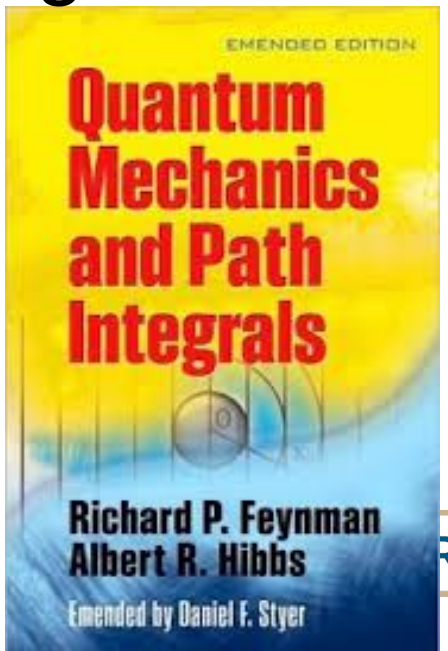
- Also called "sum over histories"
- Early application: Brownian motion (limit of random walks with infinitesimal steps)
- Gives likelihood of going from point A to point B in time t
  - Likelihood for individual paths is simple
  - Sum over all possible paths

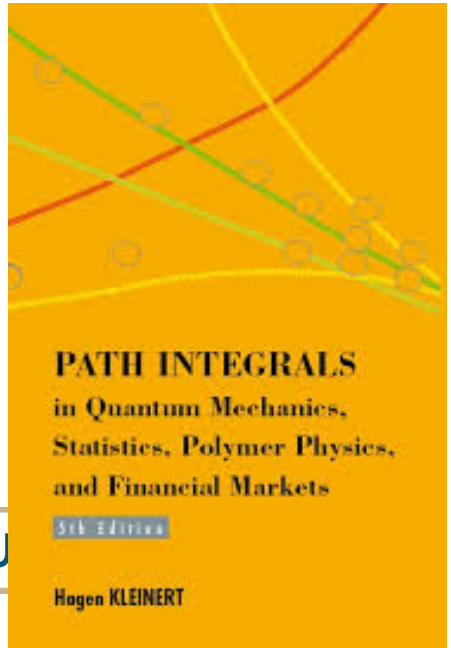
A few of the infinite number of histories to integrate



Many other applications

- Quantum and statistical mechanics
- Probability (SDEs, finance)
- Computationally intensive, can require long simulations





The new method: Sparse Laplace Approximation (SLA)

- Laplace approximation computes high-dimensional integrals by fitting a multivariate Gaussian to the integrand
- Basic version just integrates the Gaussian
- Higher-order version uses the Gaussian combined with higher-order derivatives
- **For functional integrals, the second- and higher-order derivative tensors are sparse (block-tridiagonal etc**.)

What's new here?

- Variance-stabilizing transform to get critical path
- Efficient way to get the higher-order terms: $O(Nd^4)$ instead of $O(N^4d^4)$

Application: Estimating Parameters in Dynamical Systems

- Dynamical systems are everywhere
- We want to estimate their parameters
- Traditional and recent methods
- How to use functional integrals for this
- Results and conclusions

Dynamical systems (differential equations models) are ubiquitous

- Life science, chemistry, economics
- These models incorporate:
  - *Variables*, which evolve over the time frame of the data
  - *Parameters*, which should be constant for the system – we want to estimate these.

Systems modeled by differential equations are ubiquitous

- Predator-prey models: numbers next year depend on numbers this year
  - Variables: numbers of predators and prey
  - Parameters: fertility and predation rate
- Chemical reactions
  - Variables are concentrations
  - Parameters are reaction rates

Systems modeled by differential equations are ubiquitous

- Infectious disease models
  - Variables: numbers of people who are susceptible, infected, recovered, etc.
  - Parameters: infectiousness, lethality, recovery rate, etc.

A simple example illustrates some of the challenges

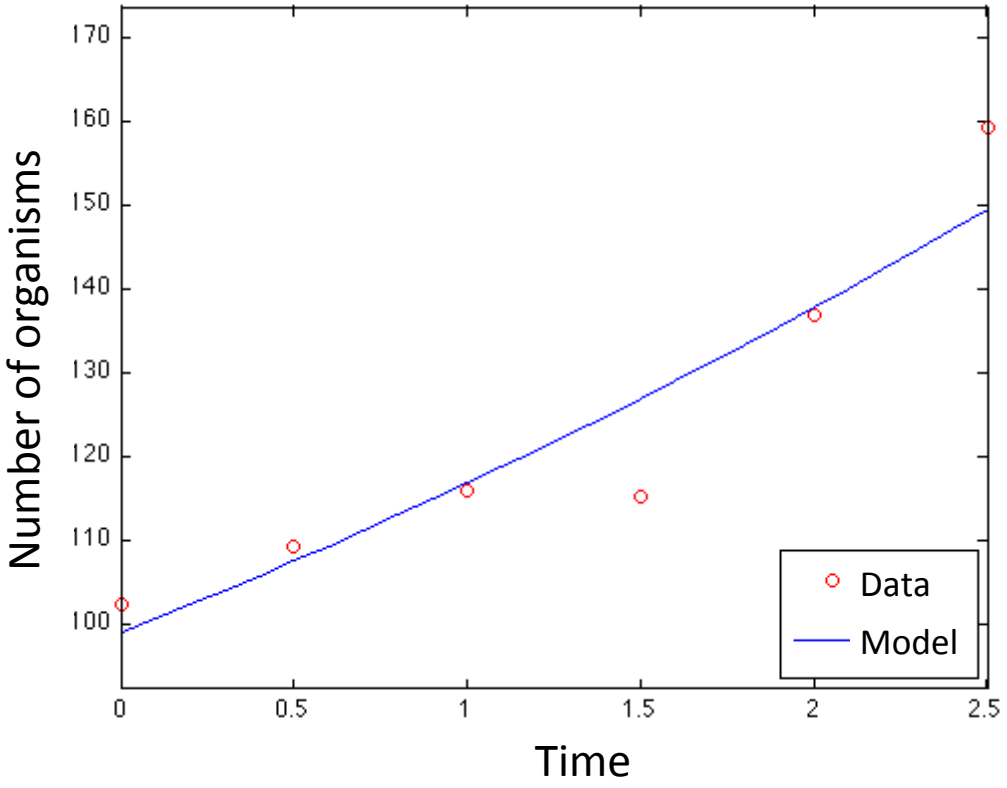
- In a bacterial colony a fixed fraction of cells divide every hour:

$$\frac{dy}{dt} = \theta y$$

where y is the number of bacteria, θ is the fraction that divide each hour, and t is time.

The traditional method solves the deterministic equations for different parameter values

- Parameter values are chosen to optimize fit to data



Traditional method has significant limitations

- It is not stochastic
- It does not allow for imperfectly followed differential equations
- In some systems, there are multiple optima of the parameters

More recent work

- Ramsay, Hooker, et al (JRSSB 2007) use spline functions and cross-validation
- Campbell (2010) uses splines and MCMC (similar to a functional integral but in a much smoother function space)

Spline-based approach

- Find a good compromise between data fit and ODE fit
- For the bacteria example, this means minimize

$$\sum_i \left(y^i_{data} - \hat{y}(t_i) \right)^2 + \lambda \int \left(\frac{d\hat{y}}{dt} - \theta \hat{y} \right)^2 dt$$

- Tradeoff (λ) is chosen by cross-validation or MCMC

Anatomy of the methods

- What all the approaches have in common:
- (1) for given params, find a "best guess" path $\hat{y}$ by minimizing "inner" objective function
- (2) given $\hat{y}$, calculate derivatives of "outer" objective function wrt parameters
- (3) repeat until outer function has been minimized

Functional Integral Approach

- Discretize time

$$N = \#\, time\ points,\ d = \#\, variables$$

- Treat true values as a latent, underlying Markov process
- This allows for rougher paths, more like Brownian motion

Overall likelihood as a functional integral

$$L(y_{data}|\theta,\sigma) = \int L_{data}(y_{data}|y_{true},\sigma)\, L_{Markov}(y_{true}|\theta)\, d^{Nd}y_{true}$$

where

y_{data} are the data values at whatever time points we have them

y_{true} is a possible history of the system

σ are parameters of measurement error

θ are dynamical parameters

Rewrite in terms of log-likelihood

- If we say

$$\ell_{data} = -\log(L_{data})$$
$$\ell_{Markov} = -\log(L_{Markov})$$
$$\ell = \ell_{data} + \ell_{Markov}$$

Then the second-order derivative matrix of ℓ is very sparse, and the higher-order derivative tensors are also sparse!

Example: bacteria colony

- L_{data} is the likelihood of the data given the true value

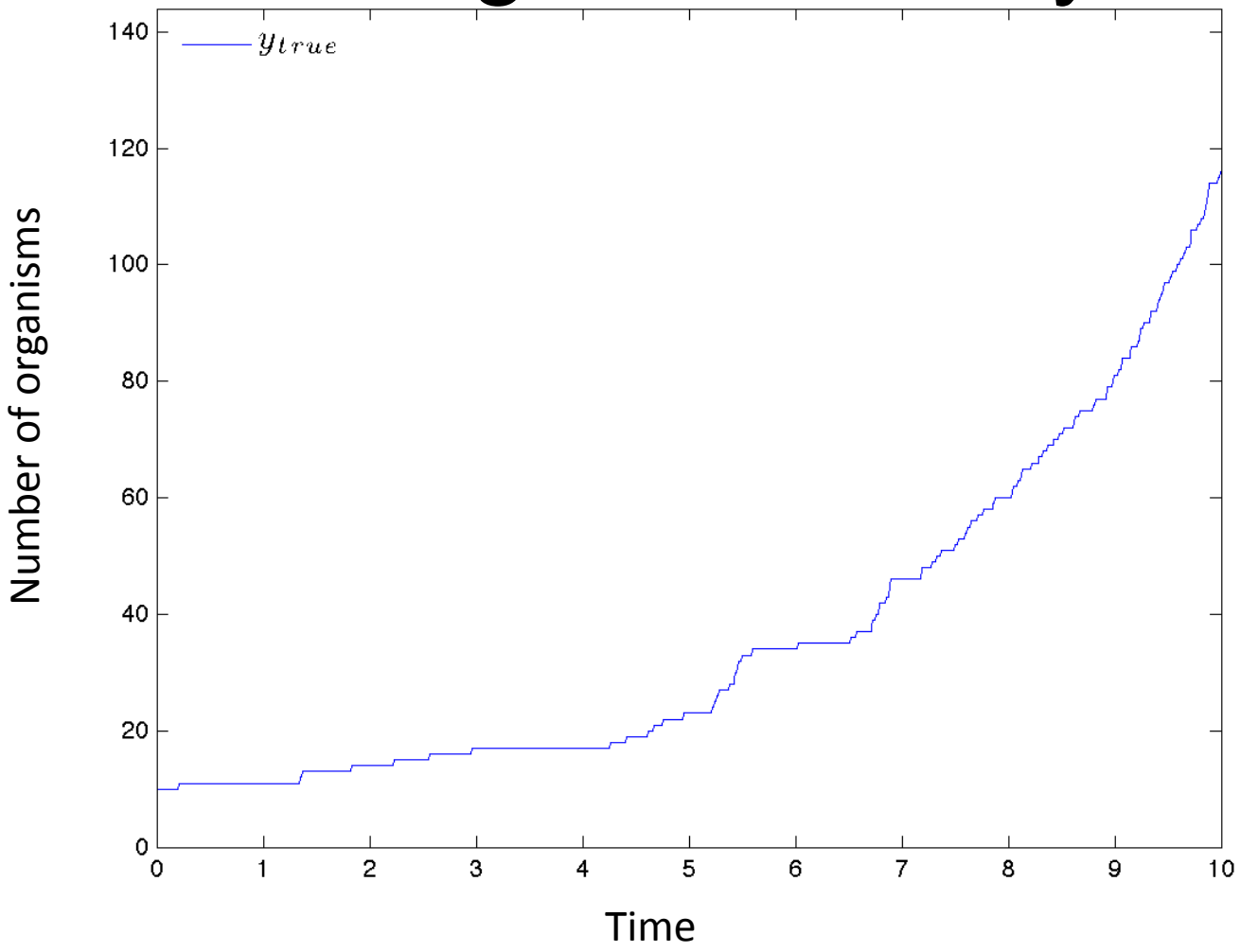
$$\log(y_{data}) \sim Normal\left(\log(y_{true}), \sigma^2\right)$$

- L_{Markov} is the likelihood of the sequence y^i_{true}

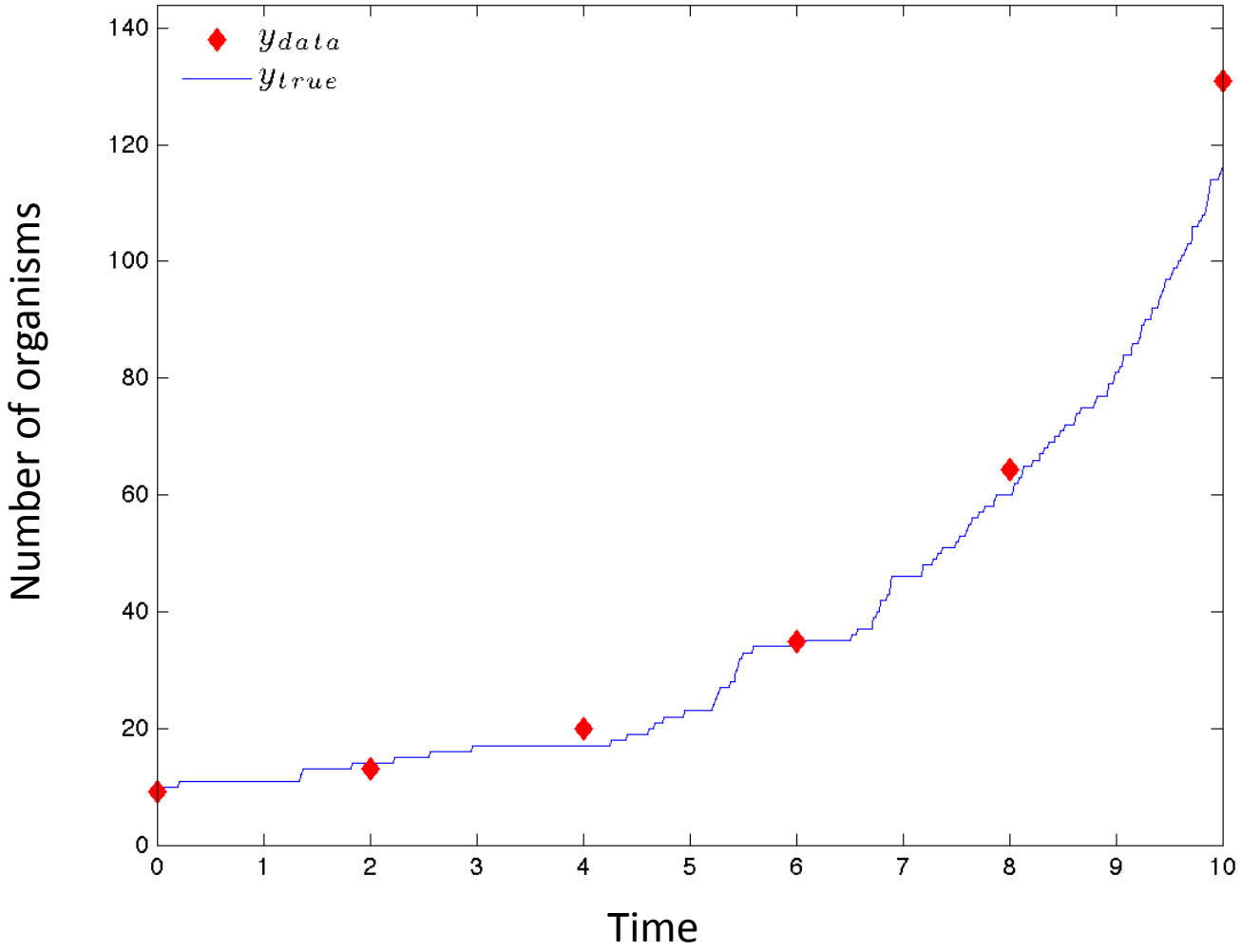
assuming that the real system follows the Markov process

$$\Delta_i y_{true} \sim Poiss(\theta \cdot y^i_{true} \cdot \Delta_i t)$$

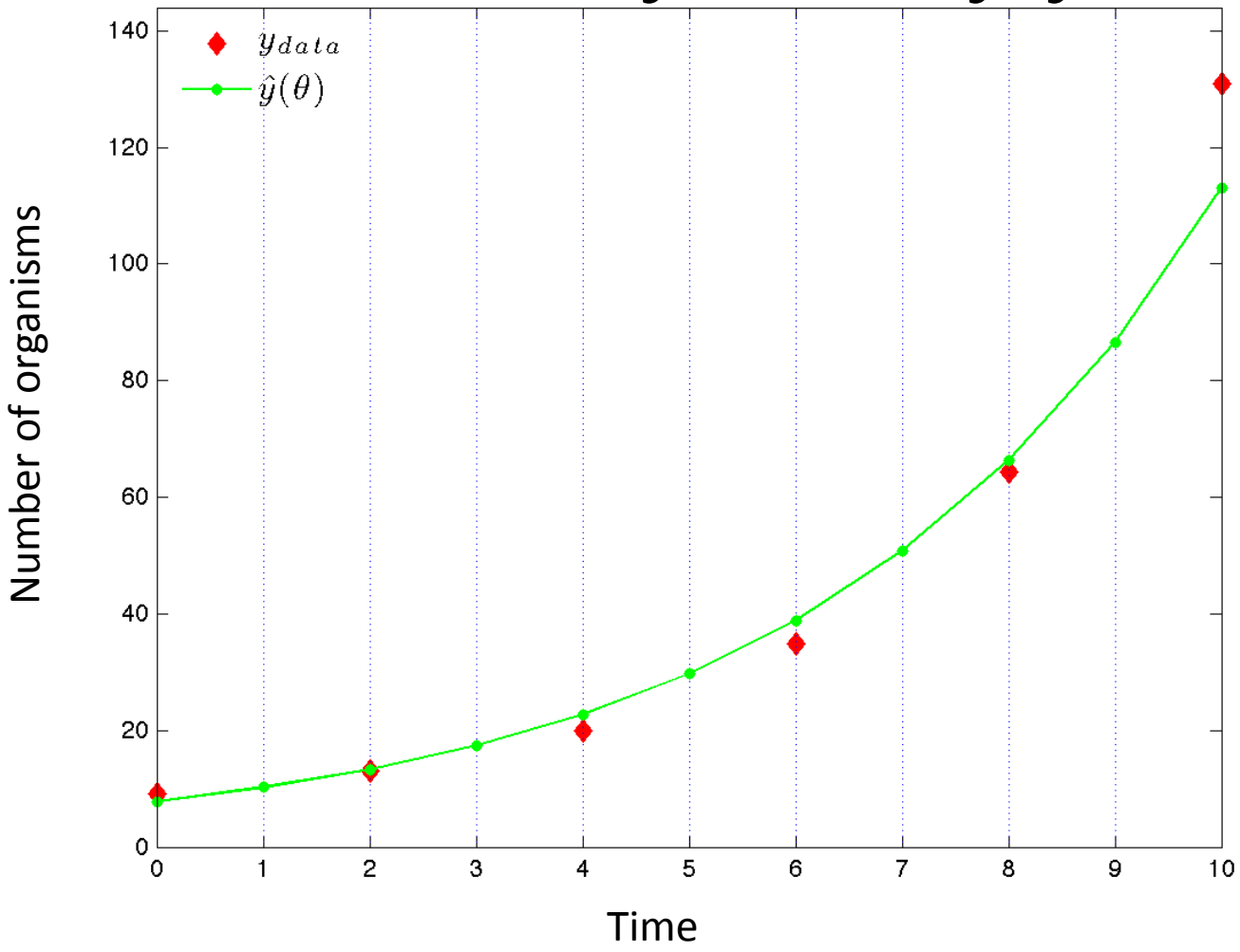
Bacterial colony example: "true" growth history



Data only at some time points, with measurement error



For given parameters, there is a most likely history ŷ



Expand around critical path

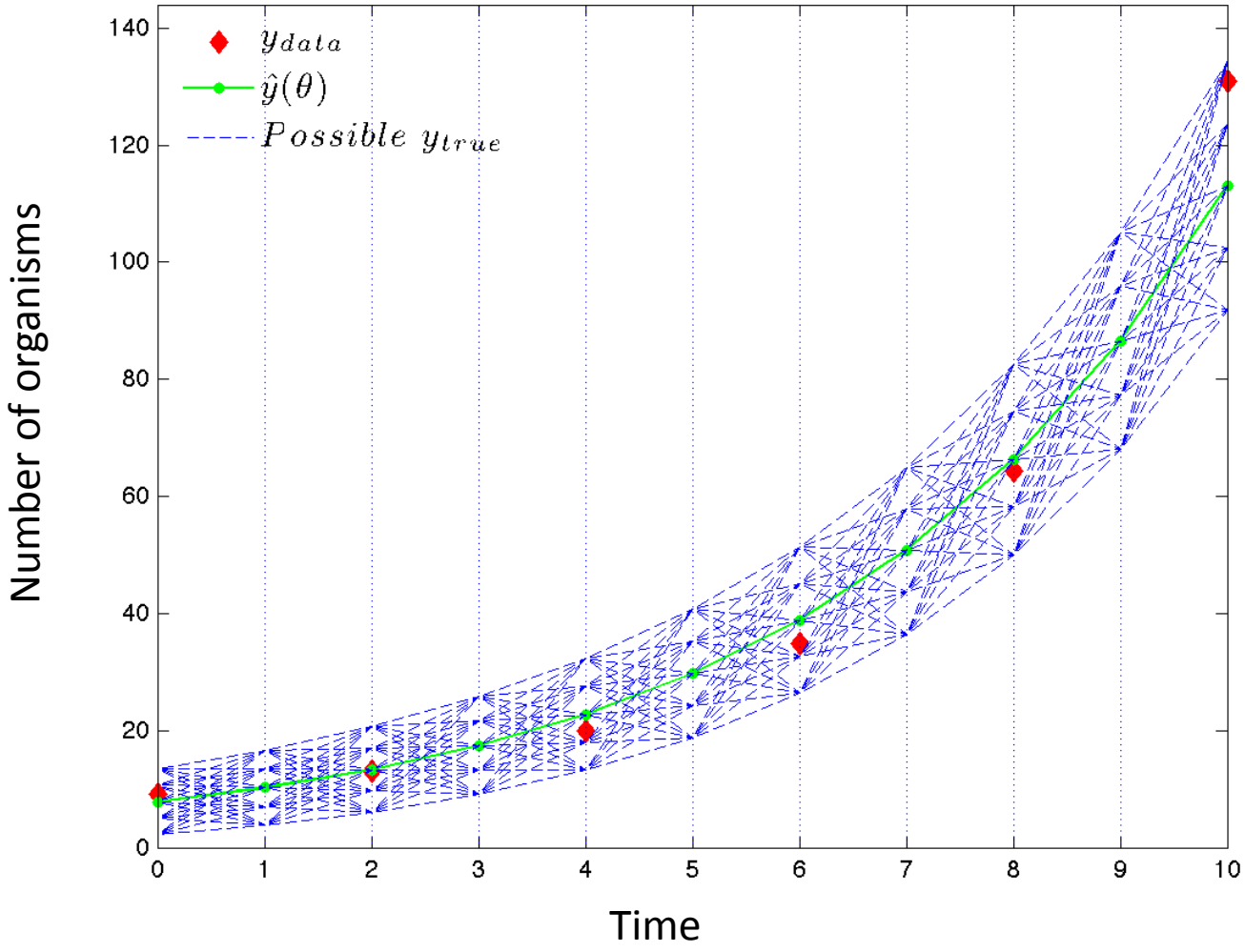
$$y = \hat{y} + \epsilon$$

$$\int_{\mathbb{R}^n} e^{-\ell(y)} d^n y = \int_{\mathbb{R}^n} e^{-\ell(\hat{y}+\epsilon)} d^n \epsilon$$

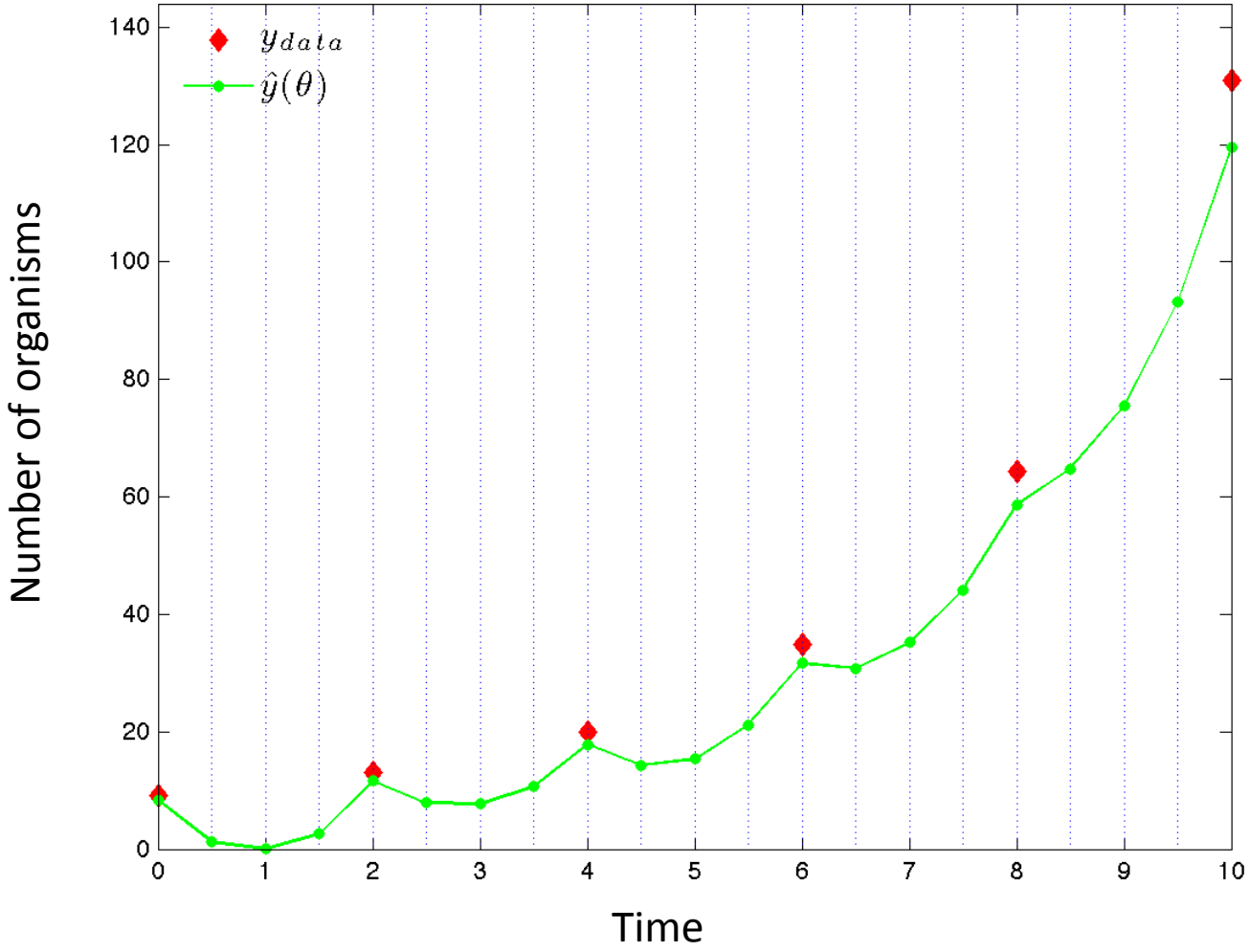
$$= \int_{\mathbb{R}^n} exp\left(-\ell\left(\hat{y}\right) - \frac{1}{2}\ell^{(2)}_{ij}\left(\hat{y}\right)\epsilon_i\epsilon_j \right.$$

$$\left. - \frac{1}{3!}\ell^{(3)}_{ijk}\left(\hat{y}\right)\epsilon_i\epsilon_j\epsilon_k - \ldots \right) d^n\epsilon$$

We use it to compute the integral over all paths



All very good, unless this happens…



What's going on?

In the normal approximation, the Markov variance is proportional to y:

$$L_{Markov} = \prod_{i<N} \frac{1}{\sqrt{2\pi\theta y_i \Delta_i t}} \exp\left(-\frac{1}{2} \frac{(\Delta_i y - \theta y_i \Delta_i t)^2}{\theta y_i \Delta_i t} \right)$$

The $\frac{1}{\sqrt{y_i}}$ means that moving y to zero increases the likelihood.

Why this is not okay

- It moves the critical path away from the realistic paths
- Likelihood *density* is maximized in a region whose *total likelihood* is small
- With the right change of variable, this problem disappears

Variance-stabilizing transform

- The solution is to make a change of variable that stabilizes the variance.

$$v_y = \sqrt{y}$$

$$L_{Markov} \prod_i dy_i \propto \prod_i \frac{e^{-q_i}}{\sqrt{y_i}} dy_i = 2 \prod_i e^{-q_i} \, dv_y = 2 \exp\left(-\sum_i q_i \right) dv_y$$

Reducing $\sum_i q_i$ does not bias y toward zero.

Cumulant form of Laplace approximation (Shun & McCullagh, 1995)

$$\log \int e^{-\ell(y)} d^N y \sim -\ell(\hat{y}) + \frac{1}{2}\log\frac{(2\pi)^N}{|H|}$$
$$- \frac{3}{24} F_{ijkl} H^{-1}_{ij} H^{-1}_{kl}$$
$$+ \frac{9}{72} T_{ijk} T_{lmn} H^{-1}_{ij} H^{-1}_{kl} H^{-1}_{mn}$$
$$+ \frac{6}{72} T_{ijk} T_{lmn} H^{-1}_{il} H^{-1}_{jm} H^{-1}_{kn}$$
$$+ \ldots$$

Basic approximation is the first line

Other terms are higher-order

Watch your accounting: higher-order terms

- There are three distinct higher-order terms
- For the first two, it is “obvious” how to use sparsity and compute efficiently
- The last one involves a complicated analytical trick
- Total time is $O(N\,d^4)$ (N = time points, d = variables)
- Without sparsity, the total time would have been $O(N^4\,d^4)$

Testing on a simple infectious disease model

- SIR Model (Kermack and McKendrick, 1927)
  - **S**usceptible
  - **I**nfected (and contagious)
  - **R**ecovered (and immune)

Usually this is solved deterministically

$$\frac{dS}{dt} = -\beta SI$$

$$\frac{dI}{dt} = \beta SI - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

SLA permits a stochastic approach

$$\text{New Infections } (t_i \text{ to } t_{i+1}) \sim Poiss(\beta S^i_{true} I^i_{true} \Delta_i t)$$

$$\text{Recoveries } (t_i \text{ to } t_{i+1}) \sim Poiss(\gamma I^i_{true} \Delta_i t)$$

Normal approximation to the Poisson distribution: write as SDE

$$dS = -\beta SIdt + \sqrt{\beta SI}\,dW_1$$

$$dI = -dS - \gamma Idt + \sqrt{\gamma I}\,dW_2$$

Variance-Stabilizing SIR

Bias is removed by this transformation:

$$v_S = \sqrt{S}$$

$$v_I = \log(I)$$

$$L_{Markov} dS_i dI_i \propto \frac{dS_i dI_i}{\sqrt{S_i \cdot I_i}} = 2 dv_S dv_I$$

Comparison with STAN on a real data set

- STAN is a new (2012) general-purpose system for Hamiltonian Monte Carlo.
- You specify the model; then it generates C++ code and compiles with optimization.
- Developed by Andrew Gelman's group at Columbia; replaces BUGS
- Try it! http://mc-stan.org

Data set

- British boarding school data set: 14-day flu epidemic
- Data is only on number infected (number susceptible is latent!)
- Still possible to implement both in STAN and SLA

Results (parameter estimates)

		β	γ	σ	Time (sec)	Opt steps
Initial guess		2.18E-03	0.440	(0.1)*	N/A	N/A
STAN	5%	1.31E-03	0.667	0.122	267	
	Mean	1.53E-03	0.760	0.152	325	N/A
	95%	1.77E-03	0.882	0.156	366	
SLA basic		1.45E-03	0.777	0.156	6	23
SLA higher		1.47E-03	0.770	0.157	42	4

*Paper doesn't specify initial sigma, so we chose 0.1. STAN runs use 4 chains each with 2000 steps. There were 100 such runs.

Results (marginal likelihood)

	Log(L)	% diff from IS estimate
SLA basic	5.353	5.7%
SLA higher	5.300	0.4%
Importance Sampling (N=6.6e8)	LB: 5.295 Est: 5.296 UB: 5.298 (99+% CI)	-0.1% 0.0% 0.2%

Day 0 removed to avoid a pathology that happens when I=1.
Importance sampling uses multivariate T, df=2.
Sample values constrained to sqrt(S) and log(I) positive.

Conclusion

- For this problem, SLA gives near-identical results to STAN, but is vastly faster
  - Basic is > 50 times faster
  - Basic + Higher is ~6 times faster
  - Real difference should be bigger, because STAN is compiled with high optimization

More to be done: methods

- Further efficiencies
- More independent variables (not just time) requires different algorithm
- Analytical error bounds
  - Notoriously hard for Laplace approximations, but methods exist
  - The usual, hand-waving explanation is not the real reason why they are so accurate (Olver, 1968)

More to be done: other applications

- Larger problems
- Bayesian model selection
- Graphical models
- Physics
  - "Likelihood" becomes complex (not that bad)
  - In some problems the path would be in a group, not $\mathbf{R}^n$

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More references

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