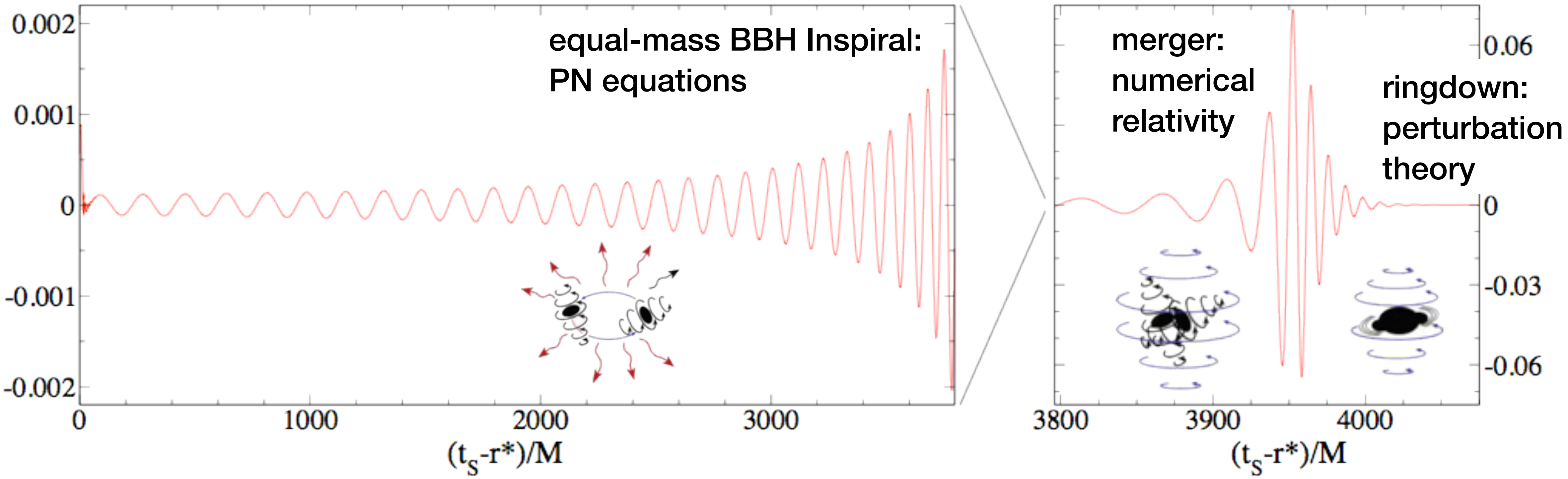
Markov Chain Monte Carlo: the ultimate multitool

Michele Vallisneri, Jet Propulsion Laboratory

GW science in a nutshell: what's in a waveform?



Caltech/Cornell/CITA NR

equal-mass BBH Inspiral: PN equations

merger: numerical relativity

ringdown: perturbation theory

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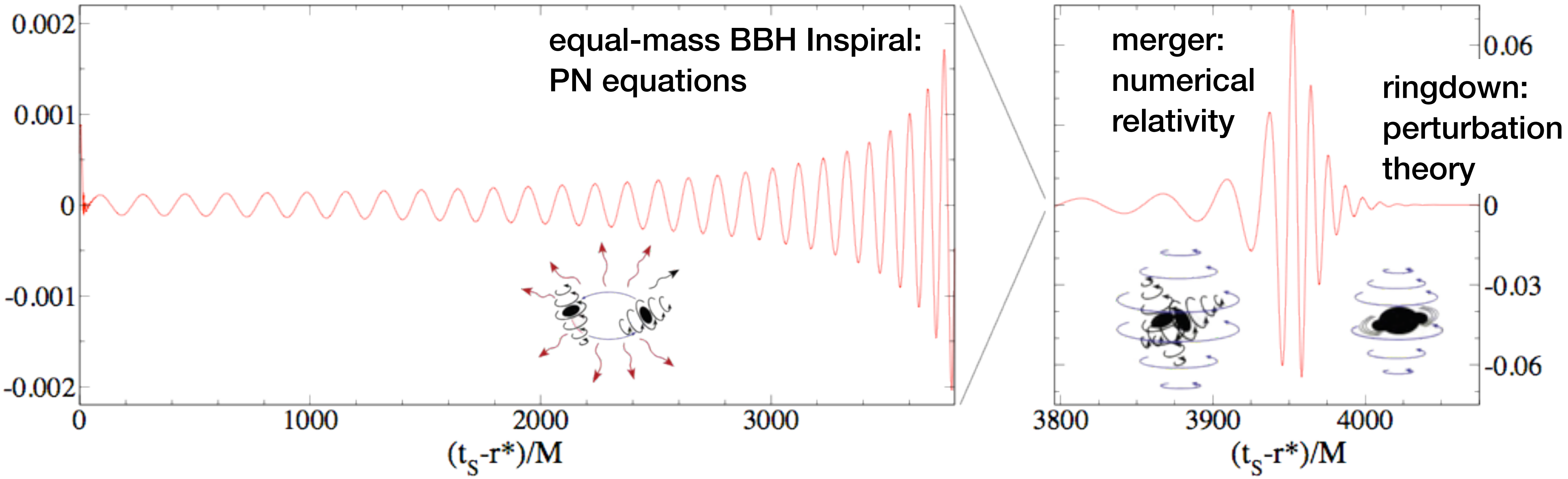

equal-mass BBH Inspiral: PN equations

merger: numerical relativity

ringdown: perturbation theory

Caltech/Cornell/CITA NR

	HF GWs: stellar masses	LF GWs: massive BHs, large separations
astrophysics	populations of compact objects; SN and GRB progenitors*	massive BH origin and evolution; Galactic WD-binary populations and interactions
nuclear physics	NS EOS, r-mode processes*	
cosmology	standard sirens*	
fundamental gravity	strong-field and radiation-sector dynamics	
black-hole structure		tests of no-hair theorem with EMRIs, ringdowns

$$p(\text{source parameters}|\text{data}) = \frac{p(\text{d.}|\text{s.p.}) \times p(\text{s.p.})}{\int p(\text{d.}|\text{s.p.}) \times p(\text{s.p.})\, d(\text{s.p.})}$$

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posterior probability:
astrophysical insight

likelihood: prob. that
noise = signal – model

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posterior probability:
astrophysical insight

evidence: relative prob.
that the model is right

Parameter estimation for compact binary coalescence signals with the first generation gravitational-wave detector network

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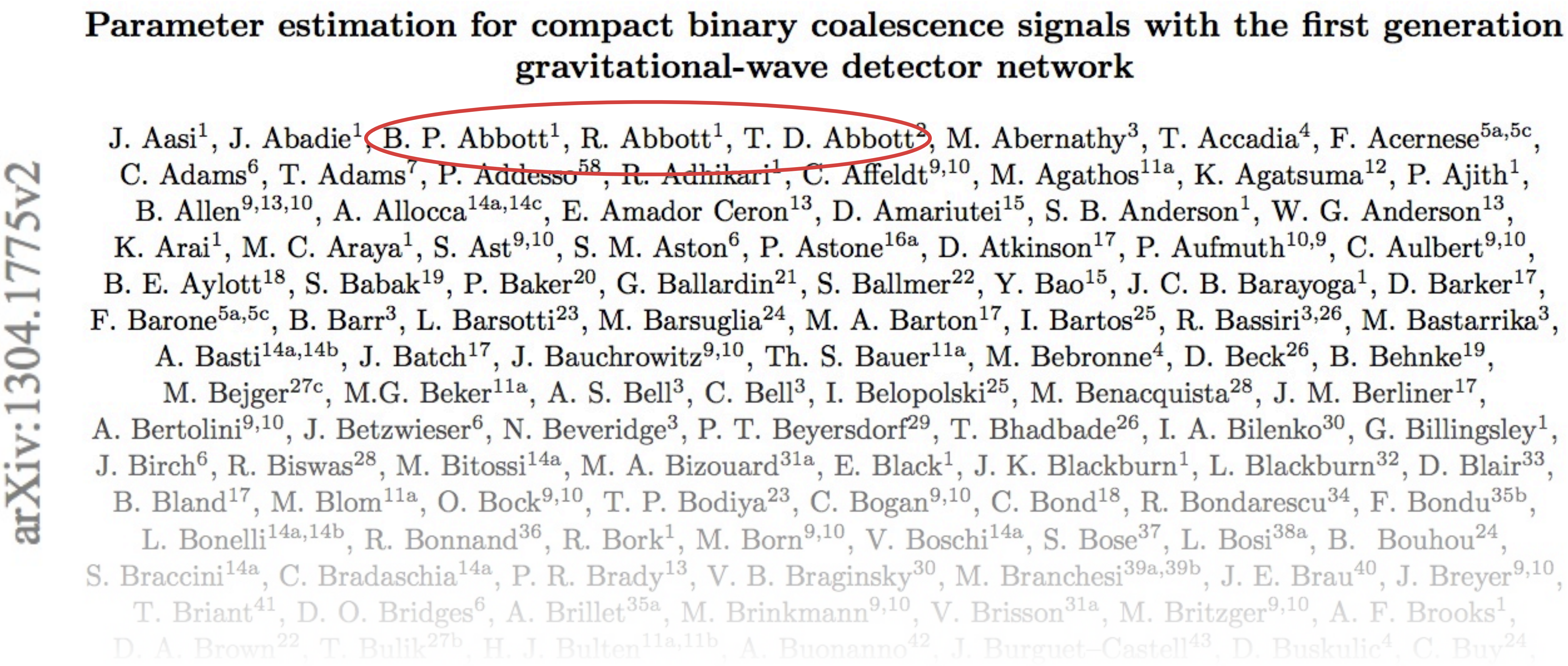

arXiv:1304.1775v2

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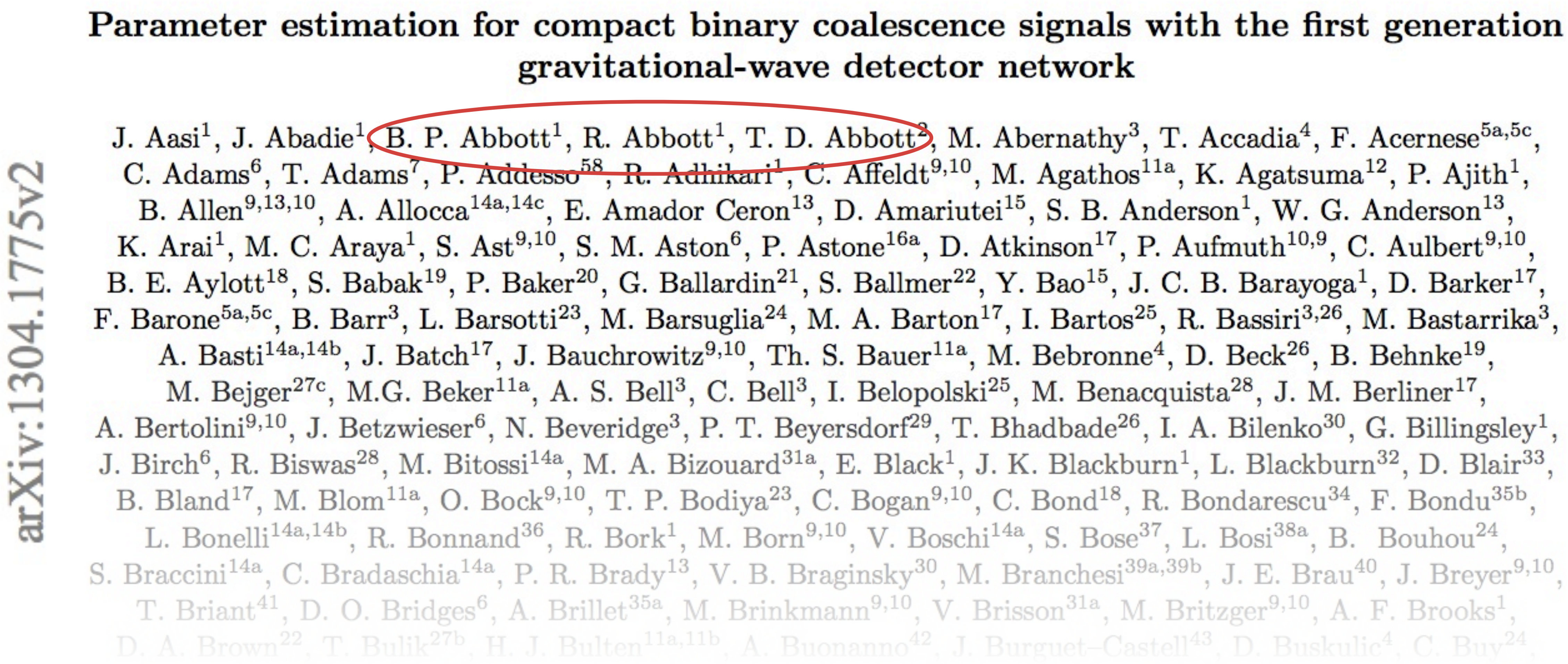

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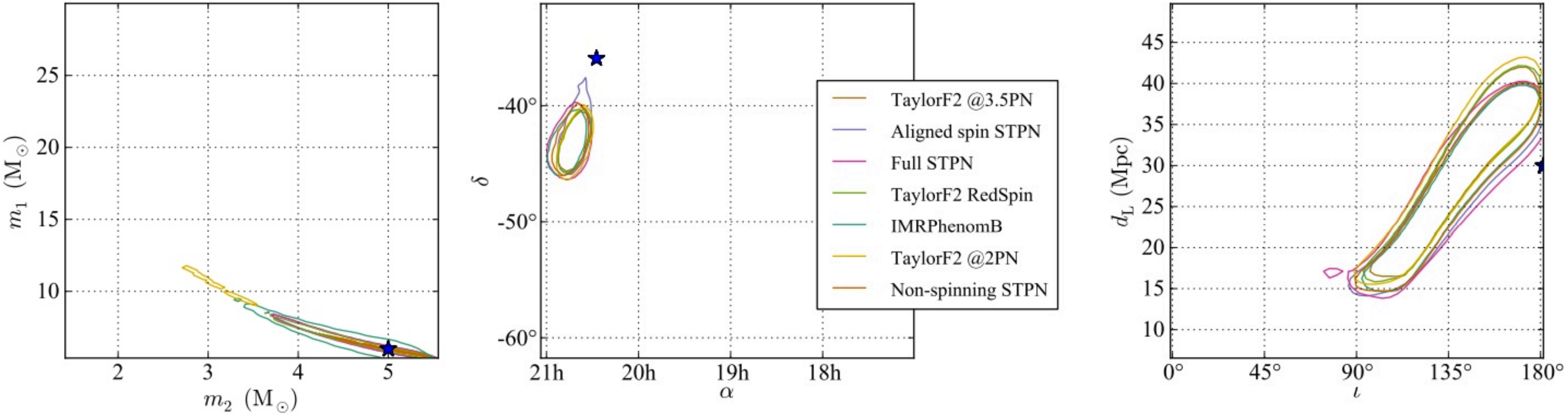
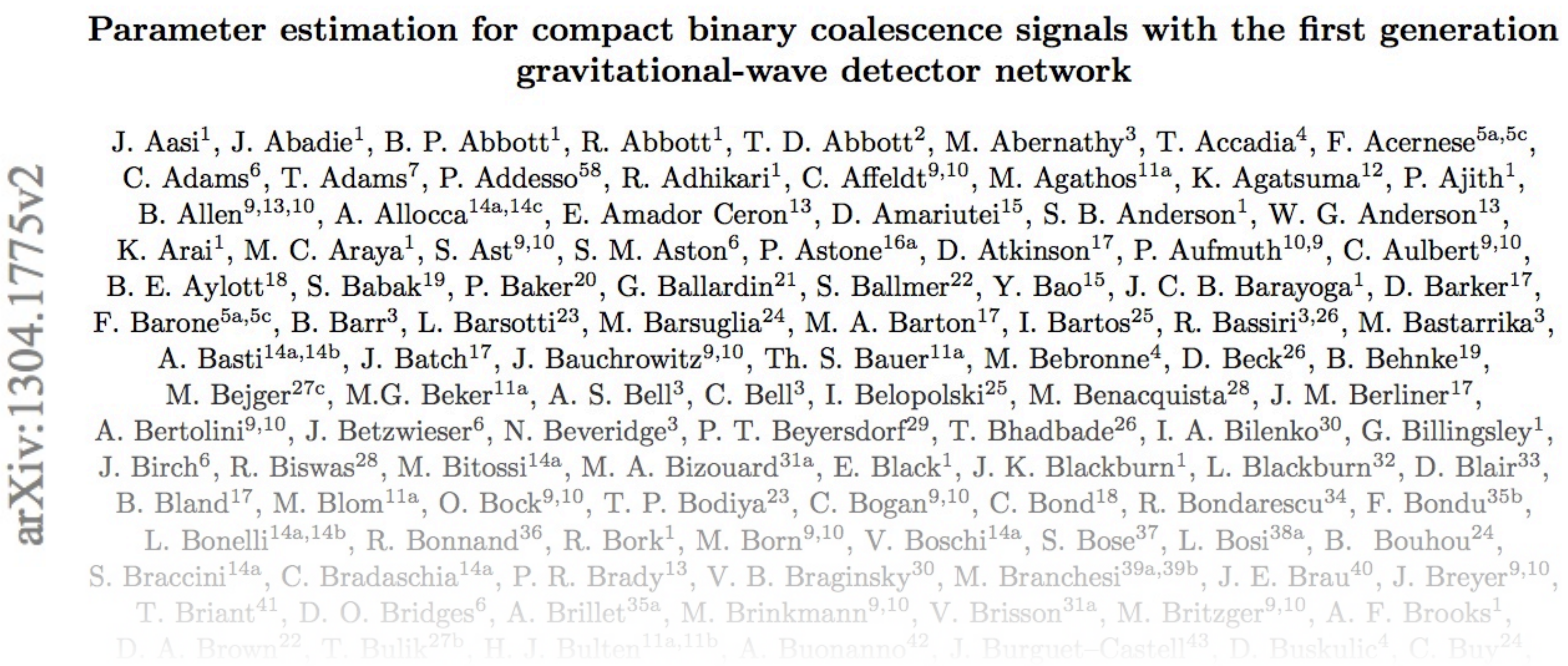


spinning BH–BH injection



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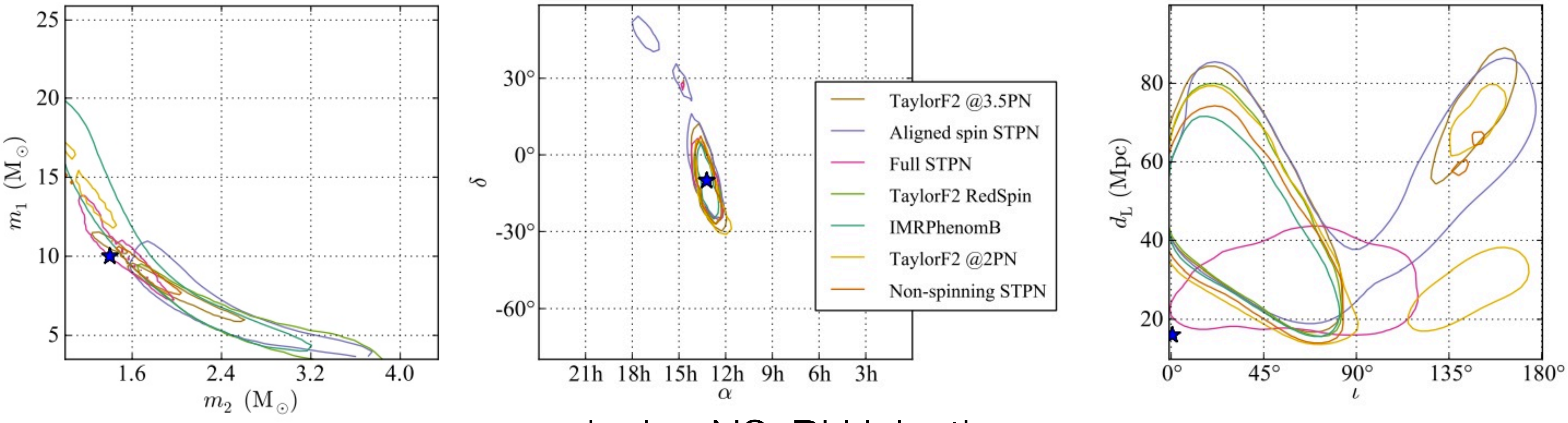

spinning NS–BH injection

Monte Carlo (Von Neumann and Ulam, 1946):
computational techniques that use random numbers

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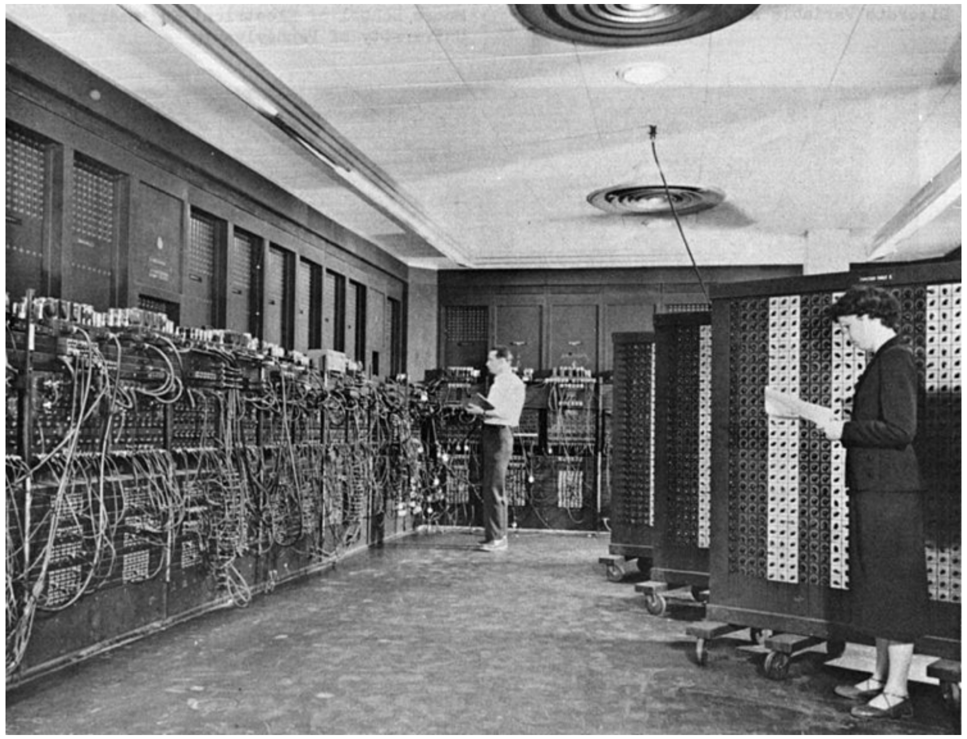

Monte Carlo (Von Neumann and Ulam, 1946): computational techniques that use random numbers

$$\int \phi(x)dx \rightarrow \hat{\phi} = \frac{1}{R}\sum_r \phi(x^{(r)})$$

accuracy depends only on variance,
not on the number of dimensions

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$$\mathrm{var}\,\hat{\phi} = \frac{\mathrm{var}\,\phi}{R}$$

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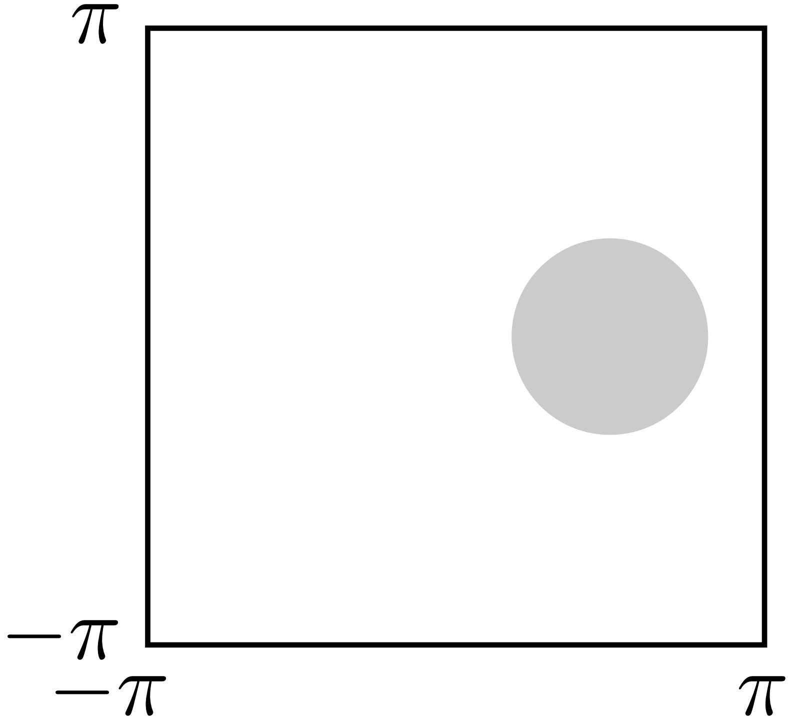


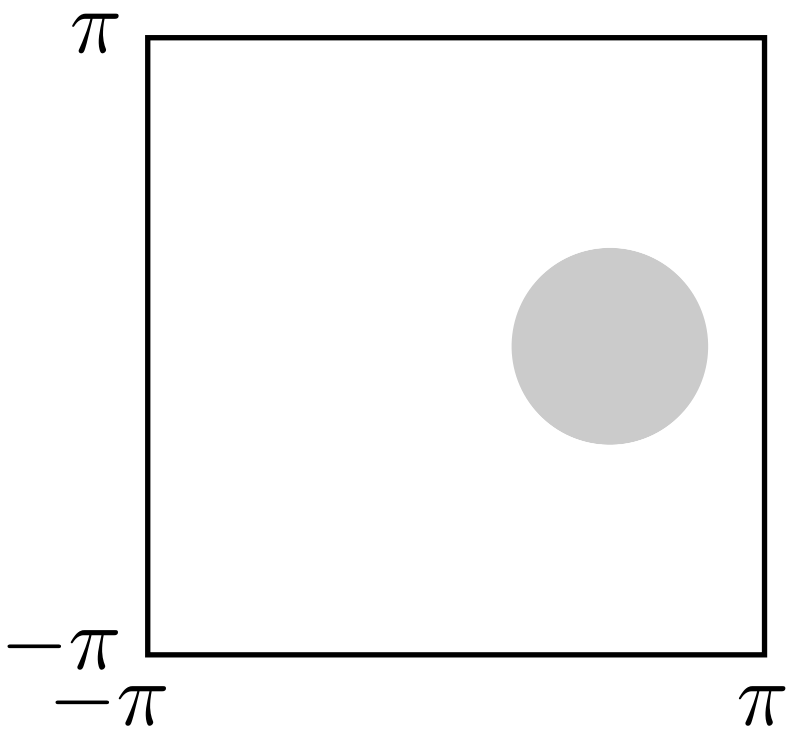
$$V_{\text{box}} = (2\pi)^d$$

$$V_{\text{ball}} = \frac{(\pi)^{d/2}}{\Gamma(n/2+1)}$$

$$\frac{V_{\text{box}}}{V_{\text{ball}}} \sim d^d$$

unfortunately uniform sampling is extremely inefficient in high-dimensional spaces

(and so are importance sampling and rejection sampling)



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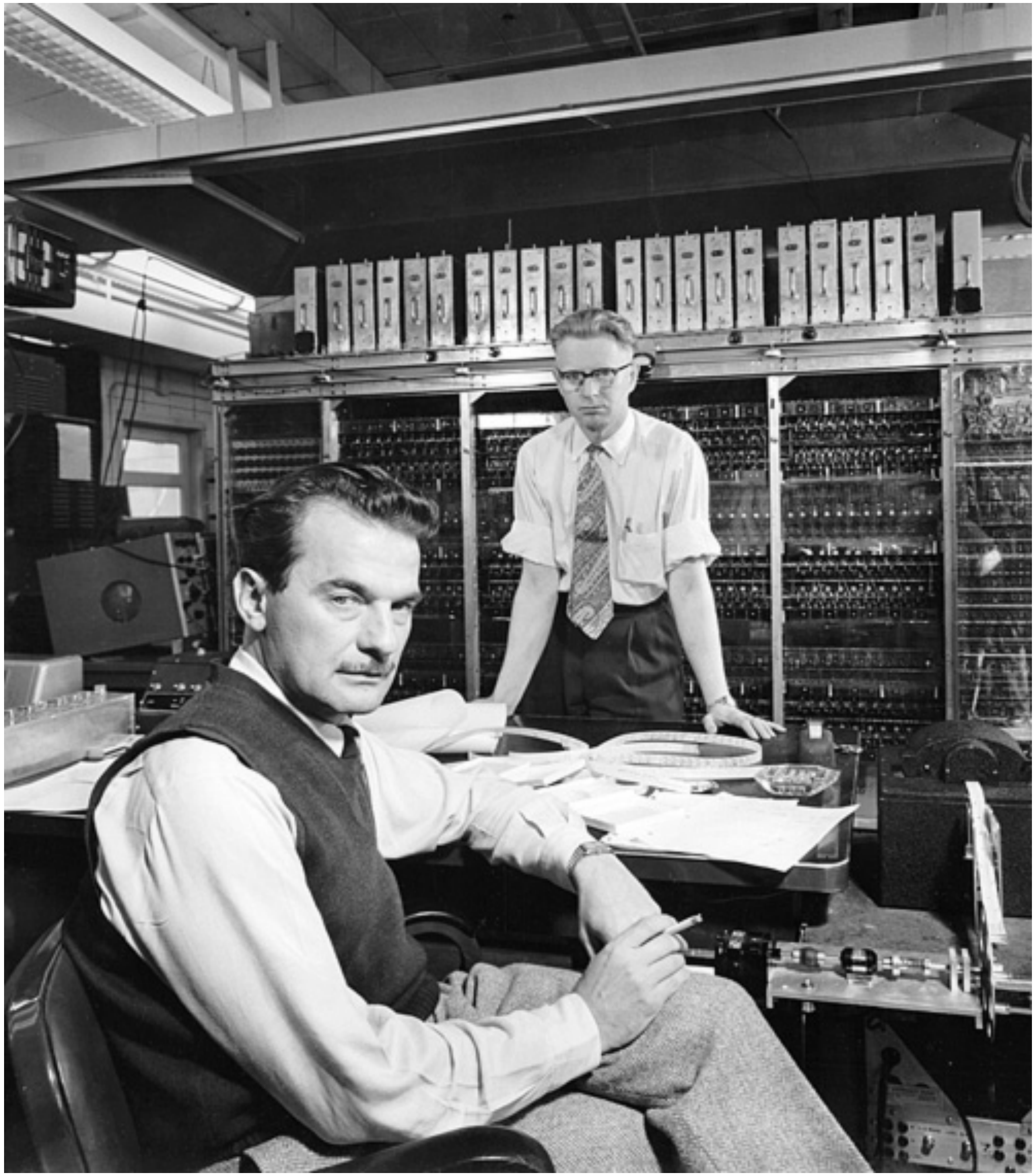
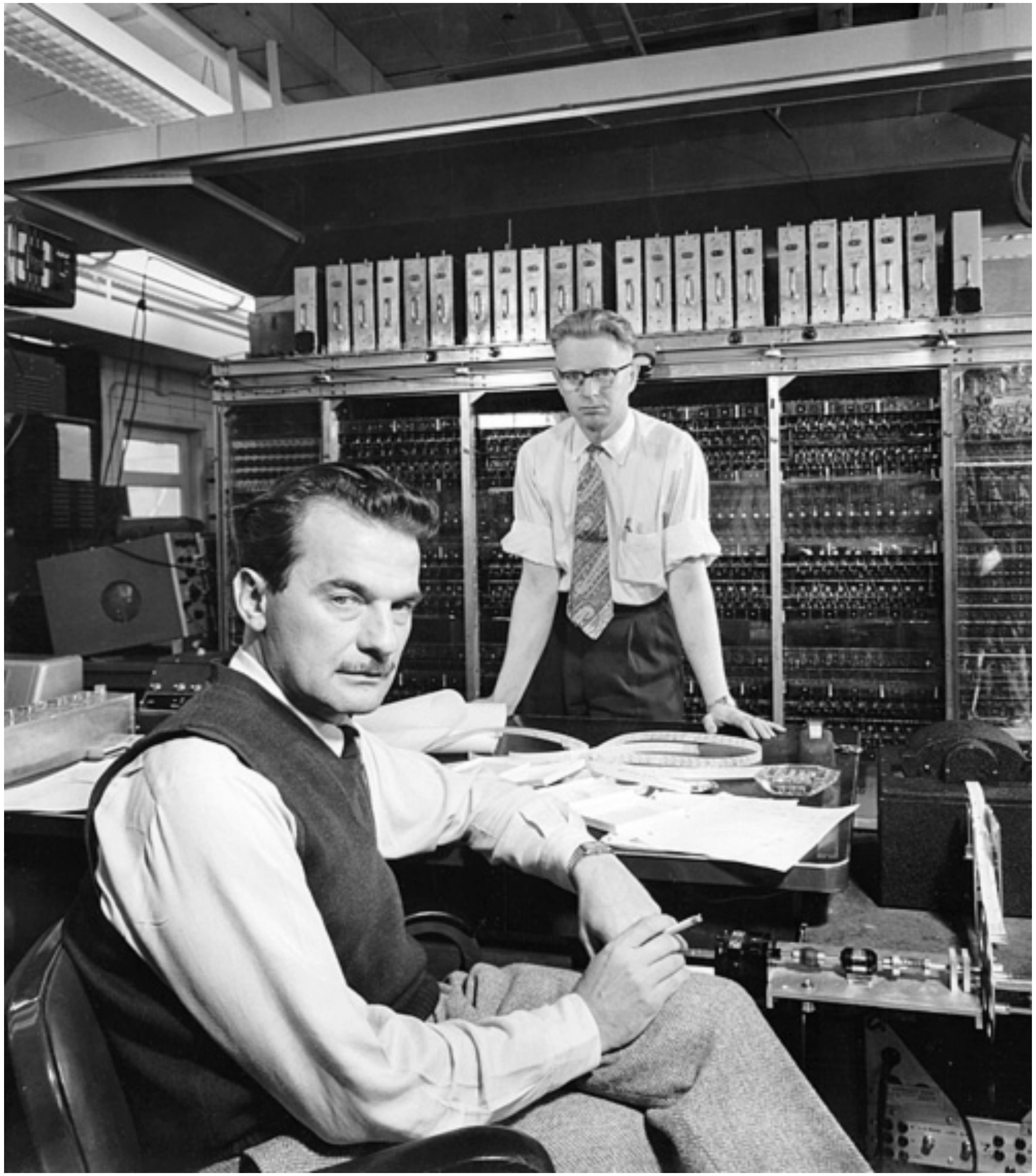
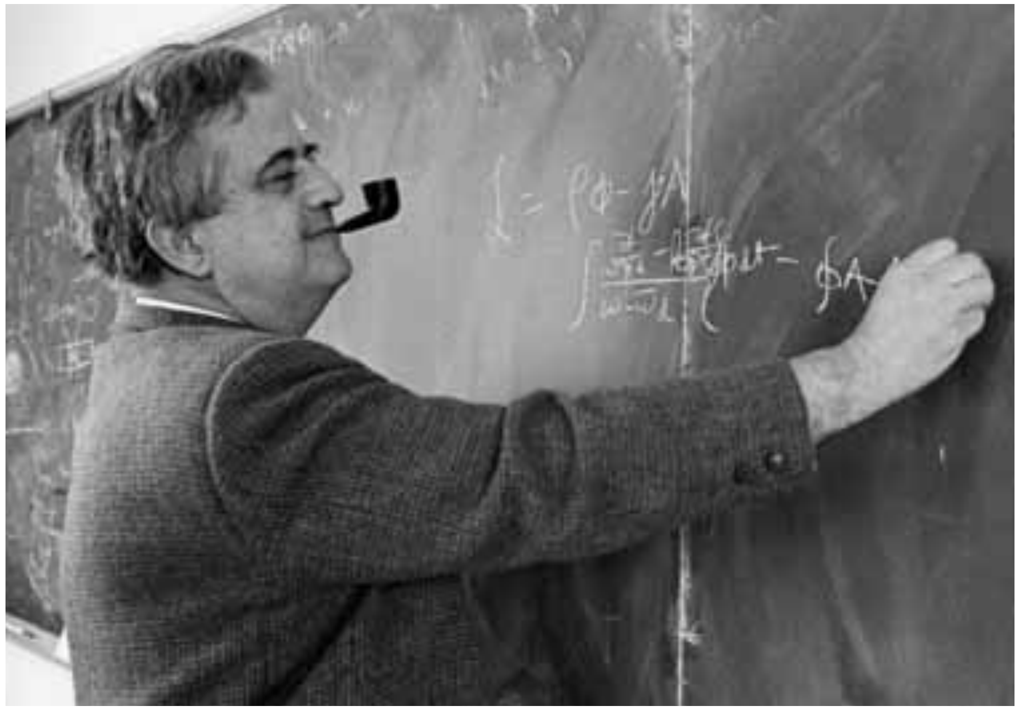
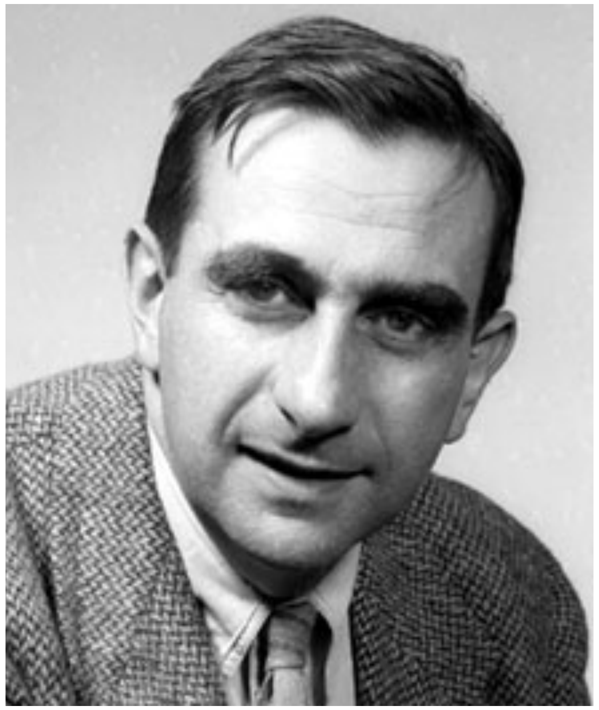
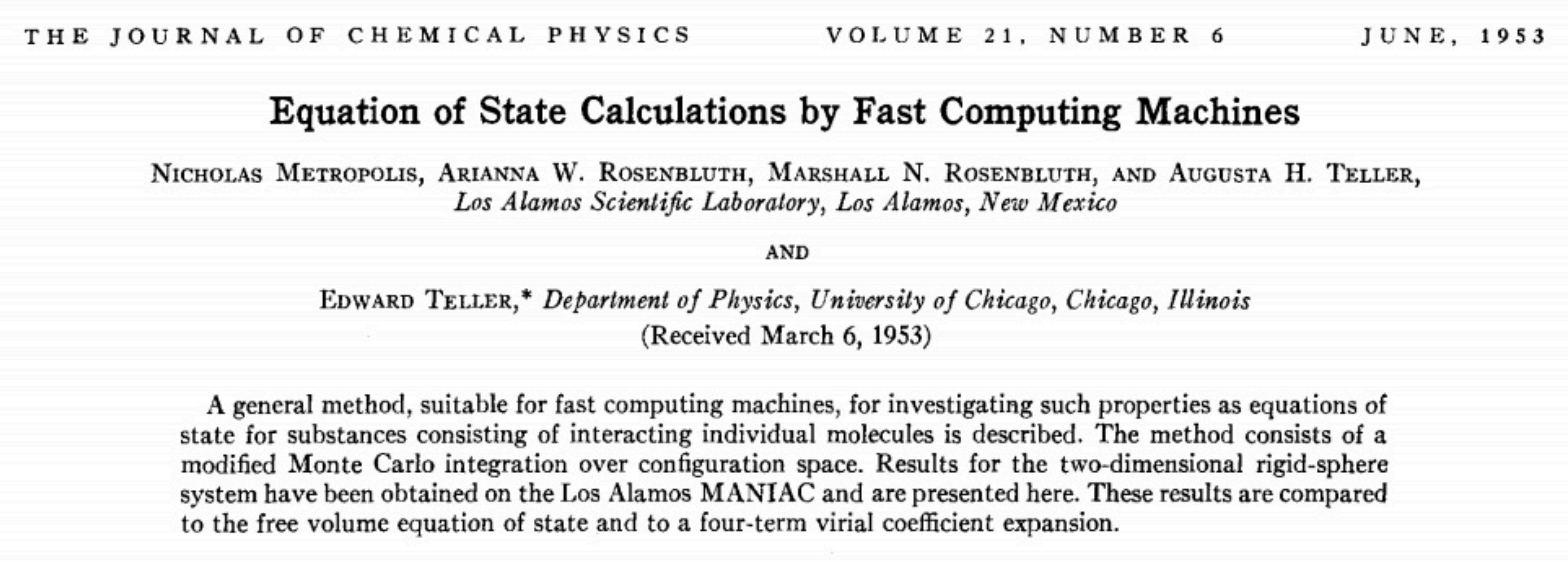




Nicholas Metropolis and his
Mathematical Analyzer Numerical Integrator And Calculator







THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

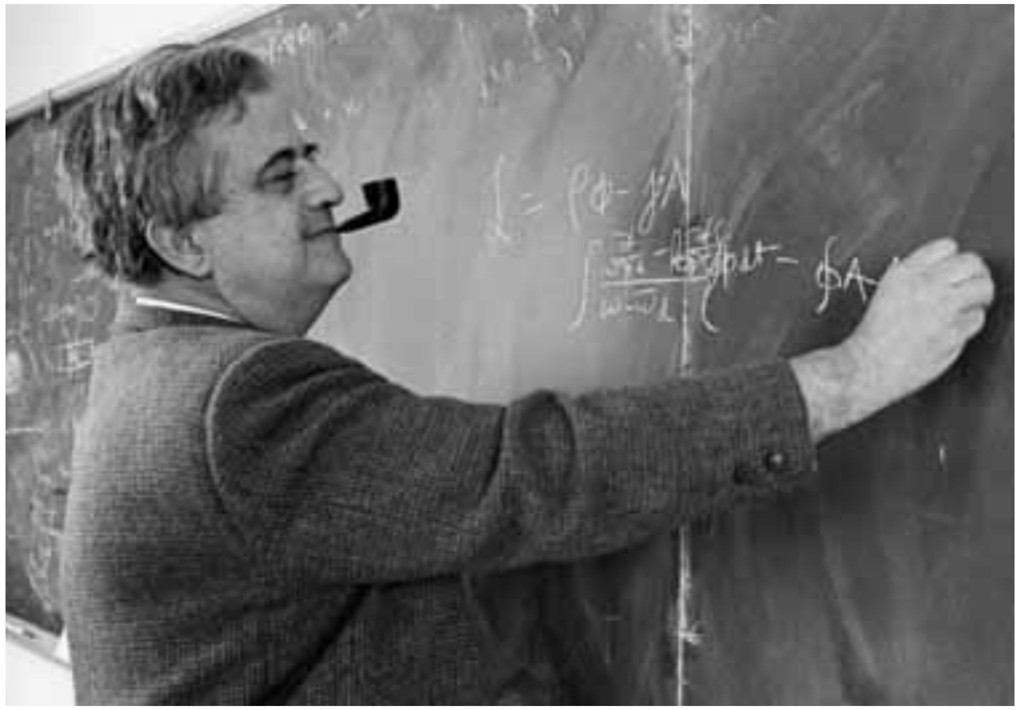
NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

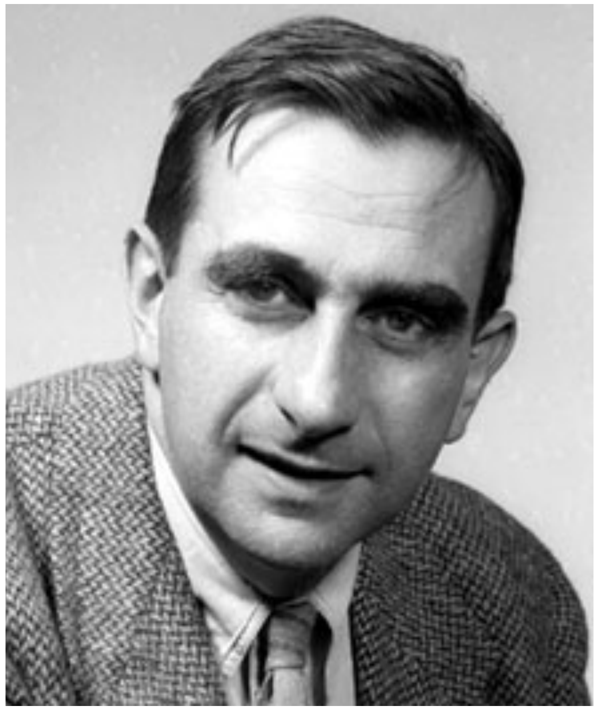
AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

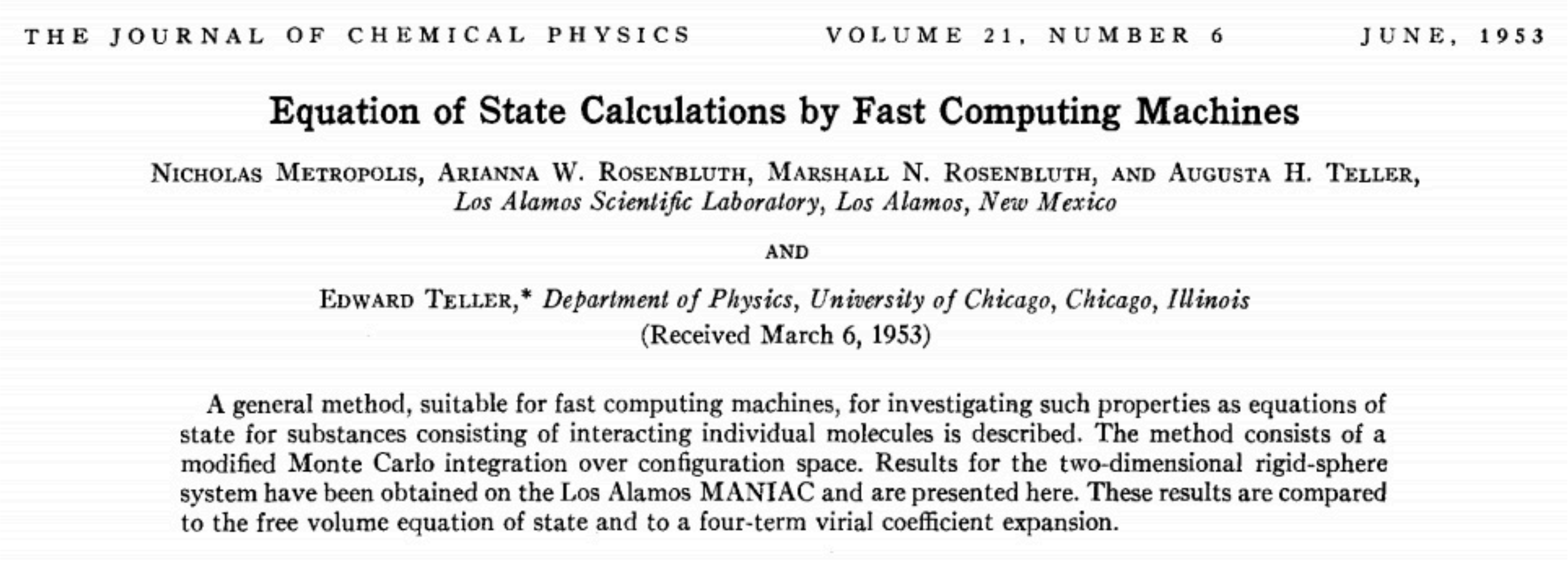
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.





Marshall Rosenbluth and Edward Teller



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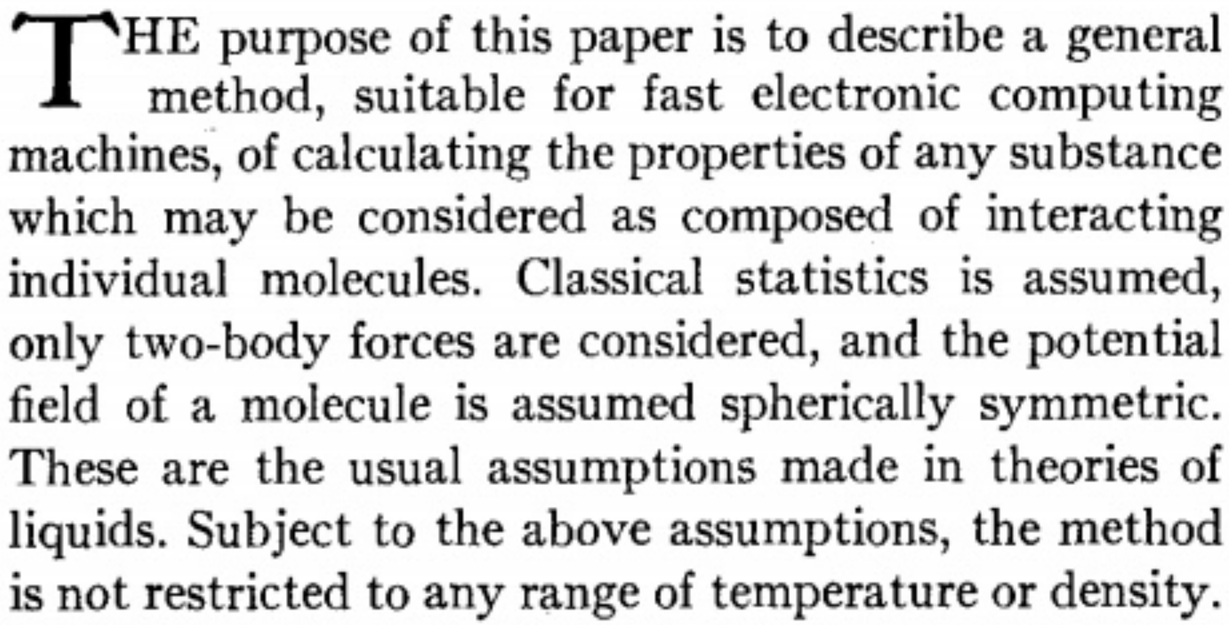


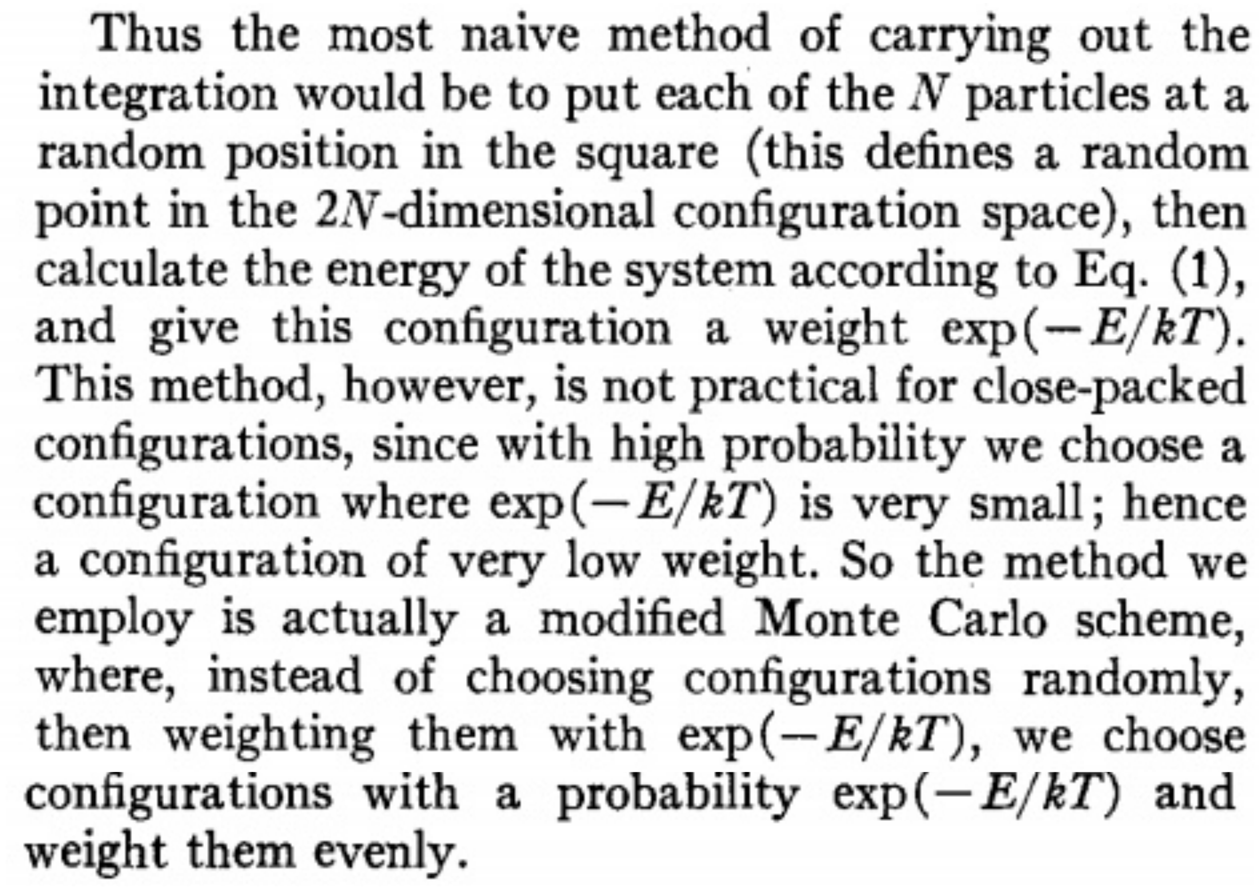
THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed, only two-body forces are considered, and the potential field of a molecule is assumed spherically symmetric. These are the usual assumptions made in theories of liquids. Subject to the above assumptions, the method is not restricted to any range of temperature or density.

Teller’s crucial suggestion: ensemble averaging...

$$\int \phi(x)p(x)dx, \quad \text{with} \quad p(x) \simeq e^{-E(x)/kT}$$

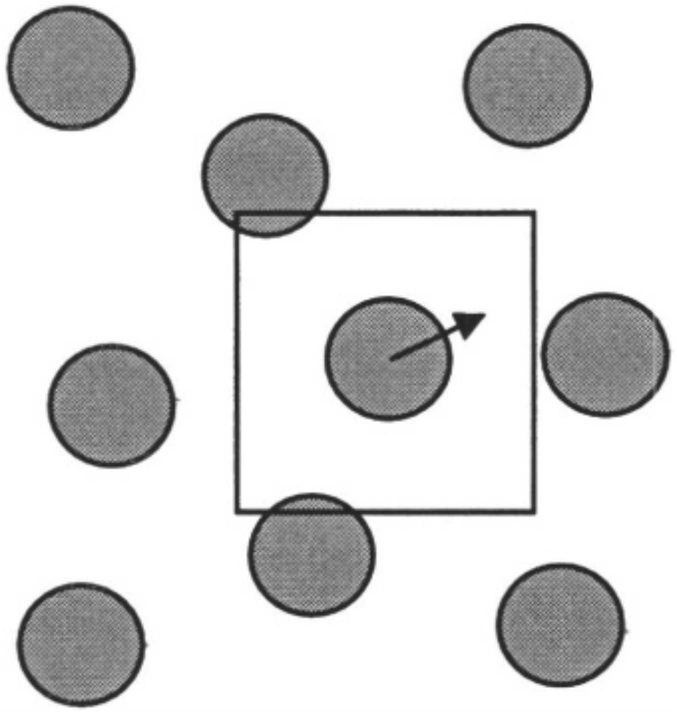
$$\Downarrow$$

$$\int \phi(x)dp(x) \simeq \frac{1}{R}\sum_R \phi(x^{(r)}) \quad \text{with} \quad \{x^{(r)}\}_P$$

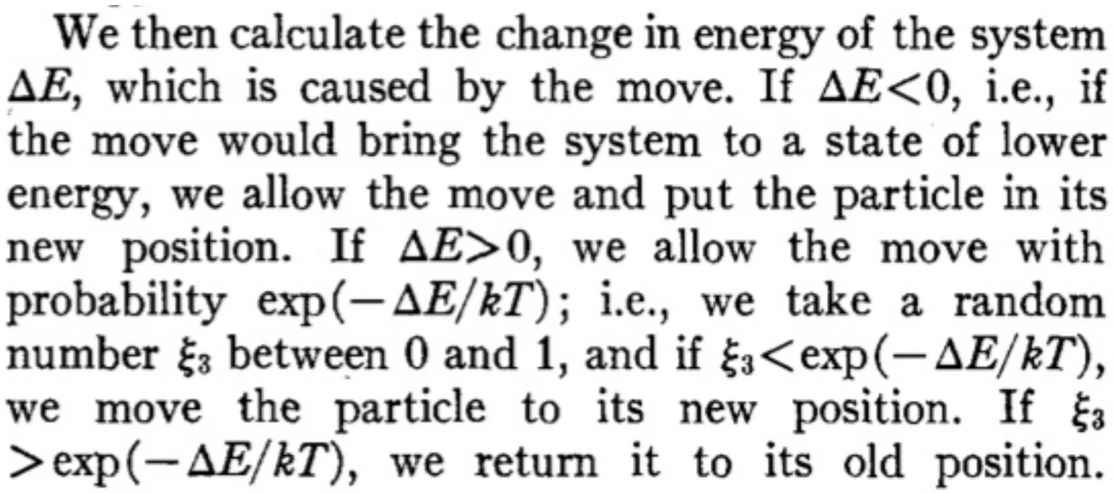


Thus the most naive method of carrying out the integration would be to put each of the N particles at a random position in the square (this defines a random point in the $2N$-dimensional configuration space), then calculate the energy of the system according to Eq. (1), and give this configuration a weight $\exp(-E/kT)$. This method, however, is not practical for close-packed configurations, since with high probability we choose a configuration where $\exp(-E/kT)$ is very small; hence a configuration of very low weight. So the method we employ is actually a modified Monte Carlo scheme, where, instead of choosing configurations randomly, then weighting them with $\exp(-E/kT)$, we choose configurations with a probability $\exp(-E/kT)$ and weight them evenly.

...with samples generated by the “Metropolis” algorithm

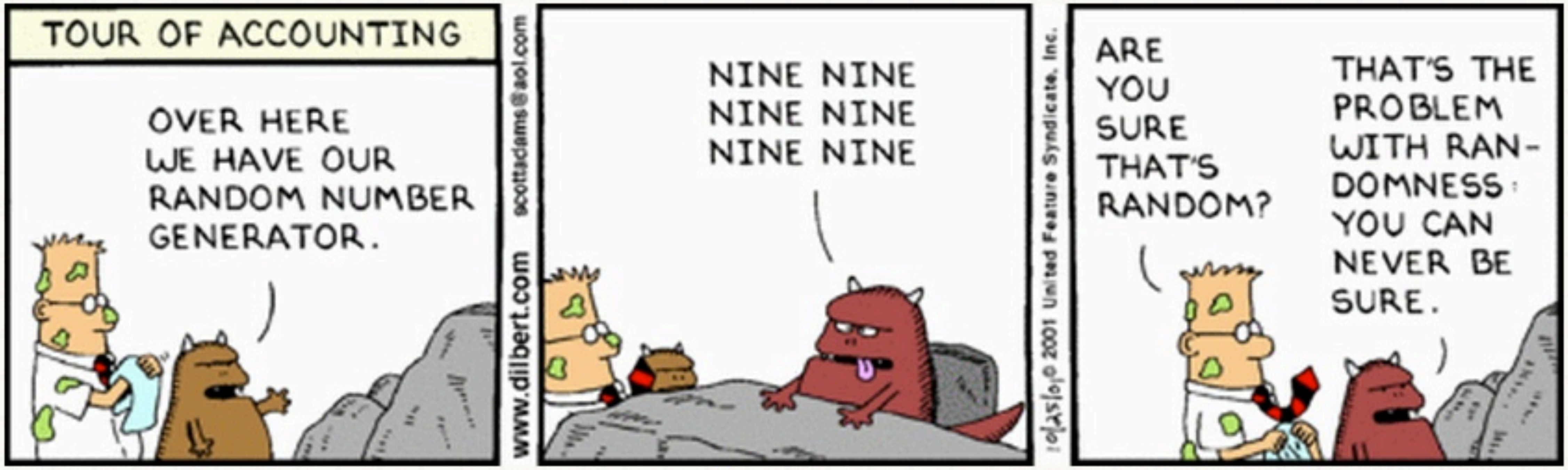


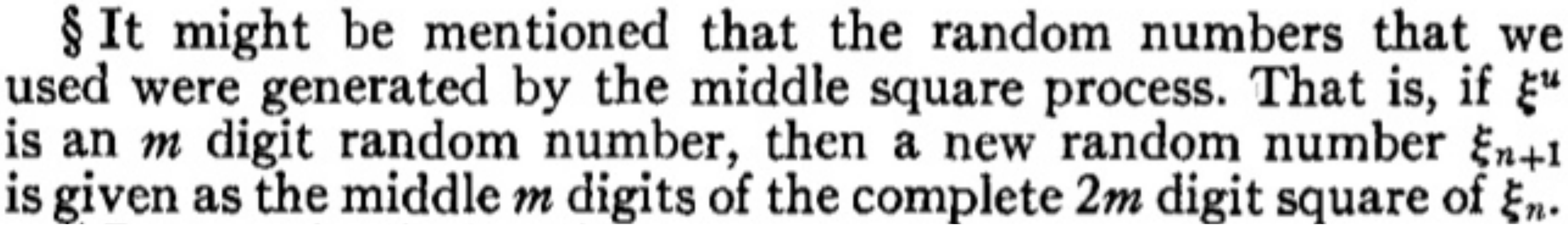
- given $x^{(r)}$, propose $x^{(r+1)}$ by random walk
- accept it if $\Delta E = E(x^{(r+1)}) - E(x^{(r)}) < 0$, or with probability $e^{-\Delta E/kT}$ if $\Delta E > 0$
- if not accepted, set $x^{(r+1)} = x^{(r)}$
- the resulting detailed balance guarantees convergence to P



We then calculate the change in energy of the system ΔE, which is caused by the move. If $\Delta E<0$, i.e., if the move would bring the system to a state of lower energy, we allow the move and put the particle in its new position. If $\Delta E>0$, we allow the move with probability $\exp(-\Delta E/kT)$; i.e., we take a random number ξ_3 between 0 and 1, and if $\xi_3<\exp(-\Delta E/kT)$, we move the particle to its new position. If $\xi_3 >\exp(-\Delta E/kT)$, we return it to its old position.

§ It might be mentioned that the random numbers that we used were generated by the middle square process. That is, if ξ^u is an m digit random number, then a new random number ξ_{n+1} is given as the middle m digits of the complete $2m$ digit square of ξ_n.


TOUR OF ACCOUNTING
OVER HERE WE HAVE OUR RANDOM NUMBER GENERATOR.
scottadams@aol.com
www.dilbert.com
NINE NINE NINE NINE NINE NINE
10/25/01 © 2001 United Feature Syndicate, Inc.
ARE YOU SURE THAT'S RANDOM?
THAT'S THE PROBLEM WITH RANDOMNESS: YOU CAN NEVER BE SURE.



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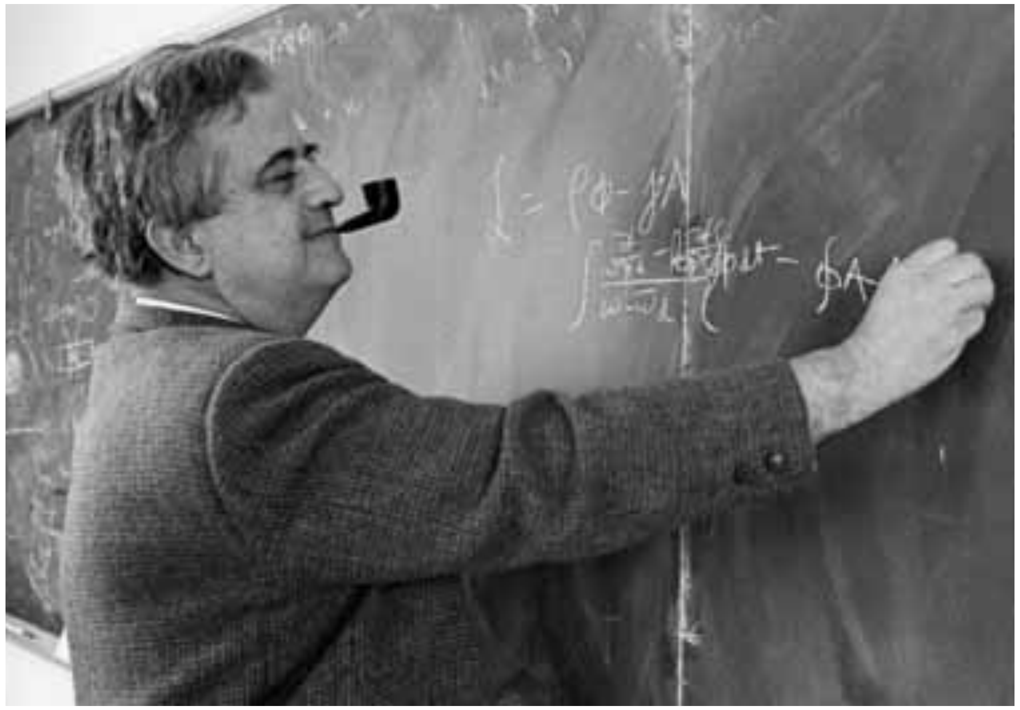

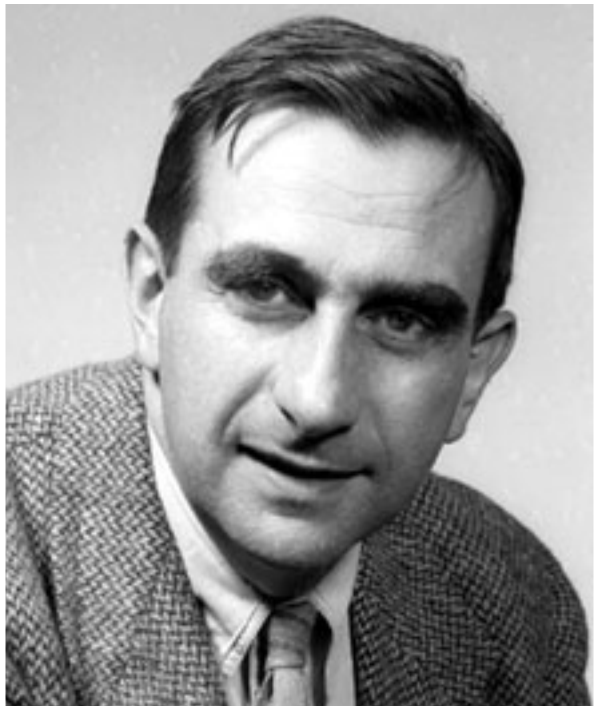

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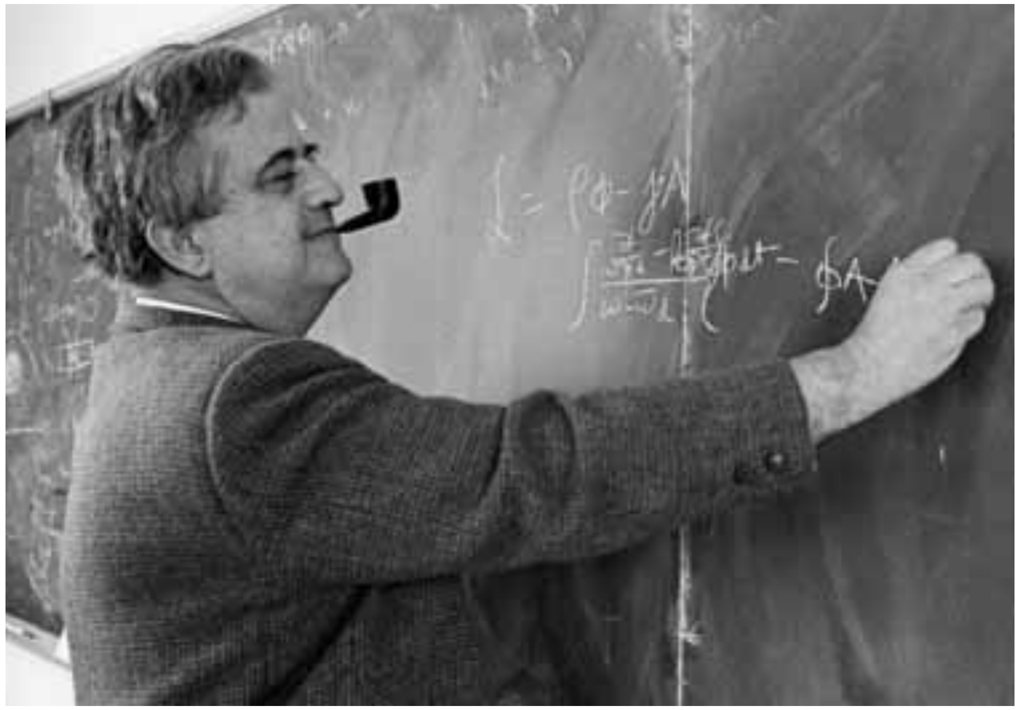

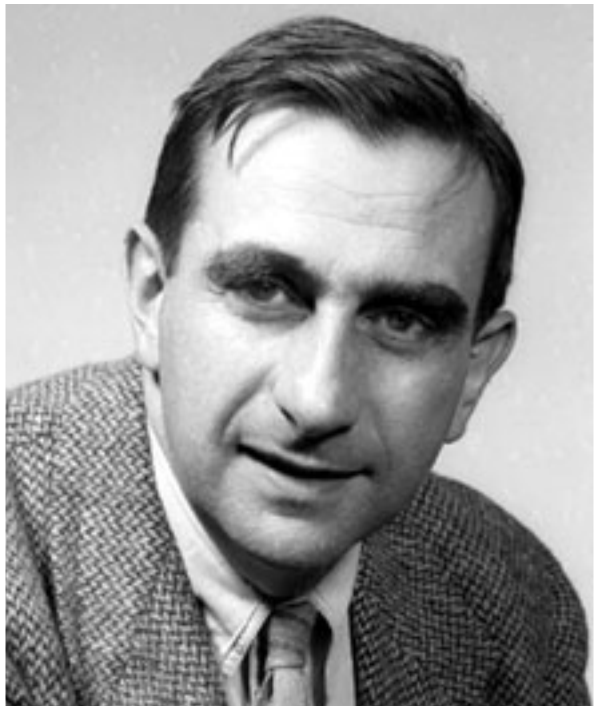

the rest is history

- (Metropolis–Hastings) algorithm for any *P:*
- given $x^{(r)}$, propose $x^{(r+1)}$ by $Q(x^{\text{next}};x^{\text{prev}})$
- accept it if
  $r = [P(x^{(r+1)})/P(x^{(r)})]\cdot[Q(x^{(r)};x^{(r+1)})/Q(x^{(r+1)};x^{(r)})] > 1$,
  or with probability r if $r < 1$
- if not accepted, set $x^{(r+1)} = x^{(r)}$

but why does it work?

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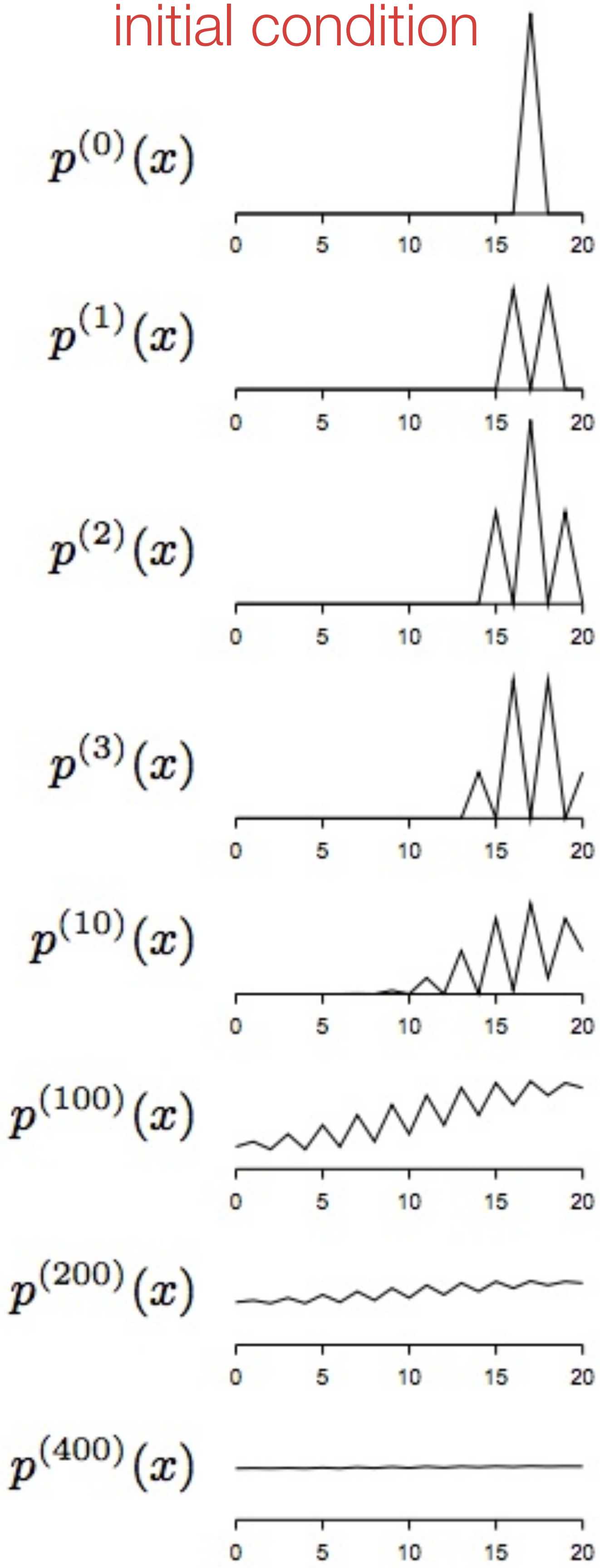
initial condition



equilibrium distribution

(MacKay 2003)

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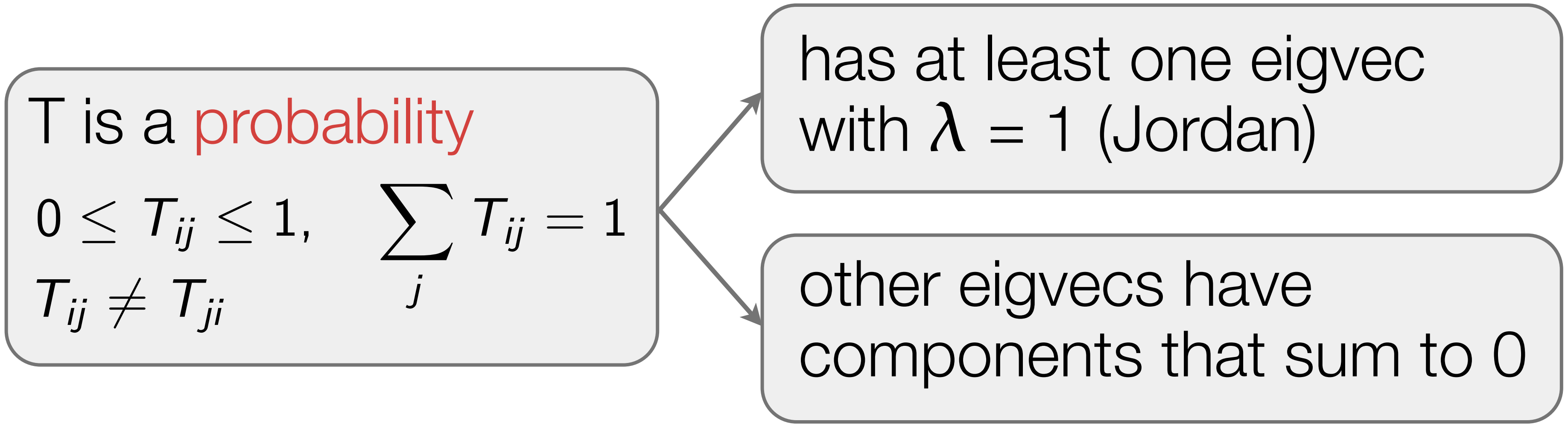

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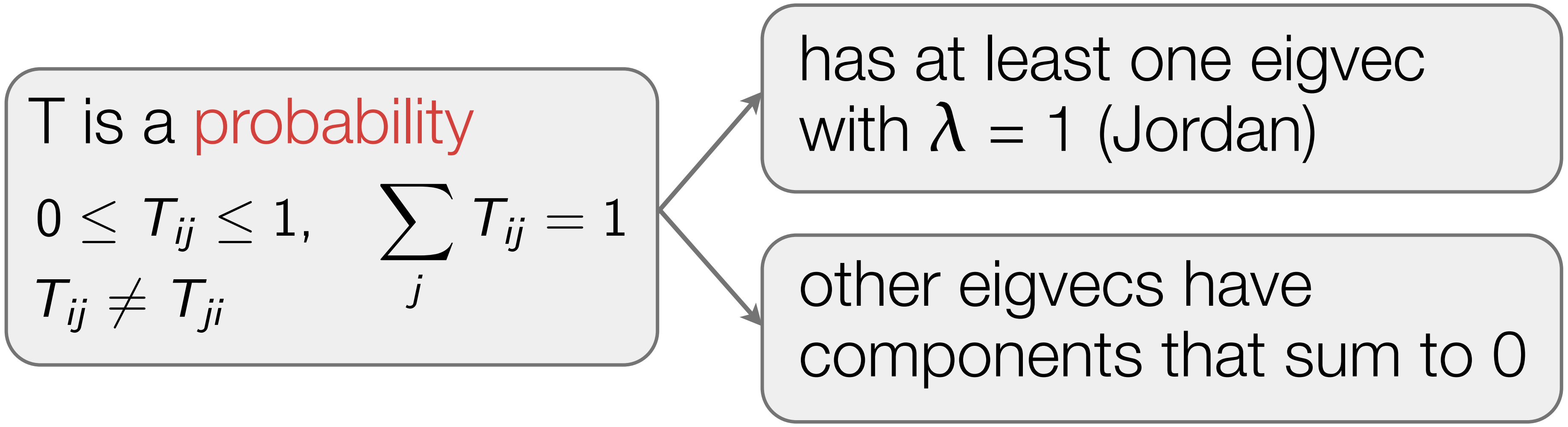

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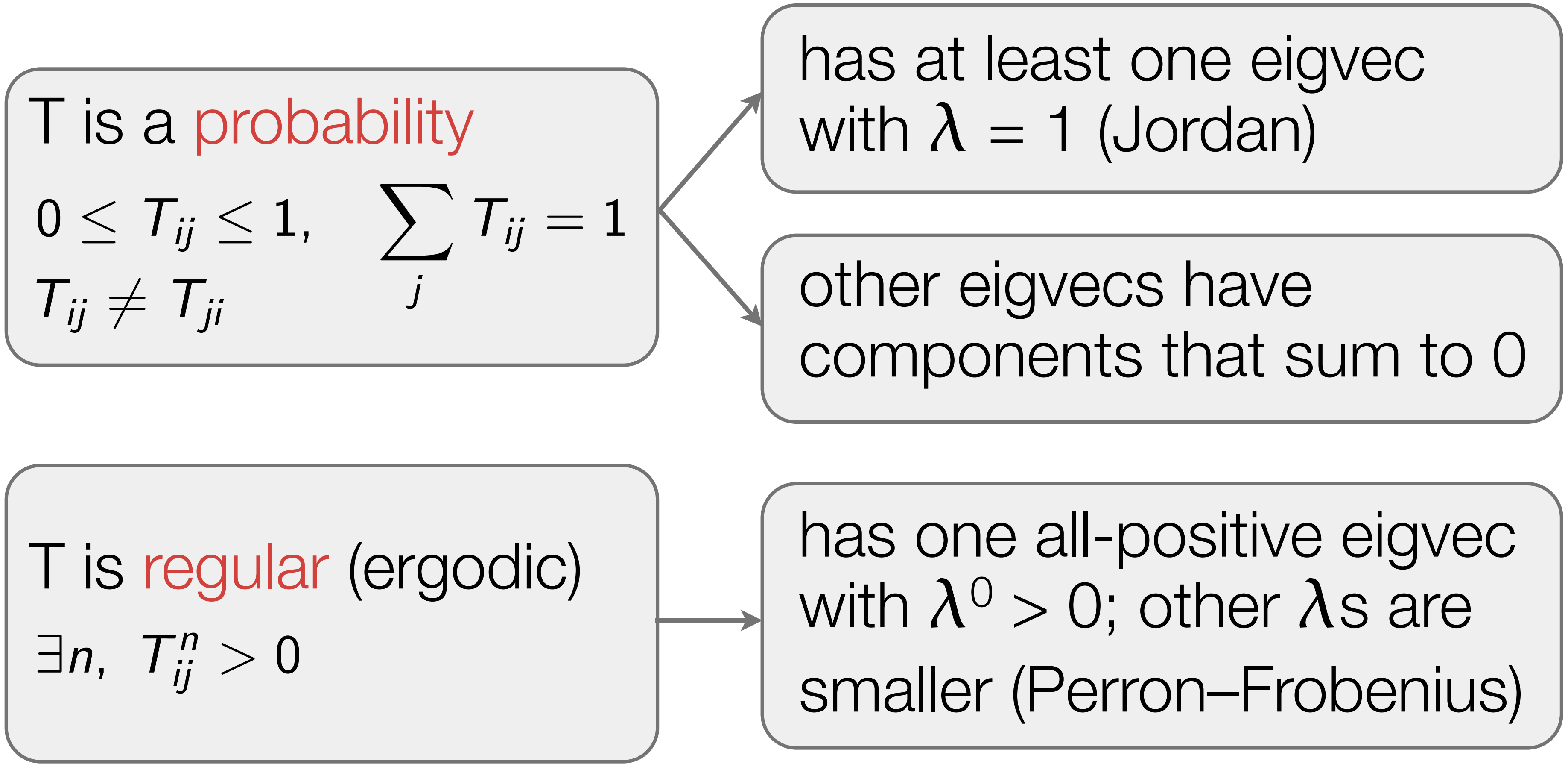

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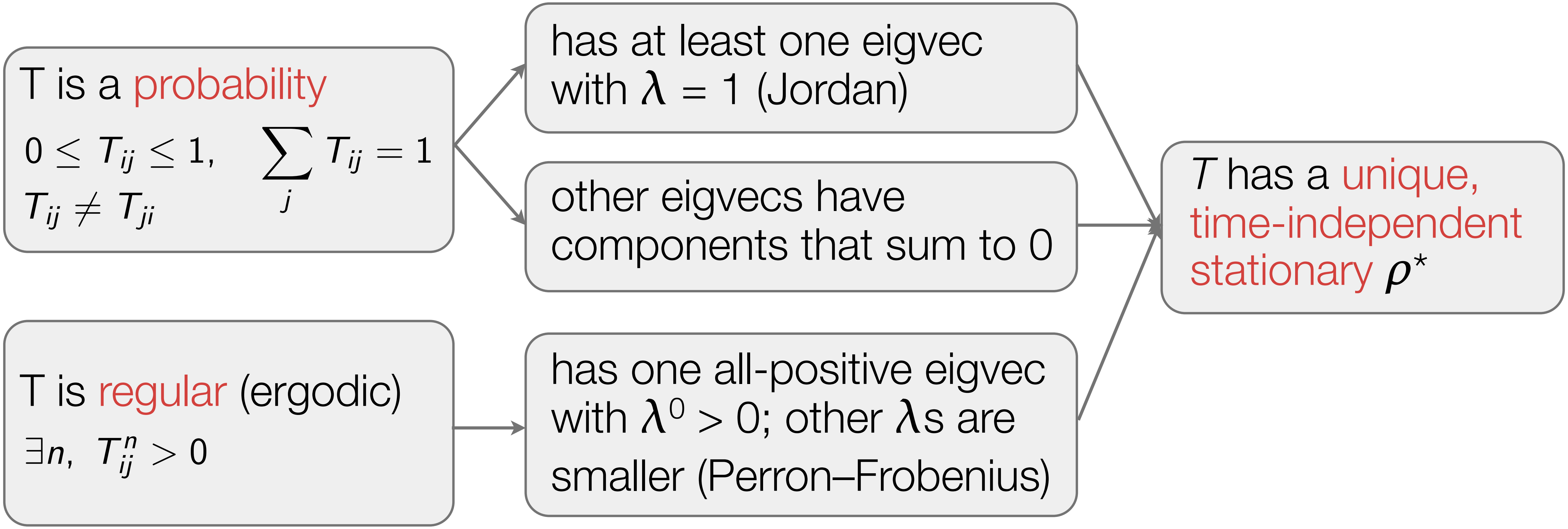

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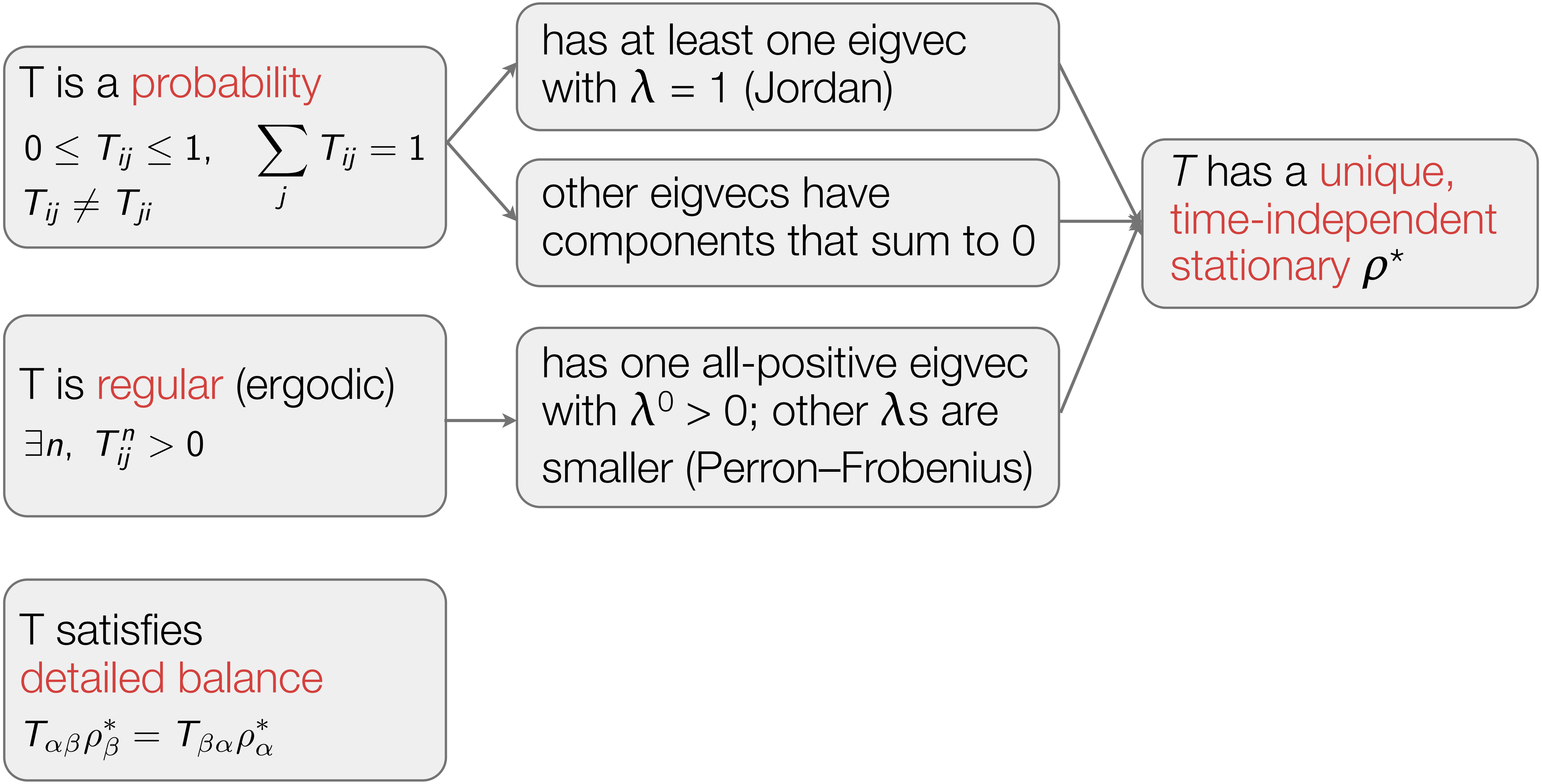

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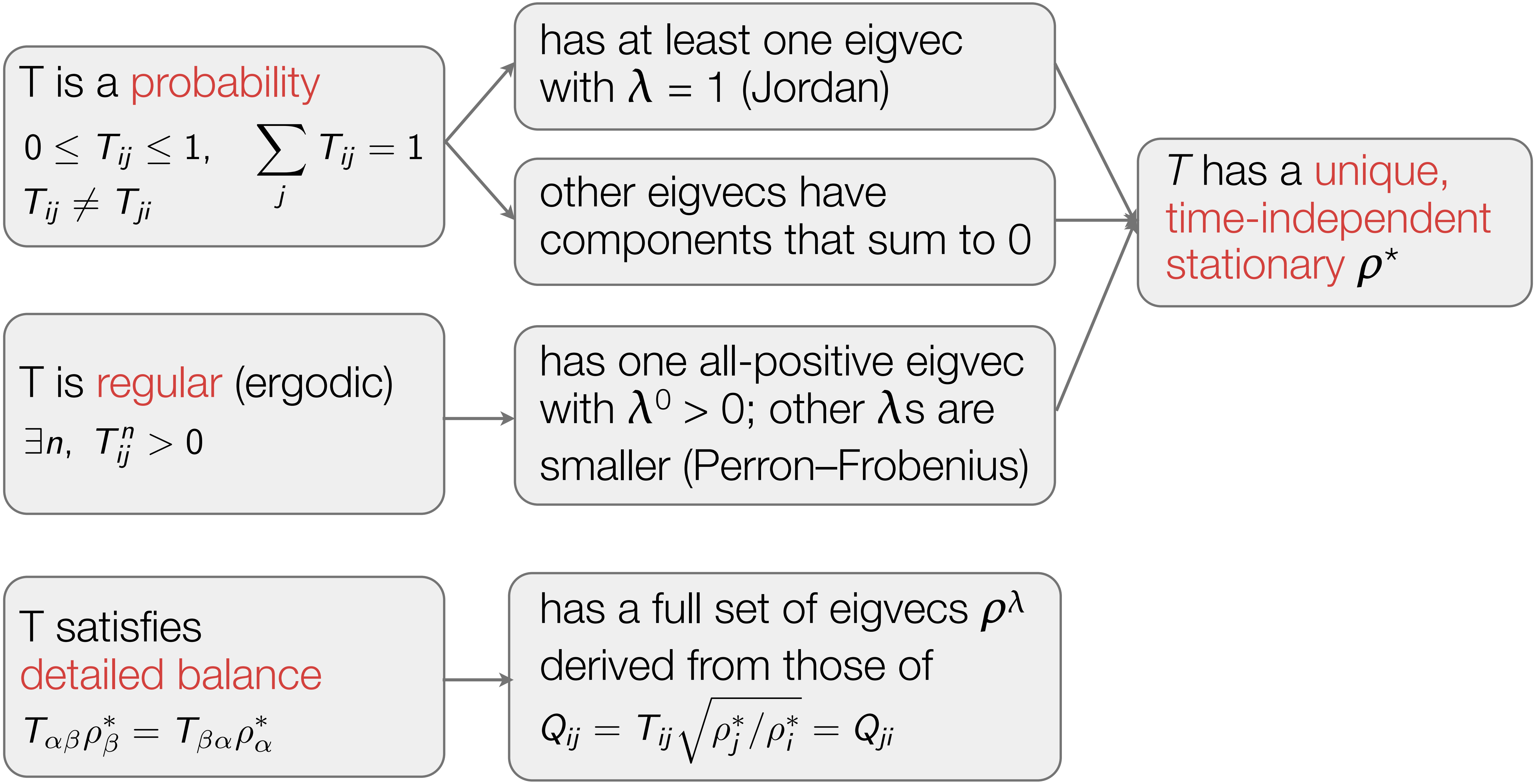

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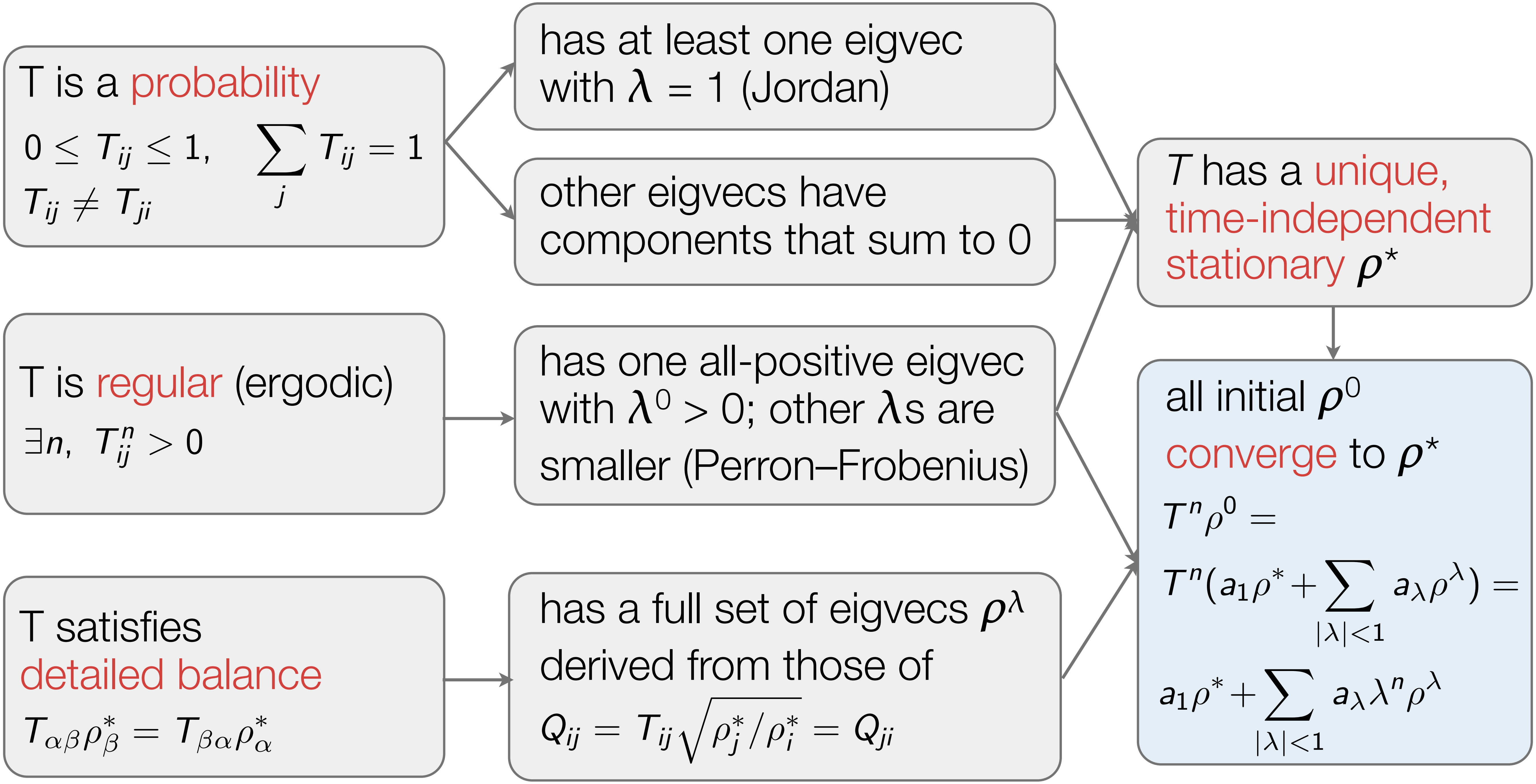

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$$T^n(a_1\rho^* + \sum_{|\lambda|<1} a_\lambda \rho^\lambda) =$$

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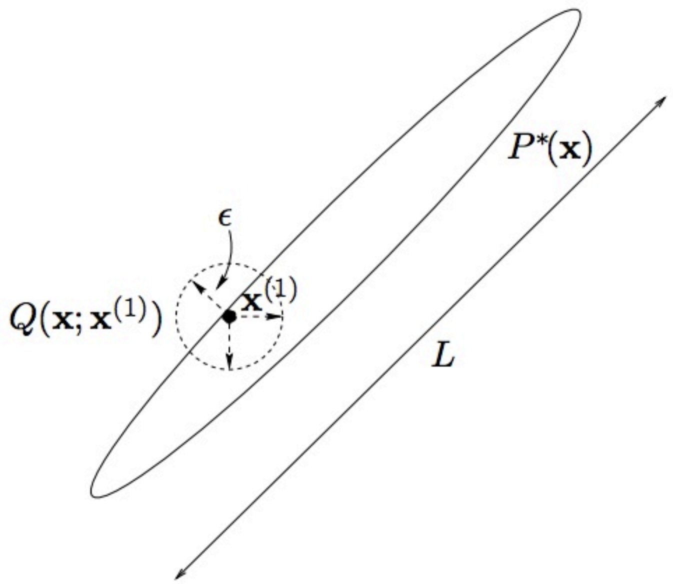

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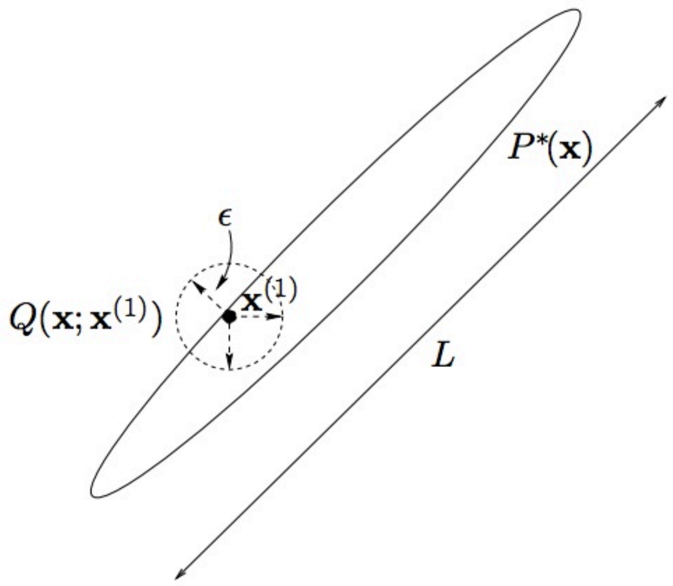

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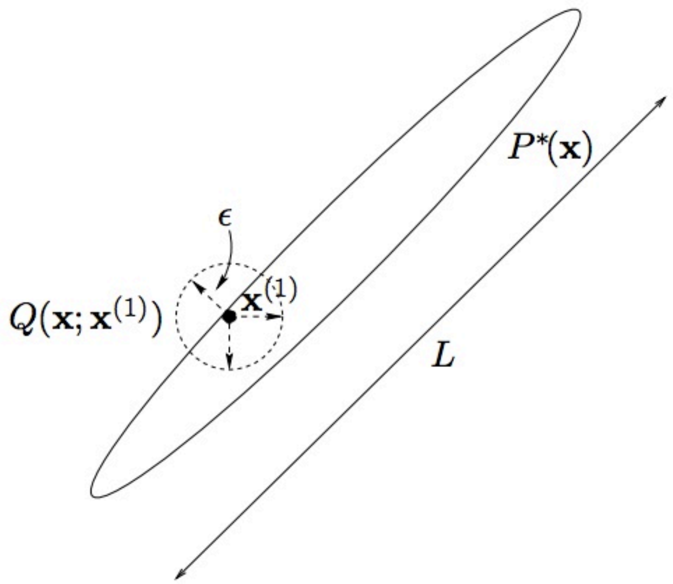

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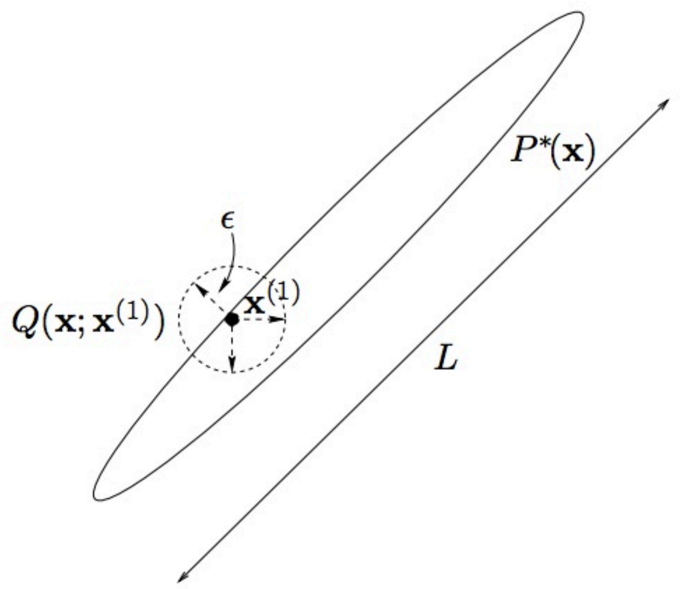

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- thermodynamic integration
- reversible-jump MCMC
- nested sampling

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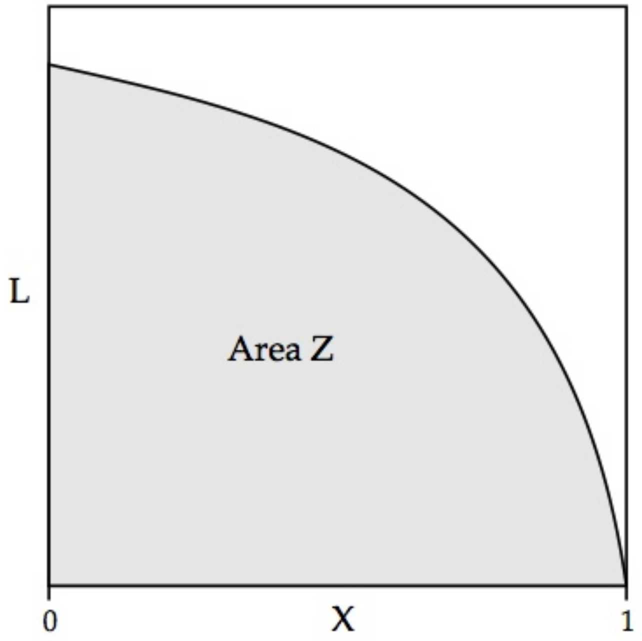

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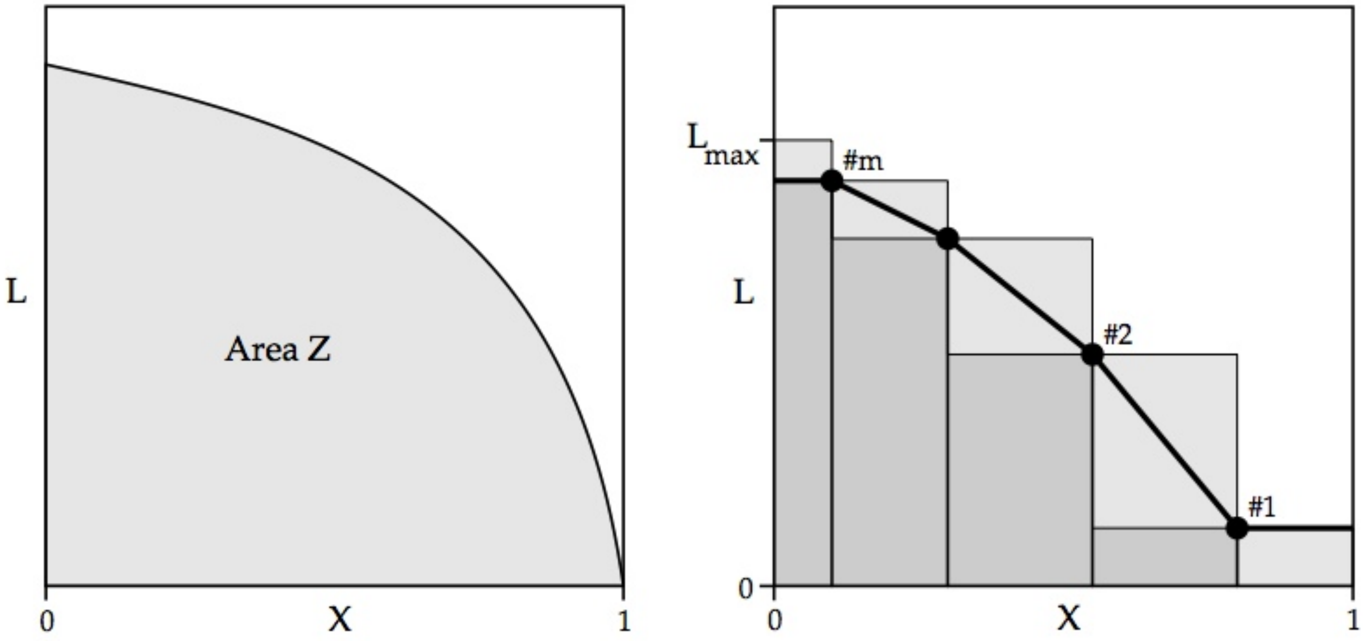

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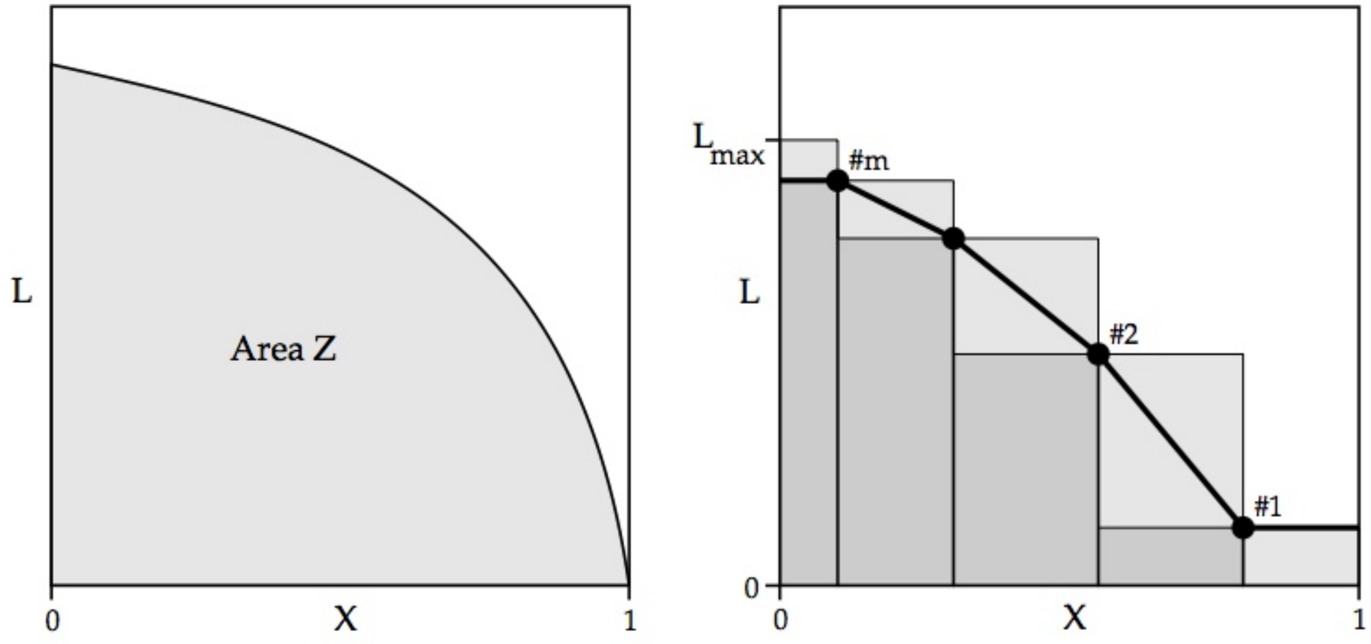

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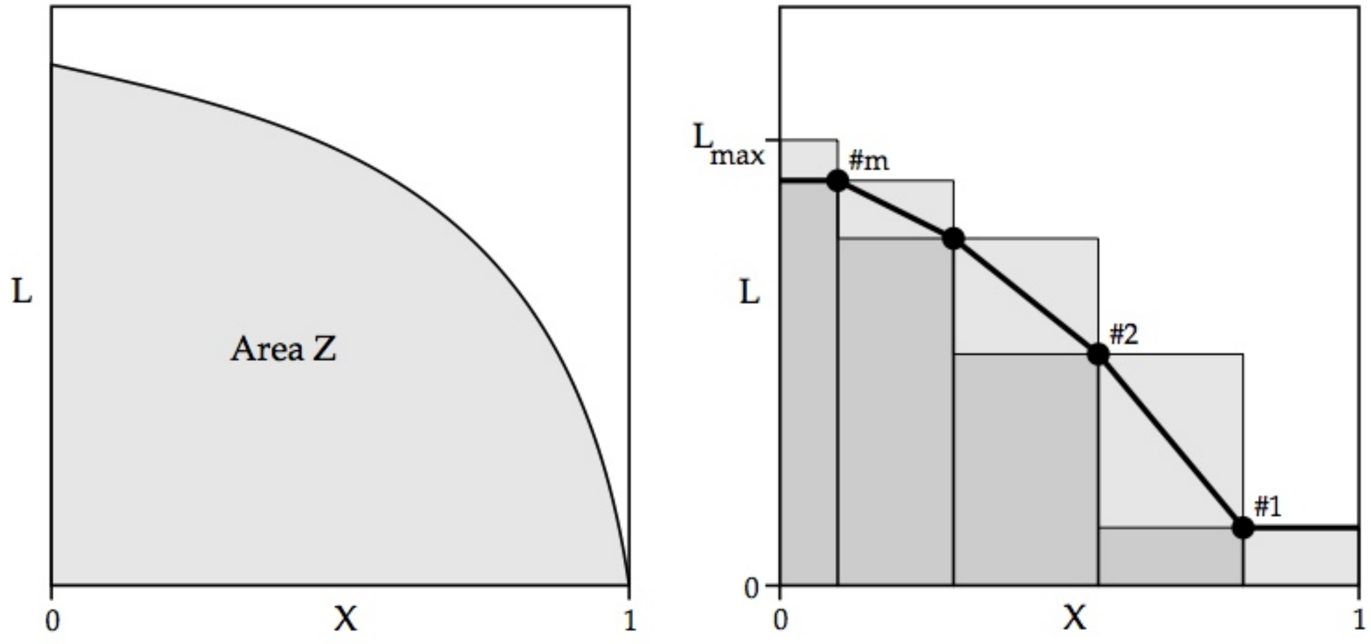

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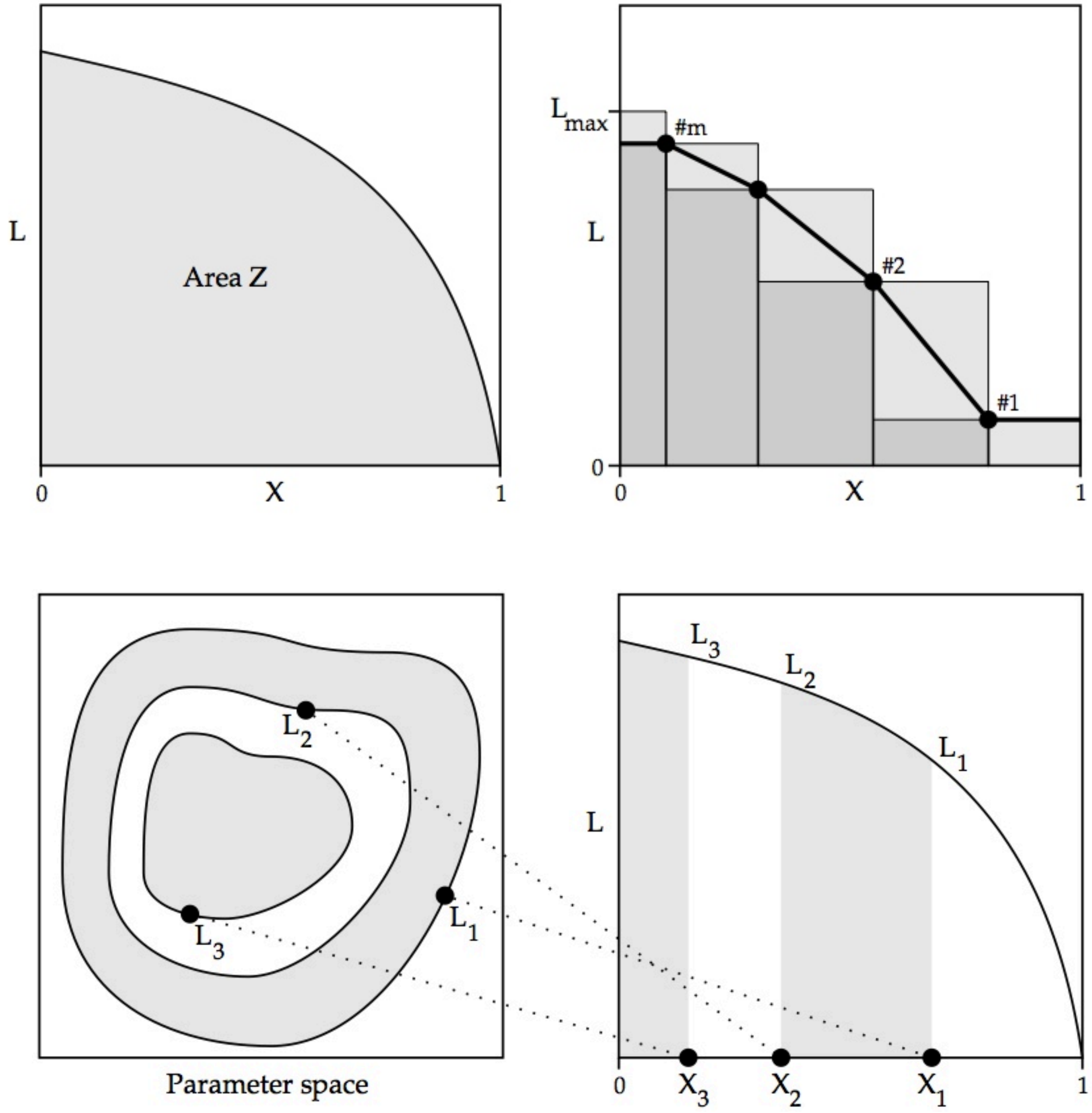

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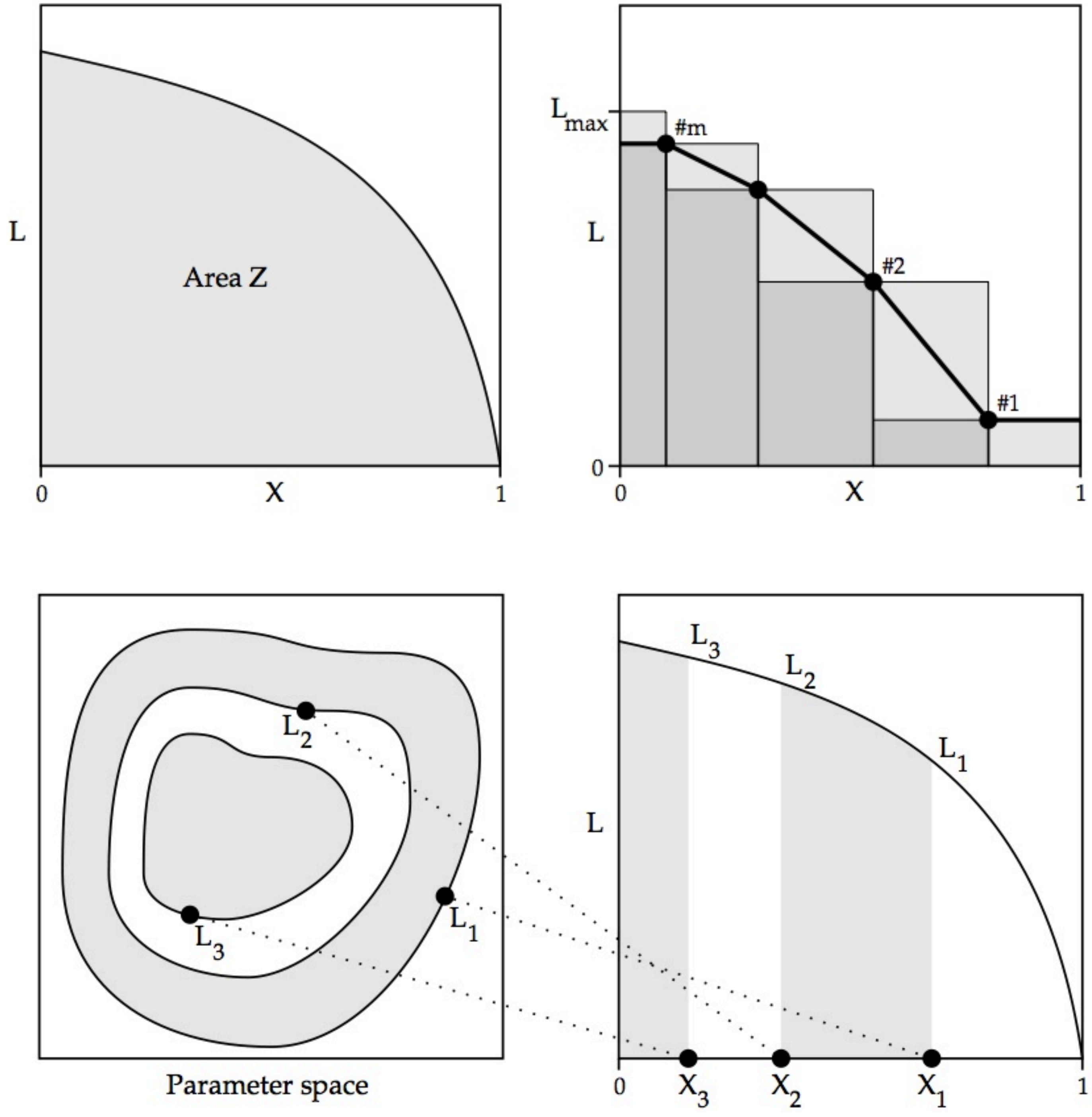

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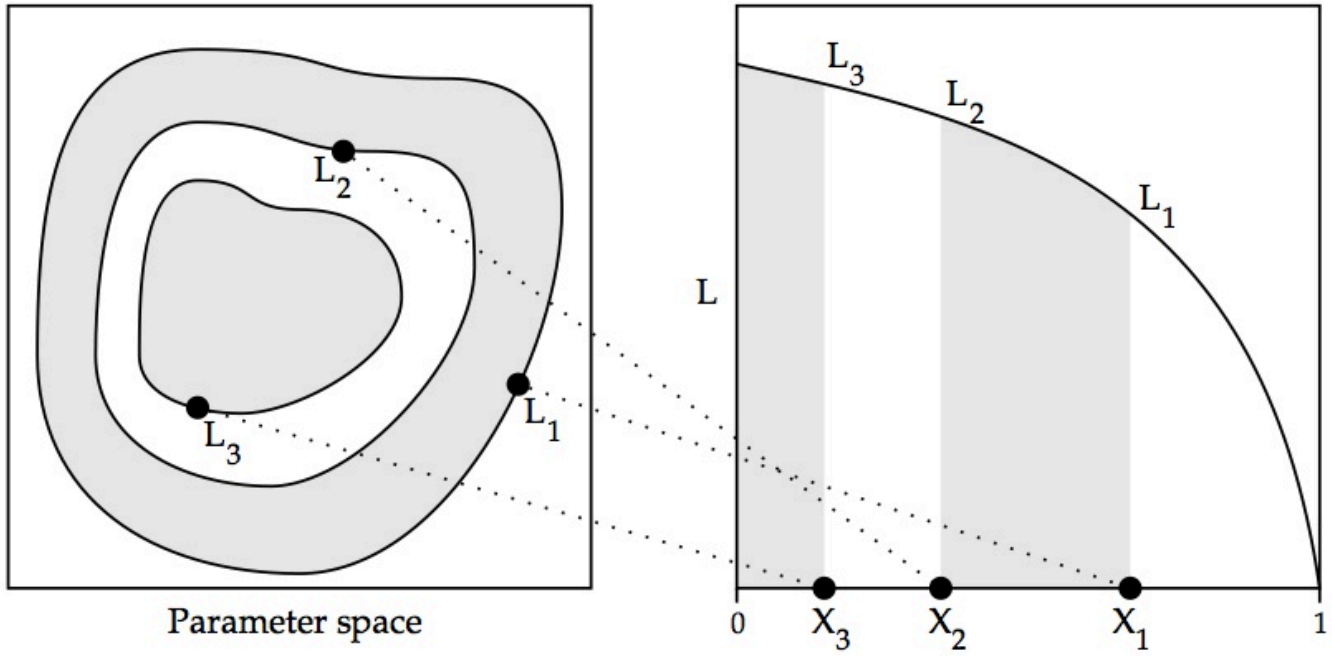

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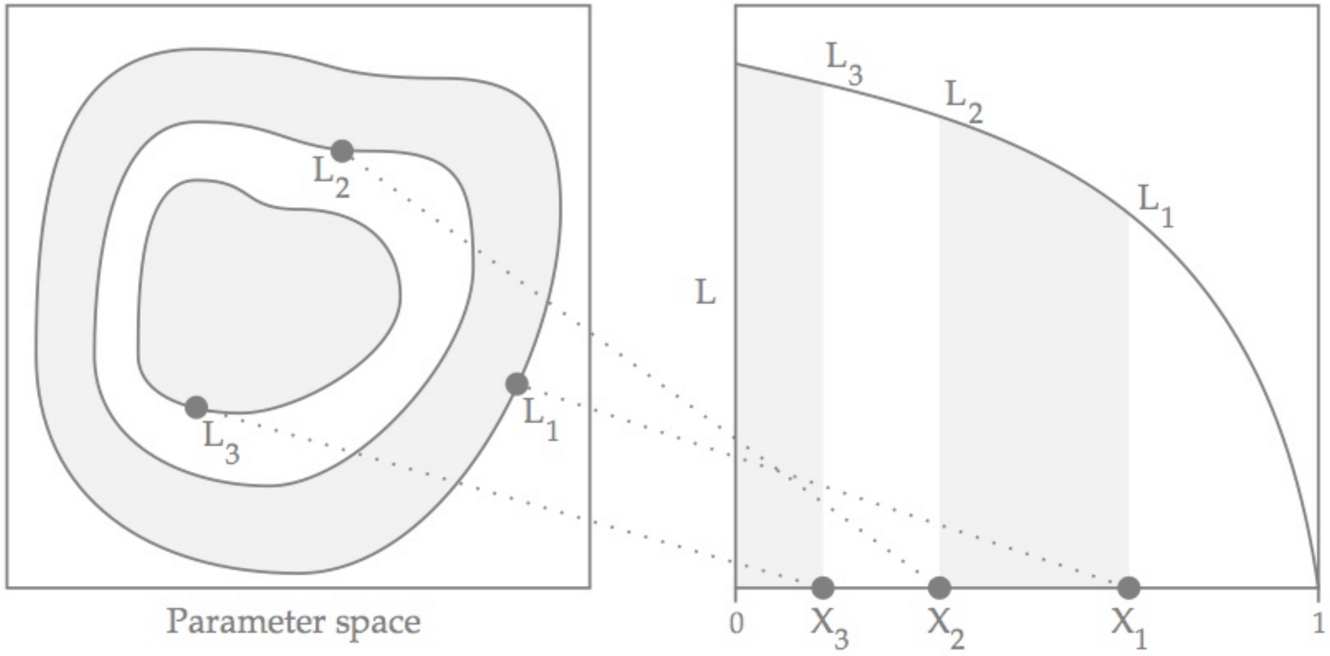

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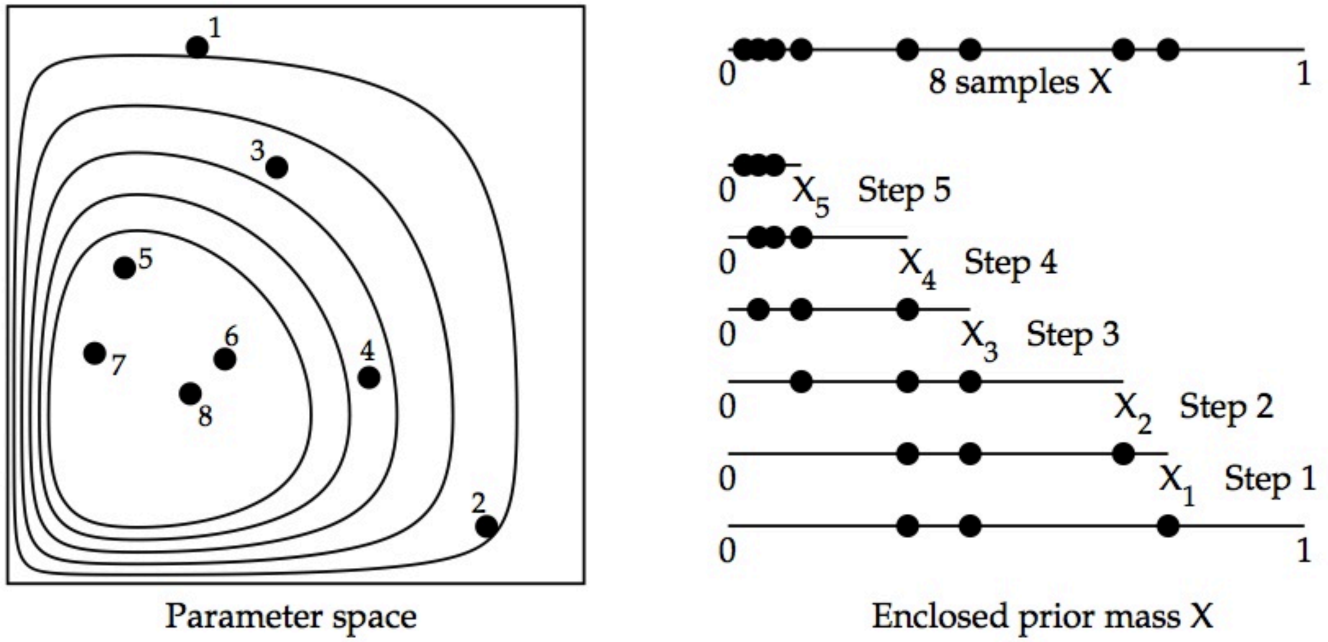

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- $\log X_i \simeq (-i \pm \sqrt{i})/N$

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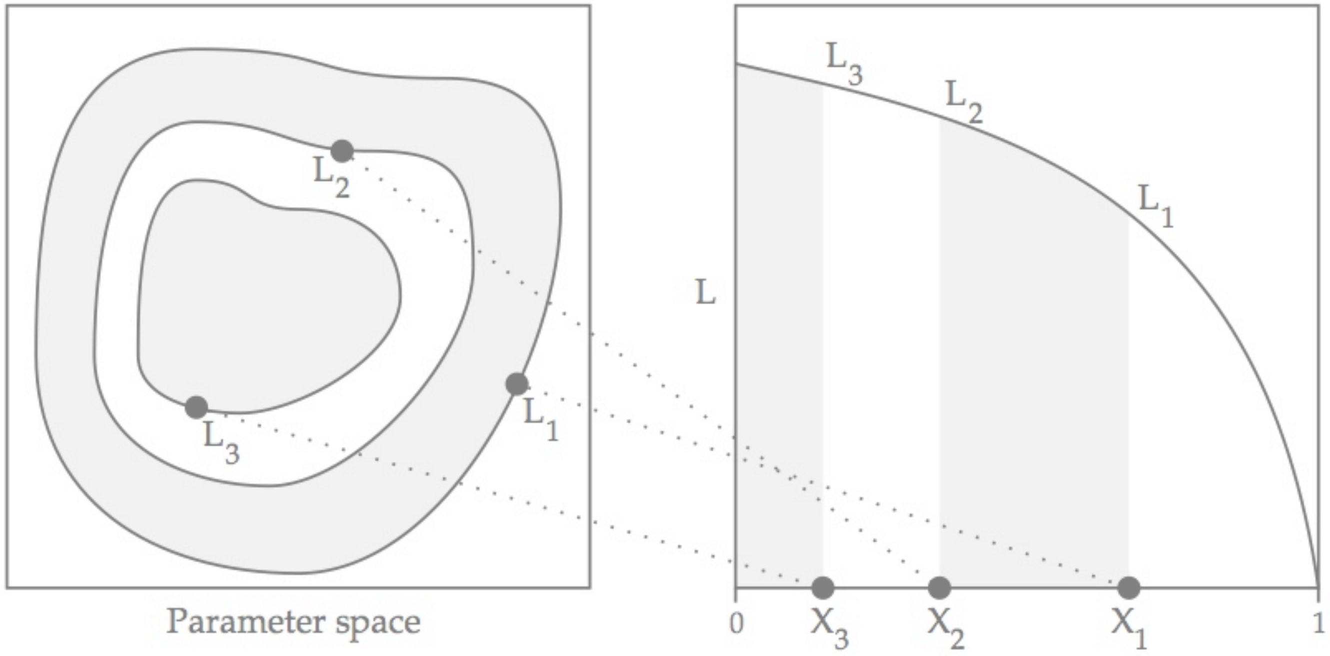

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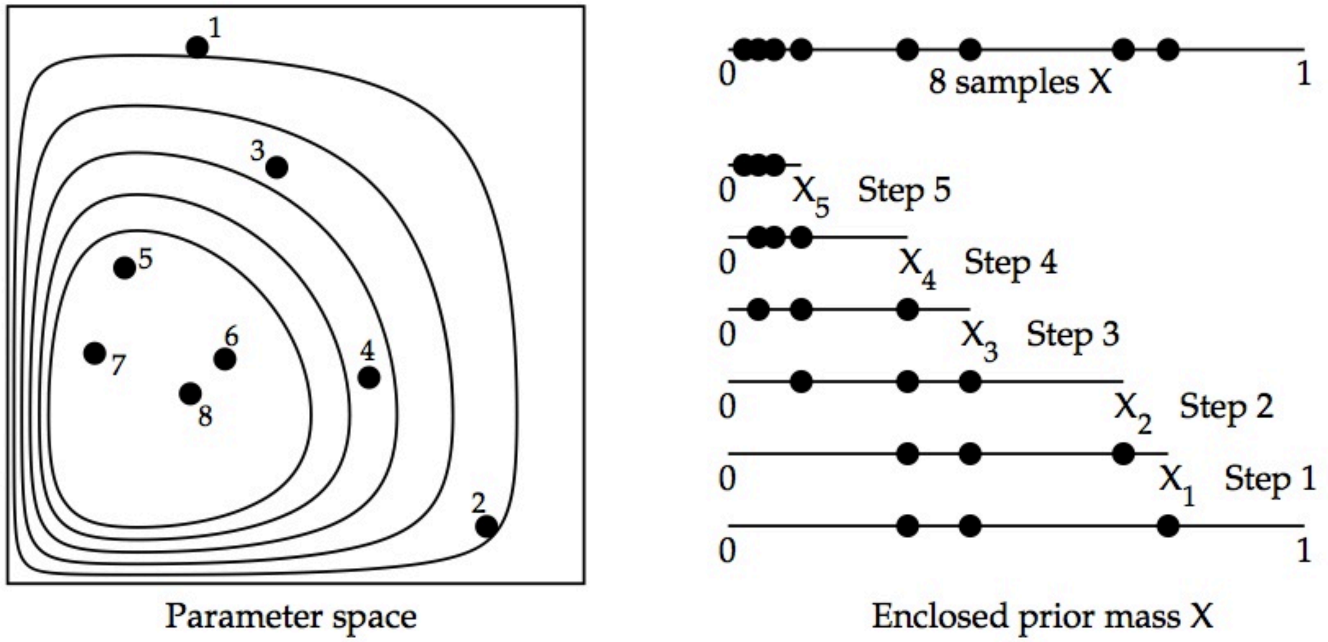

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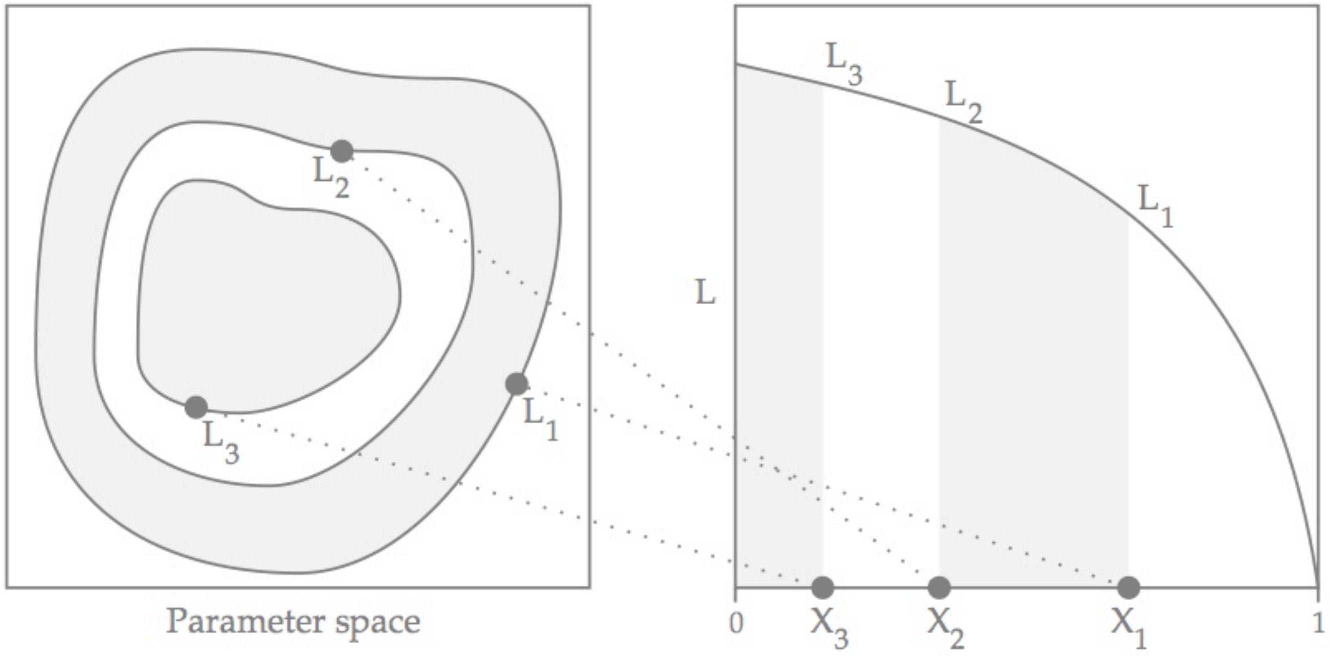

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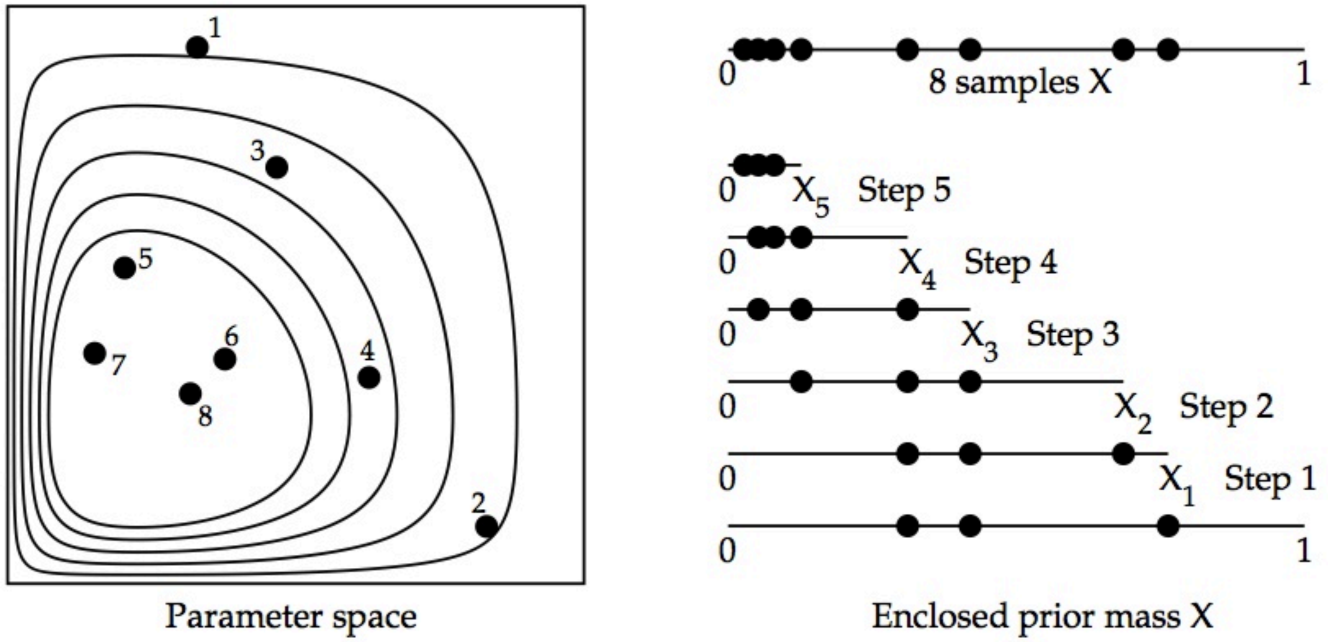
- stop when Z converges



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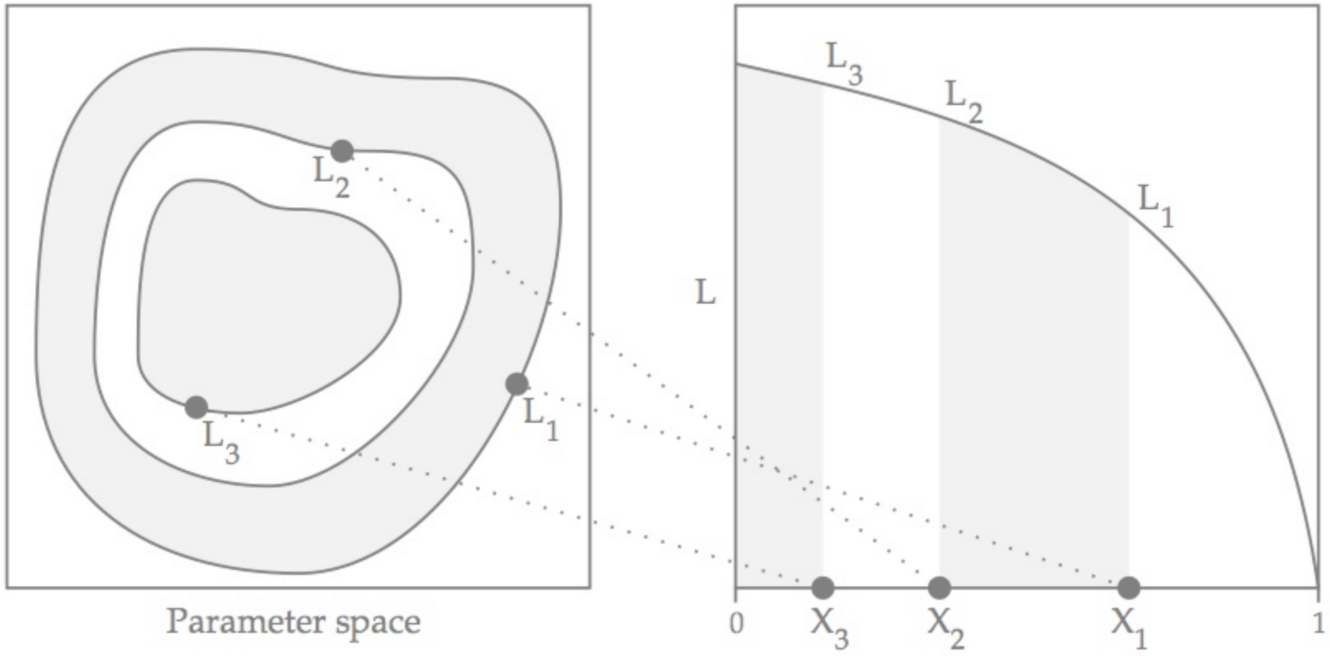
Nested sampling
(Skilling 2006)

see bit.ly/multinest
by Farhan Feroz, Hobson, Bridges

- Z is dominated by a range $-H \pm \sqrt{d}$ in $\log X$, so we explore X linearly in $\log X$
- choose each X_i randomly, subject to $X_i < X_{i-1}$
- in practice, choose θ from $\pi(\theta)$, subject to $L(\theta_i) > L(\theta_{i-1})$

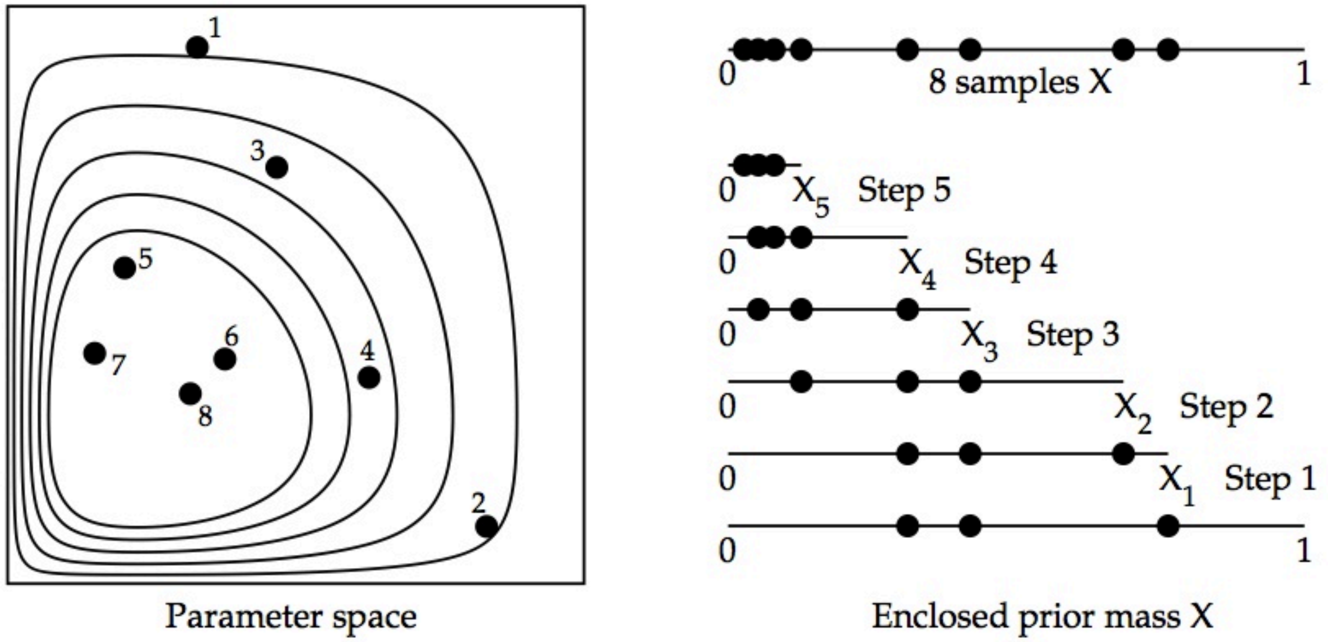


$$X_0 = 1, \quad X_i = t_i X_{i-1}, \quad t_i \in [0,1]$$

- working with a cloud of N live points, keep replacing the least-L member, use it as X_i
- $\log X_i \simeq (-i \pm \sqrt{i})/N$

$$Z = \sum_i w_i L_i, \;\; w_i = \frac{X_{i-1} - X_{i+1}}{2}$$

- stop when Z converges



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Affine–invariant sampling

(Goodman–Weare 2010)

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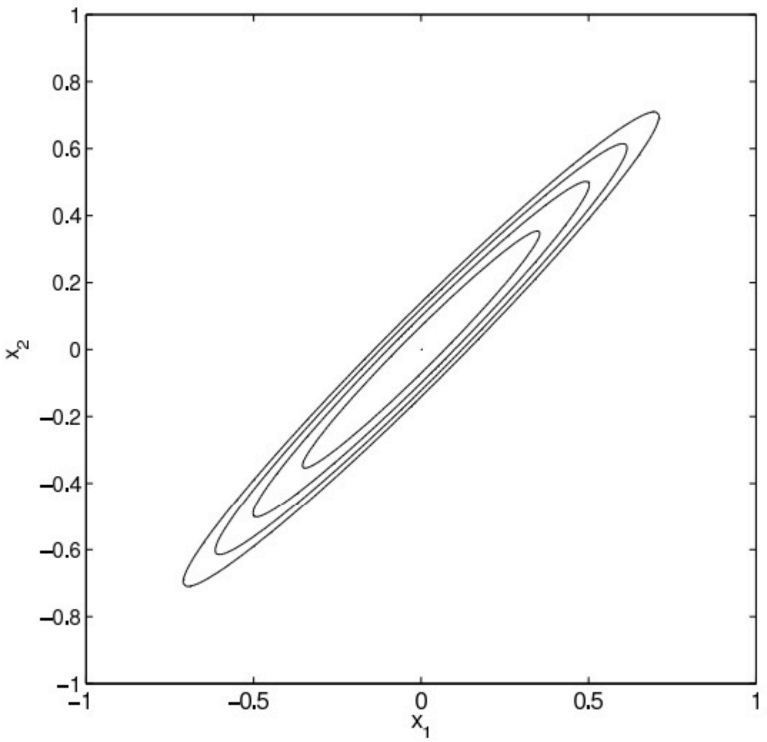

$$\pi(x) \propto \exp\left(\frac{-(x_1 - x_2)^2}{2\epsilon} - \frac{(x_1 + x_2)^2}{2}\right)$$

hard to sample!

Affine–invariant sampling

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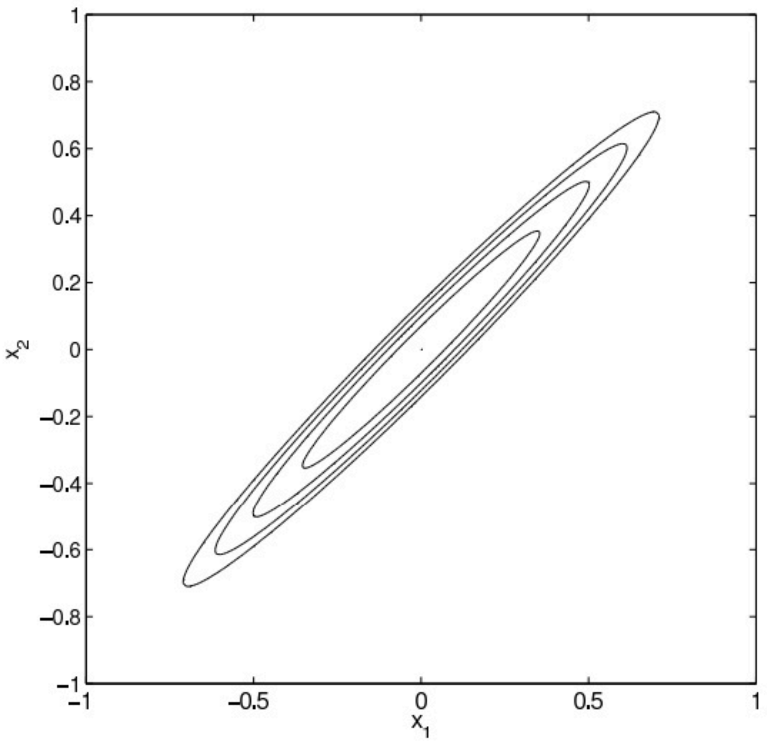

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$$y_1 = \frac{x_1 - x_2}{\sqrt{\epsilon}}, \qquad y_2 = x_1 + x_2$$

$$\pi_A(y) \propto \exp\left(-\frac{(y_1 + y_2)^2}{2}\right)$$

much better!

Affine–invariant sampling
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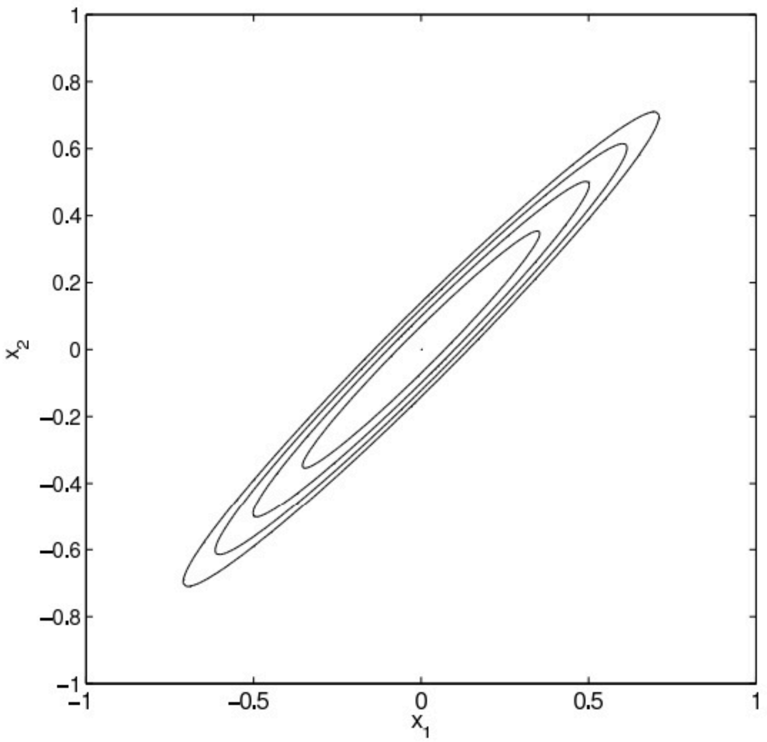

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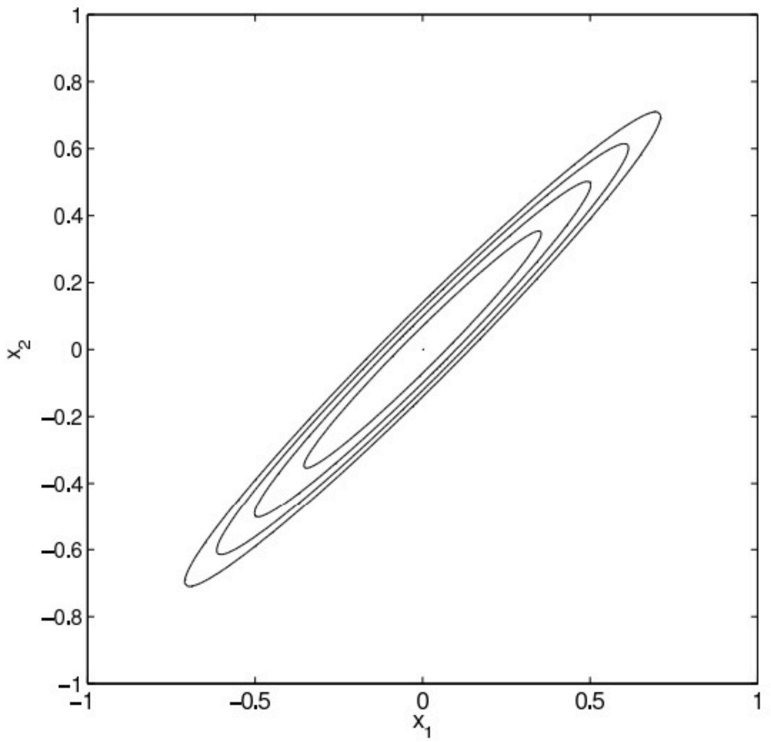

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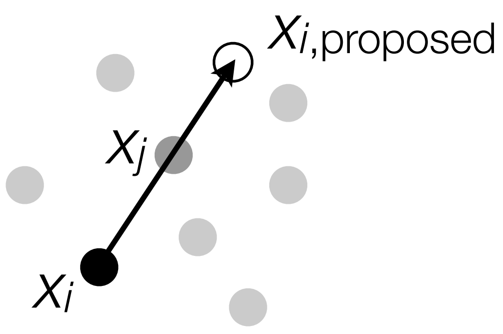
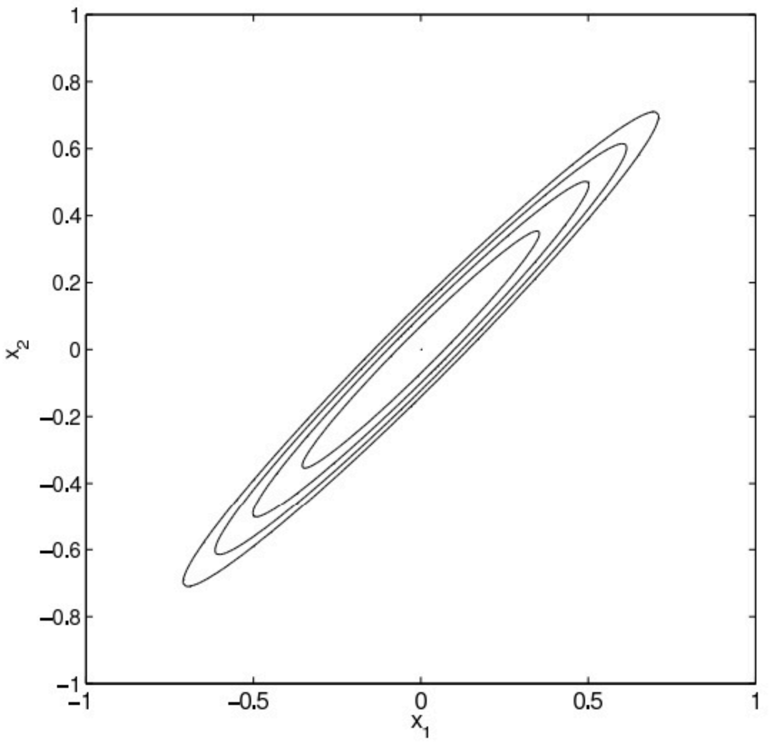


propose $x_i \longrightarrow x_j + z\cdot(x_k - x_j),\ k \neq j$

with density $g(z) \propto 1/\sqrt{z}$ for $z \in [1/a, a]$

accept with Metropolis

Affine–invariant sampling
(Goodman–Weare 2010)



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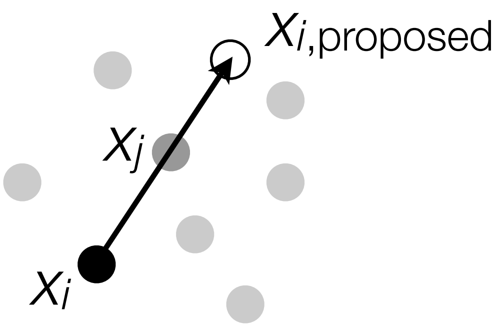

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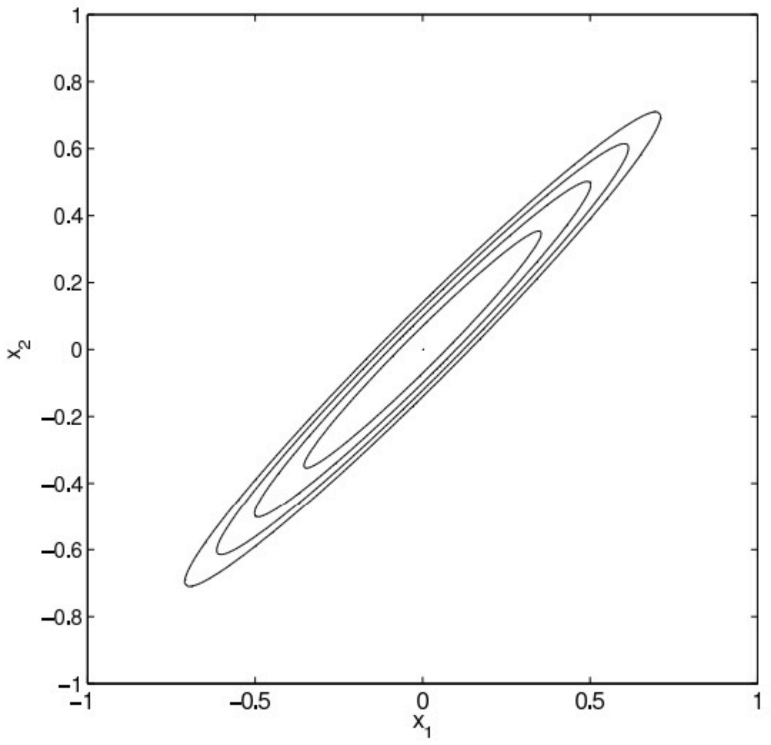
- the final ensemble approximates the posterior

Affine–invariant sampling
(Goodman–Weare 2010)

see dan.iel.fm/emcee
by Daniel Foreman-Mackey *et al.*



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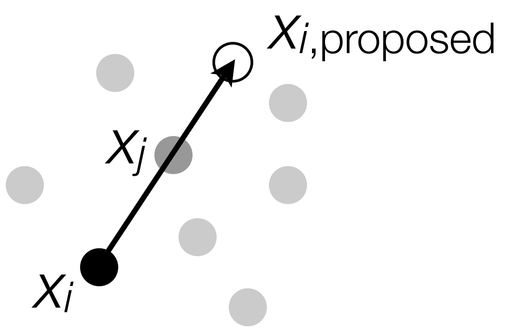

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Discussion

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God is always in the details...

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...but the transcendent is experienced, never proved

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...but Gaussian integrals are easy

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(not even with genetically engineered algorithms)

Parallelization is hard...

...but Gaussian integrals are easy

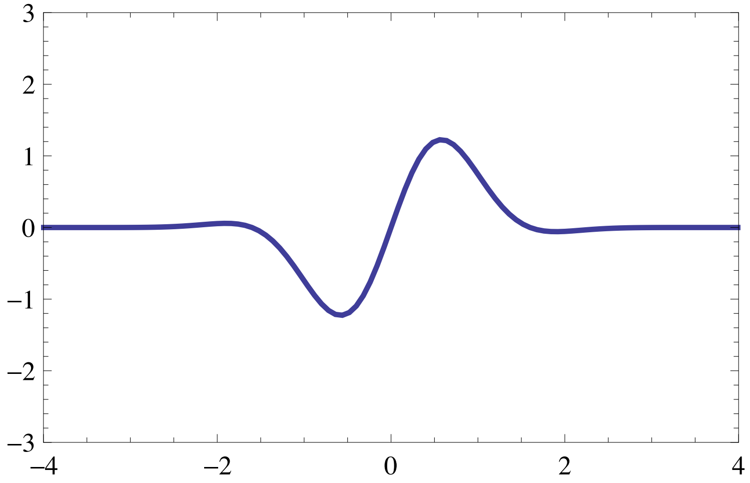
But harnessing the power of stochastic physical systems, that’s just cool!

Backup slides

Michele Vallisneri, Jet Propulsion Laboratory

GW science in a nutshell:
GW detection with addition, subtraction, and multiplication

data = signal + noise



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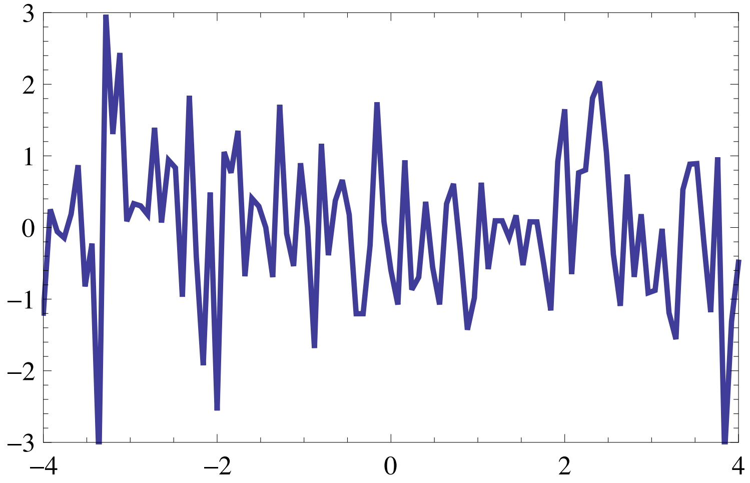

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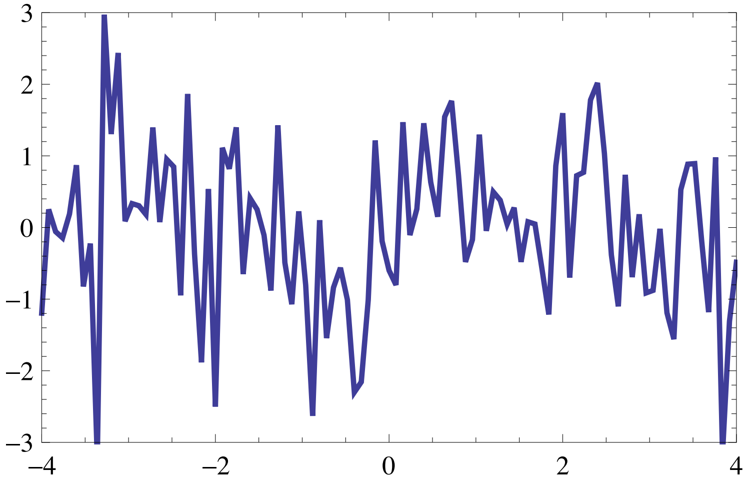
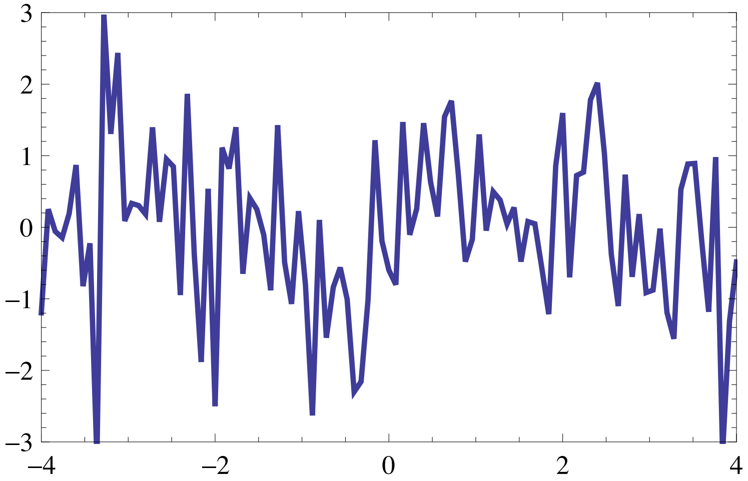


(SNR = 5)

therefore: noise = data – signal; to assess detection, we ask which instance of noise is more probable?



(no signal)

or

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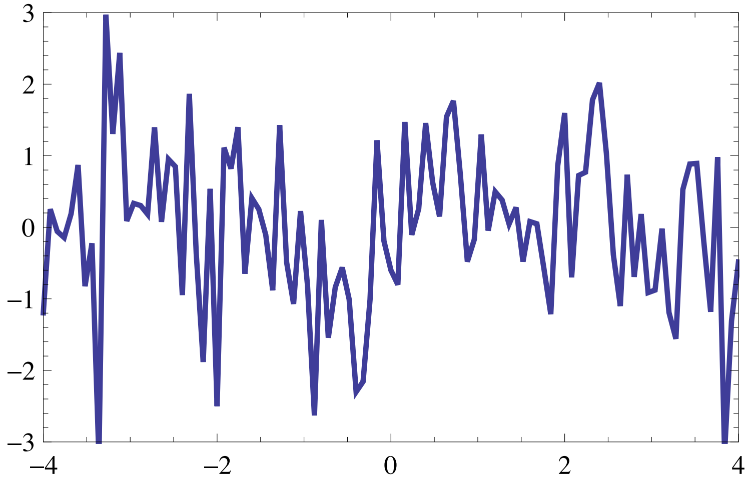
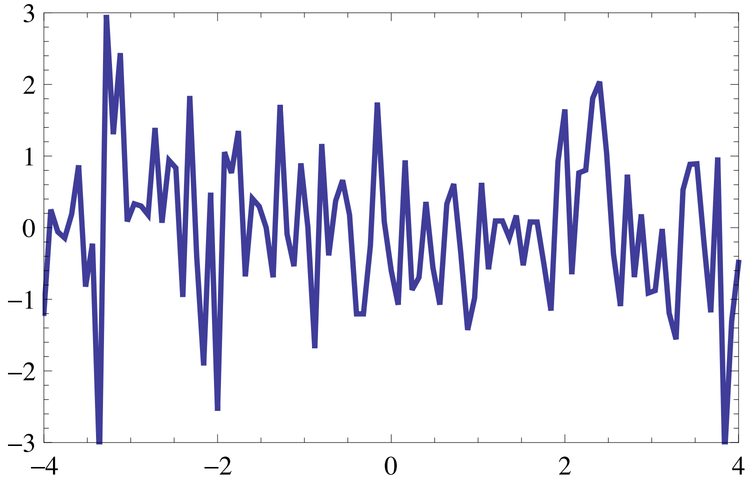


(no signal)

or

(signal hidden in noise, so we subtract it out)



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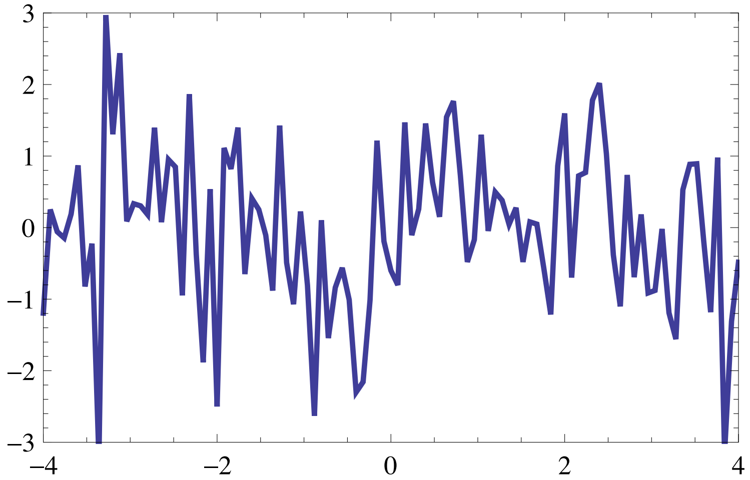

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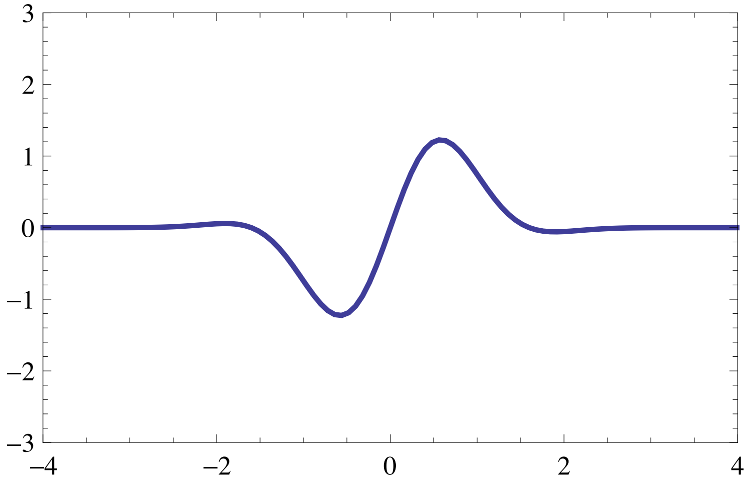

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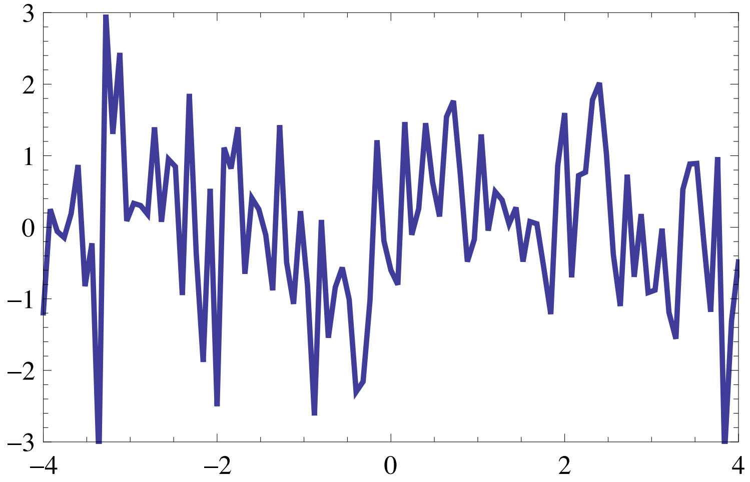

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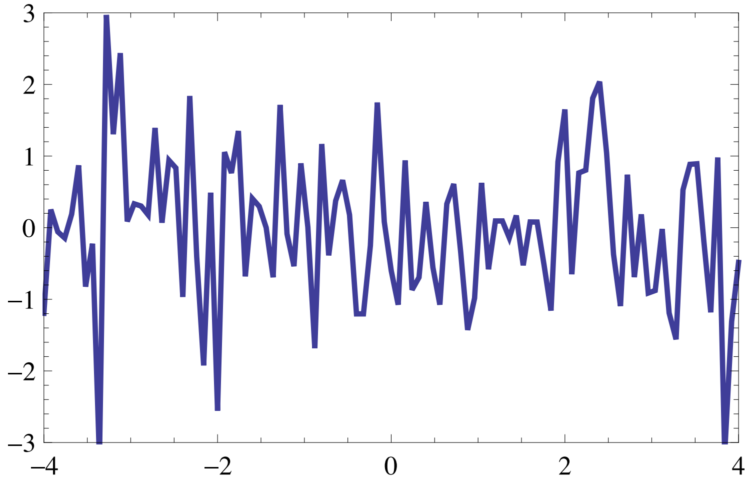

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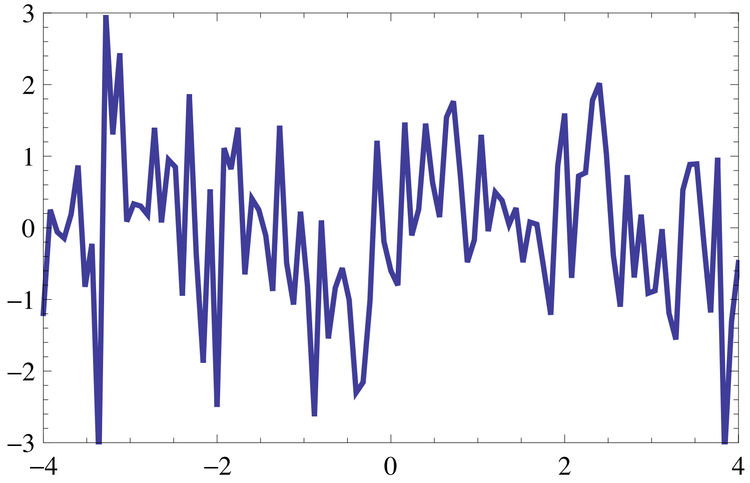

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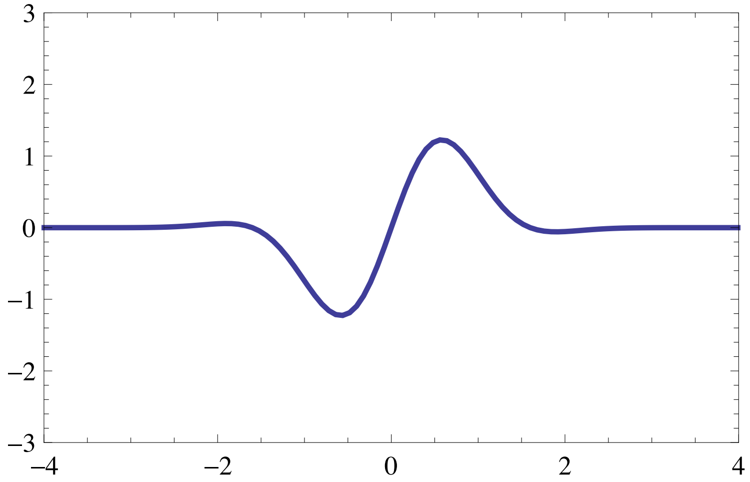
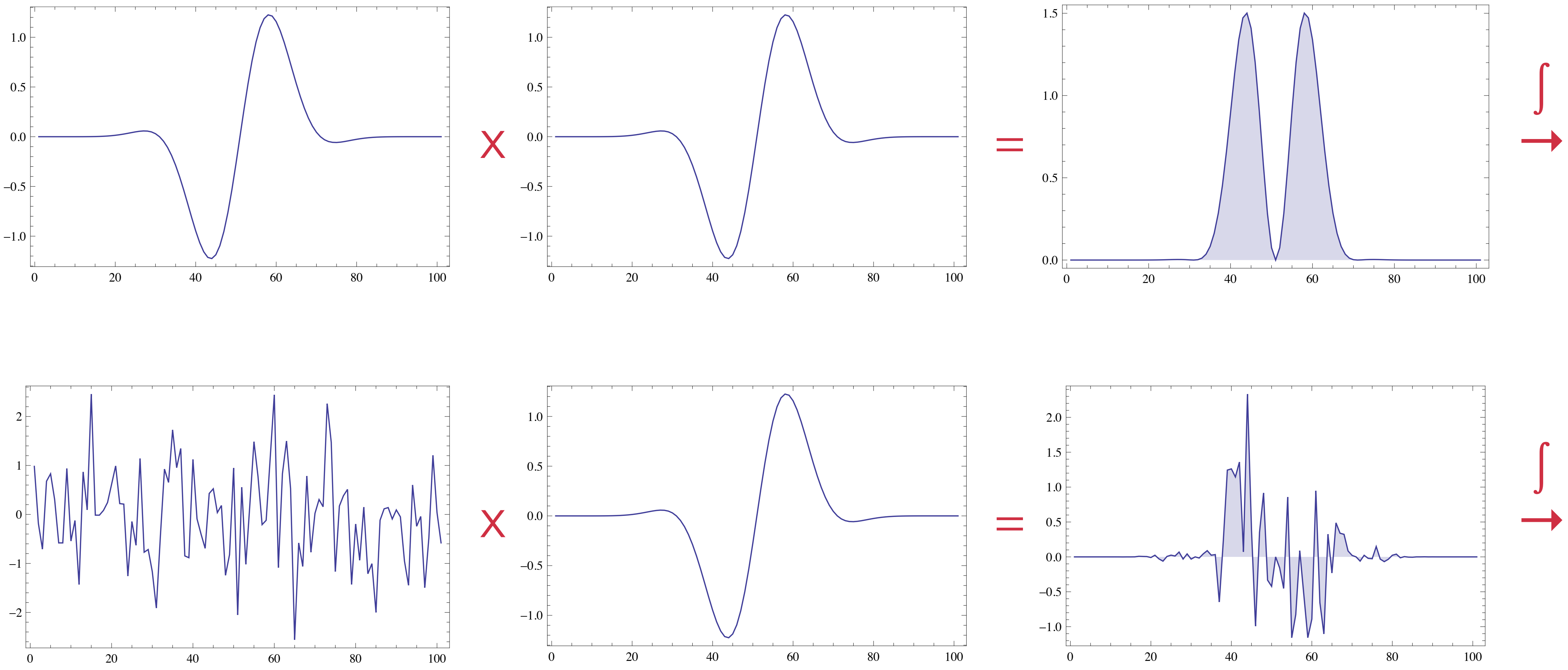


the ratio of probabilities is ~ exp SNR^2/2,
(here ~ 270,000)

an intuitive interpretation of this process is in terms of correlation products/matched filtering



∫ → 25

∫ → 3.39

an intuitive interpretation of this process
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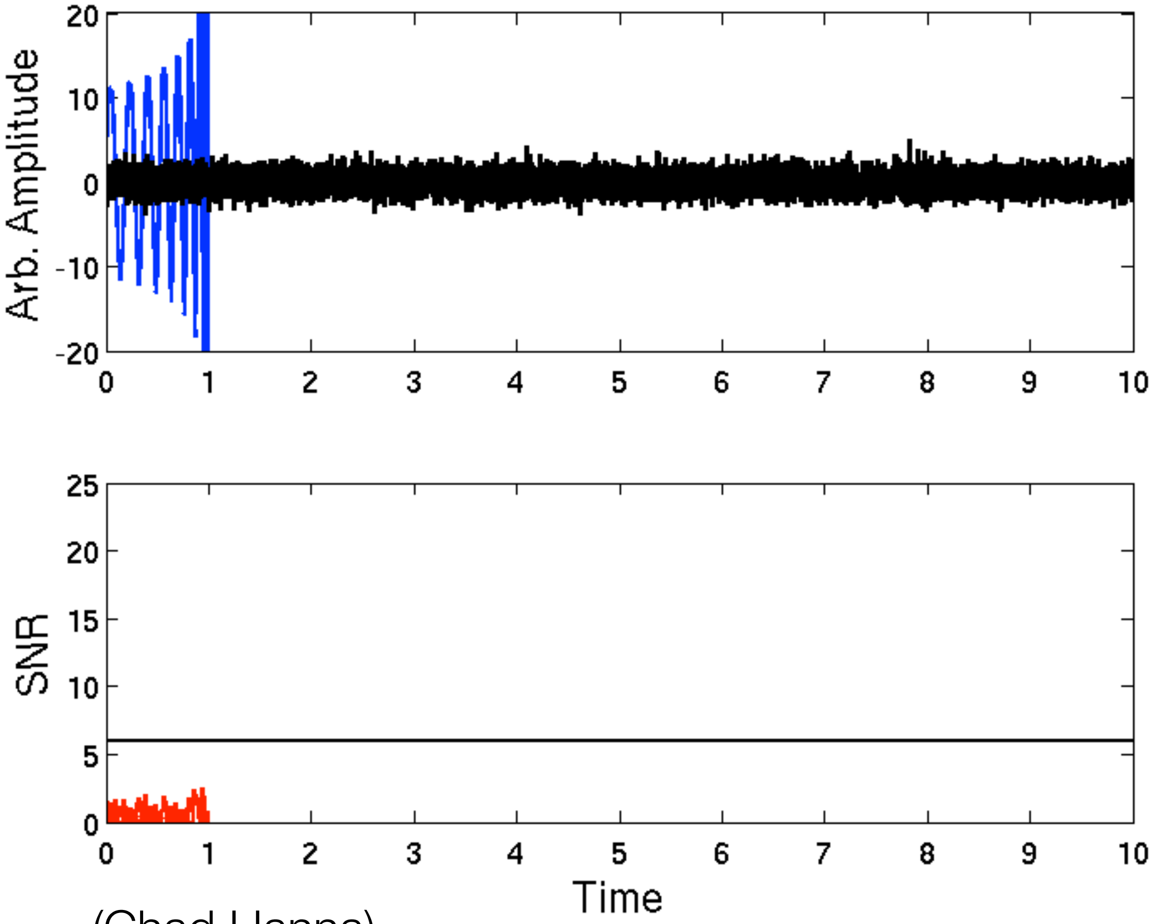
detector
data

$$\mathrm{SNR}(t_0) = \int_0^{\Delta t} s(t+t_0)h(t)dt$$

signal
“template”



(Chad Hanna)

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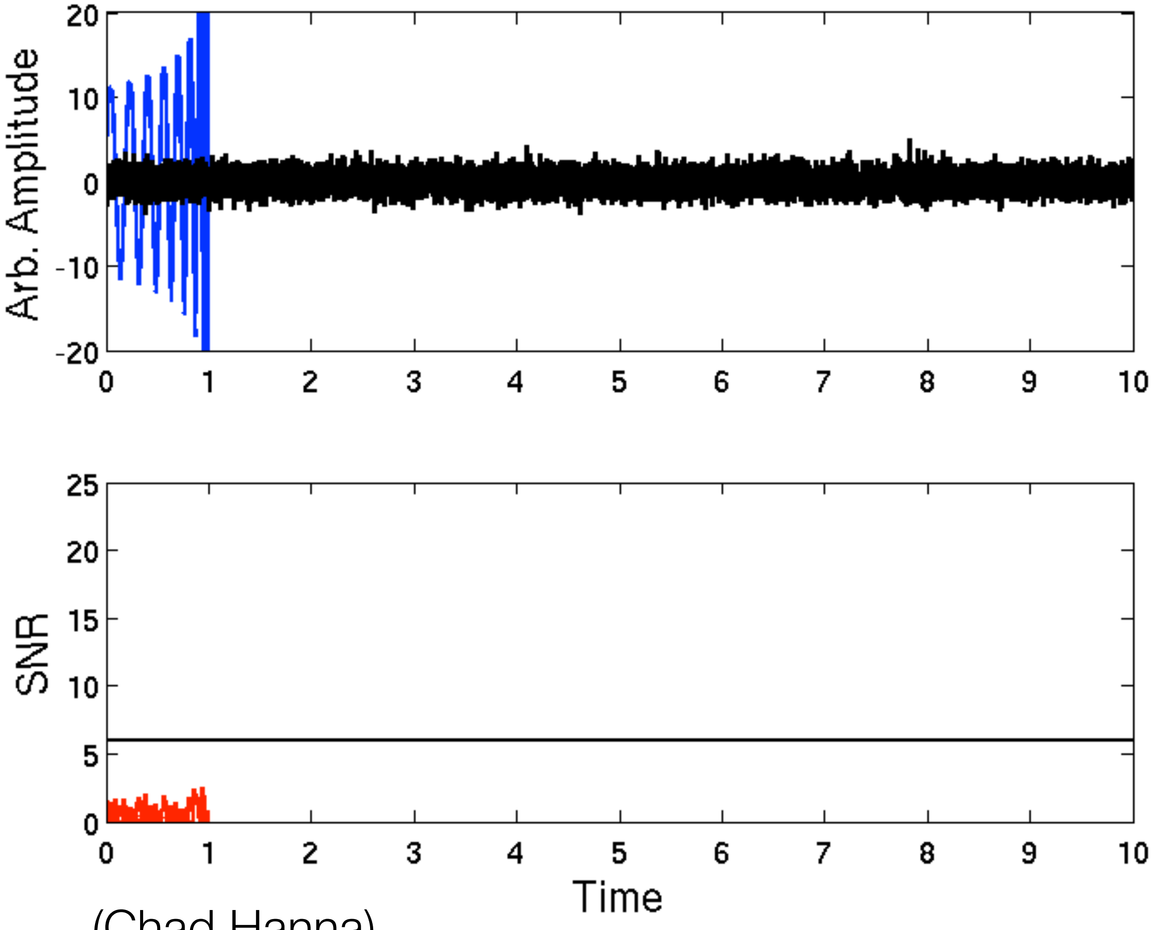

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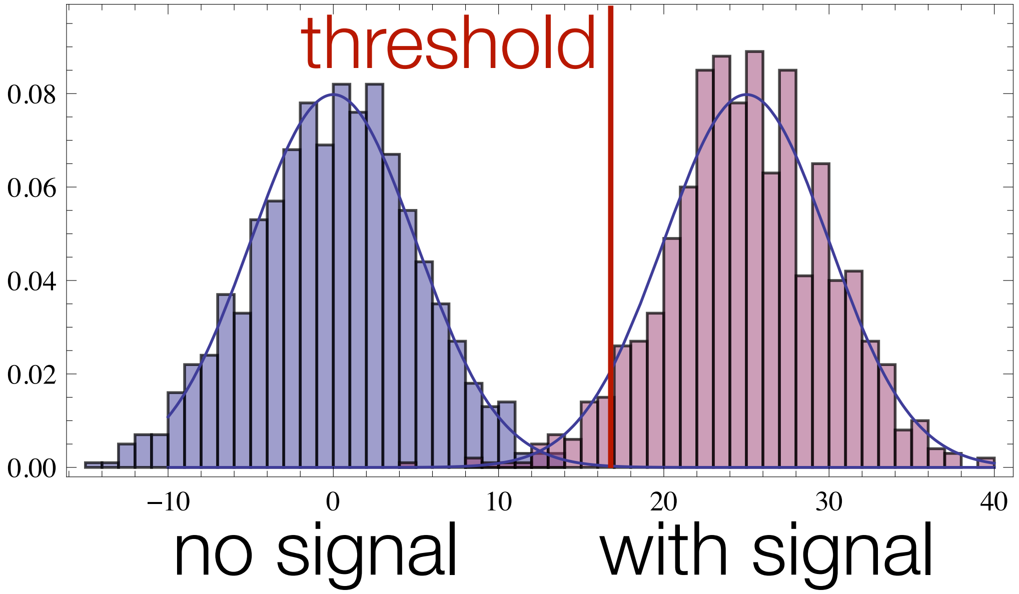

GW detection in practice [see PRD 87, 024033, 2013]

filter detector output
with theoretical templates

GW detection in practice [see PRD 87, 024033, 2013]

condition and calibrate detector output

filter detector output with theoretical templates

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estimate statistical significance

(estimate background, using coincidence between time slides)

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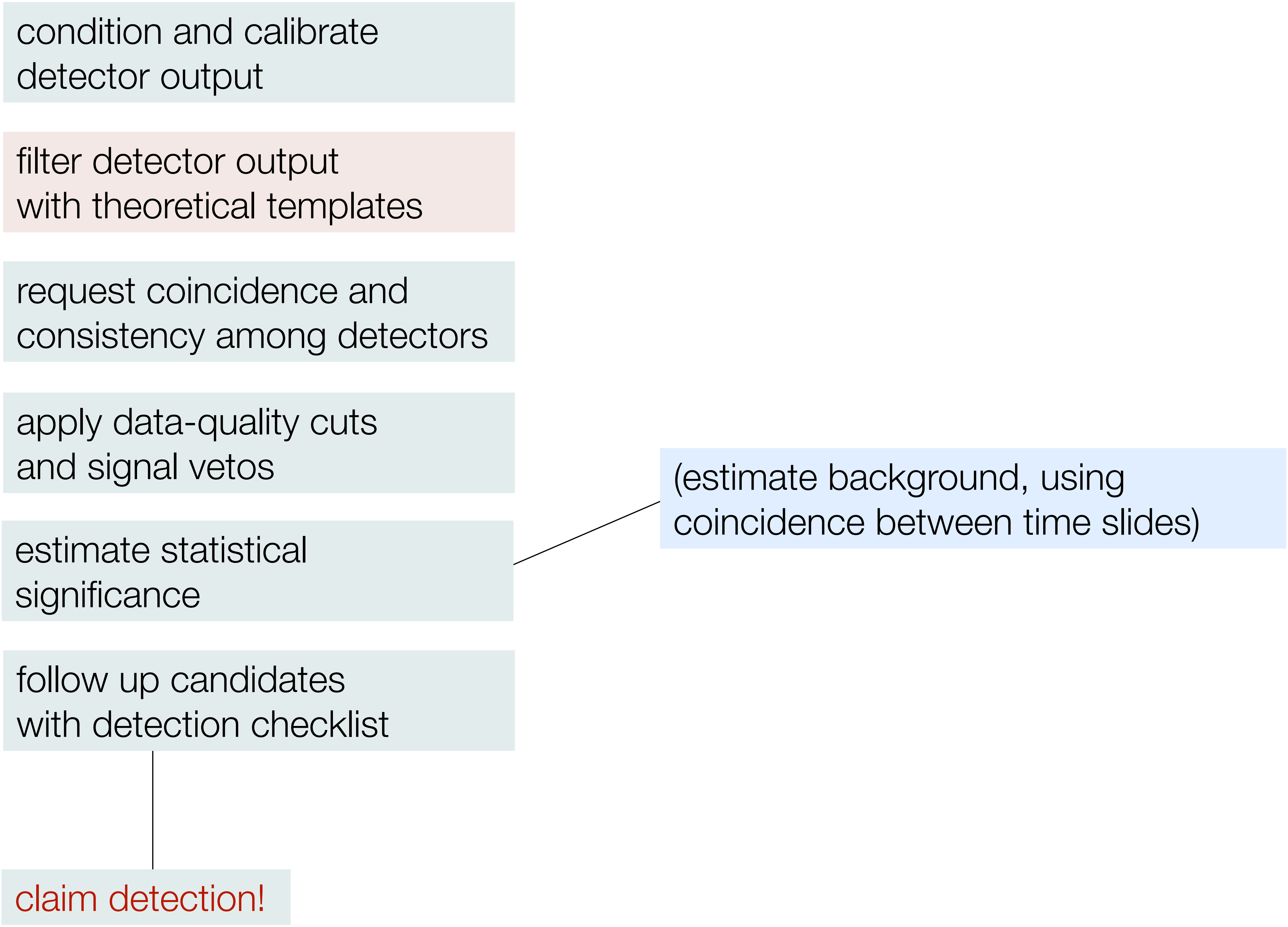

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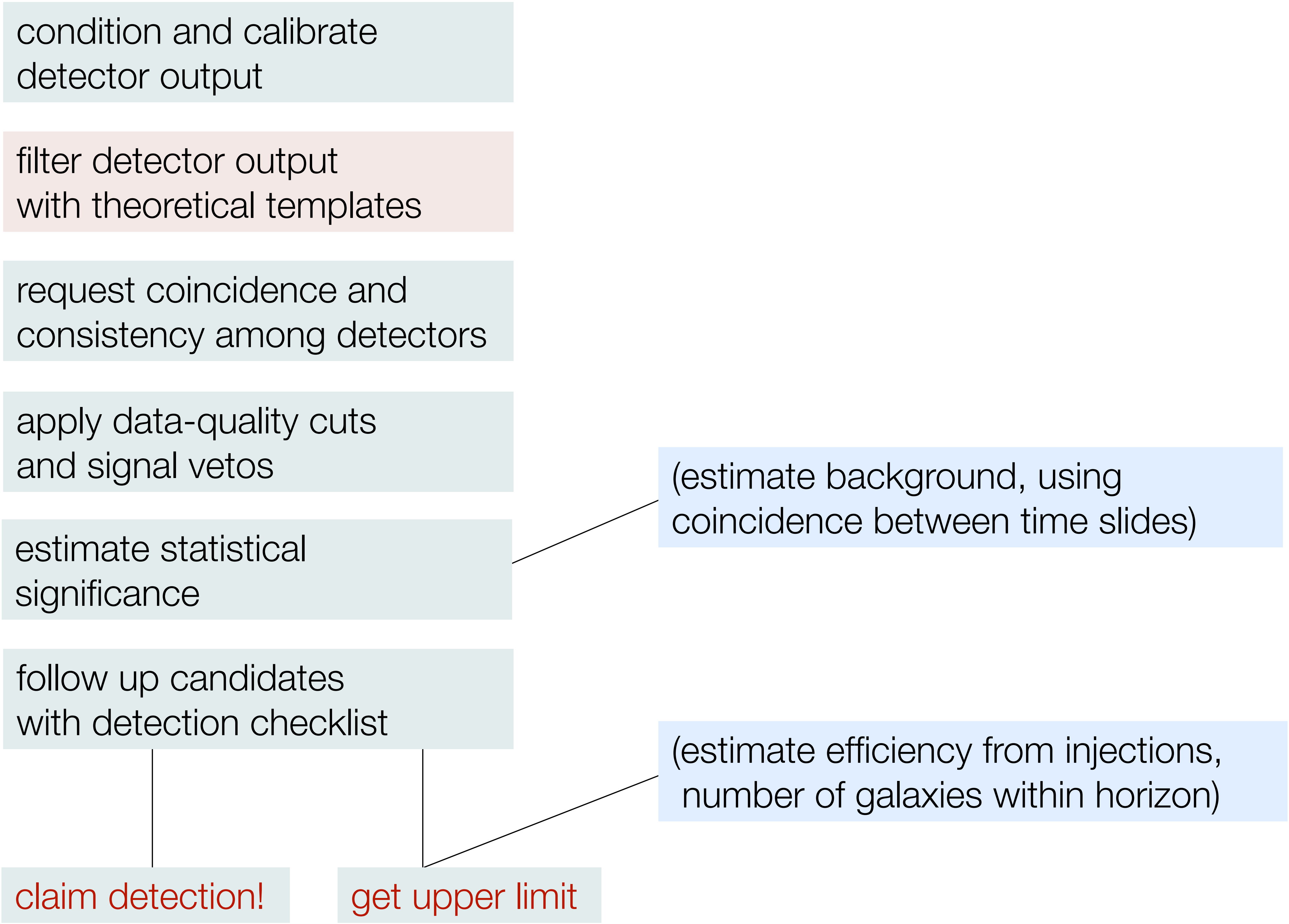
claim detection!

GW detection in practice [see PRD 87, 024033, 2013]



condition and calibrate detector output

filter detector output with theoretical templates

request coincidence and consistency among detectors

apply data-quality cuts and signal vetos

estimate statistical significance

(estimate background, using coincidence between time slides)

follow up candidates with detection checklist

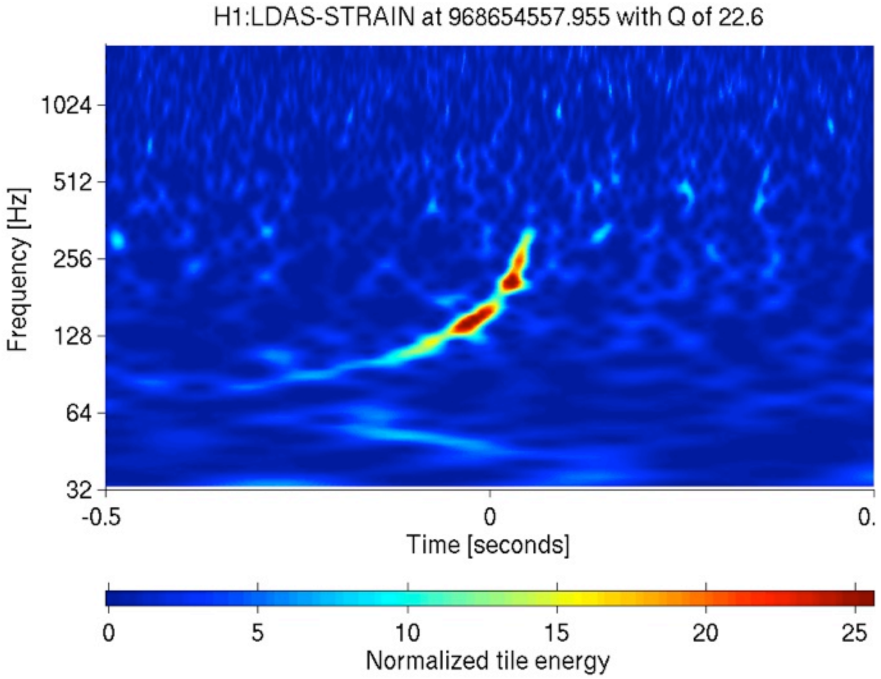
(estimate efficiency from injections, number of galaxies within horizon)

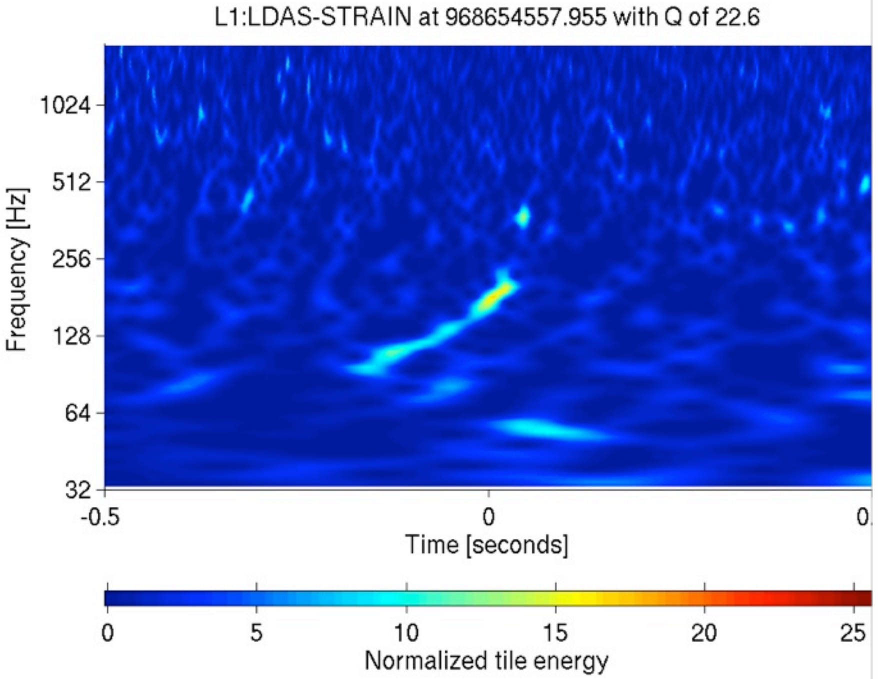
claim detection!

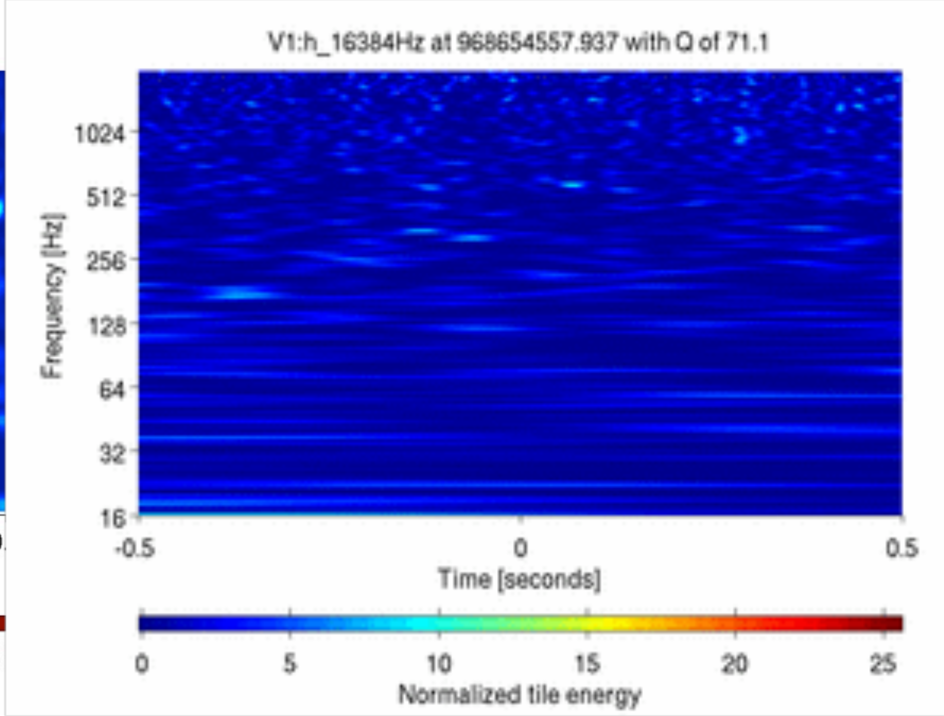
get upper limit

GW100916, the Big Dog

GW100916, the Big Dog

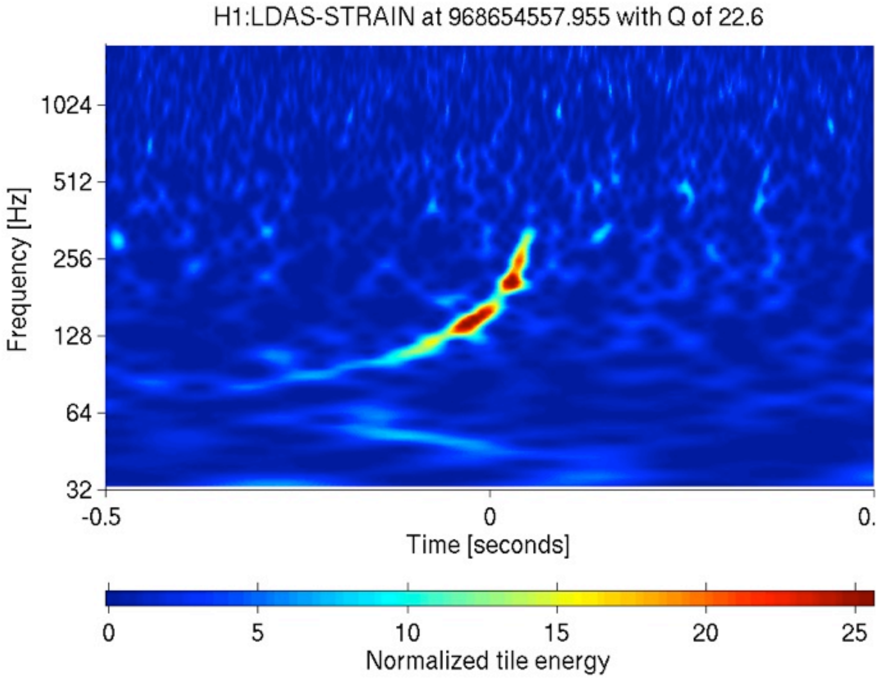

H1:LDAS-STRAIN at 968654557.955 with Q of 22.6

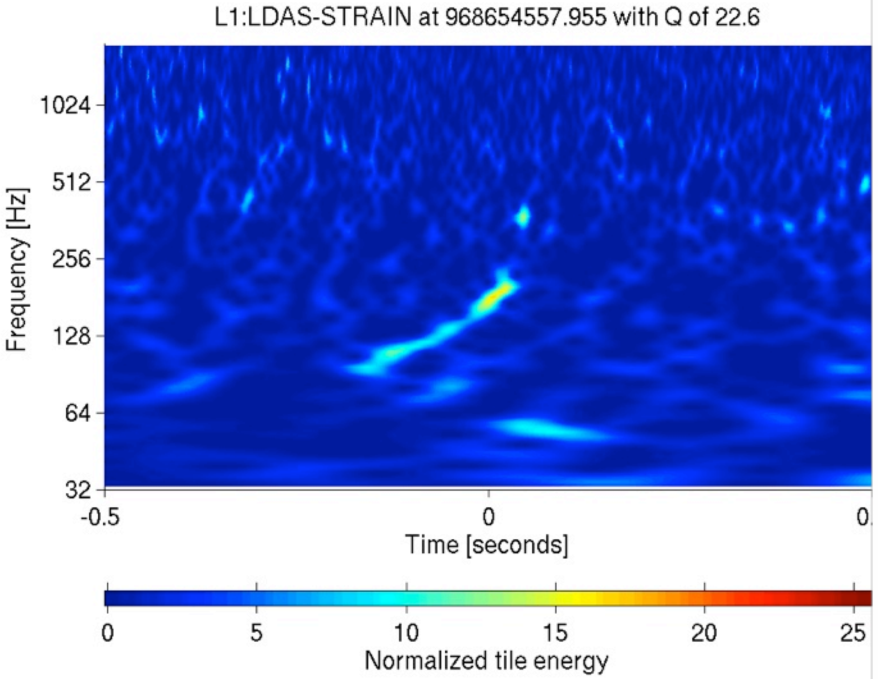

L1:LDAS-STRAIN at 968654557.955 with Q of 22.6

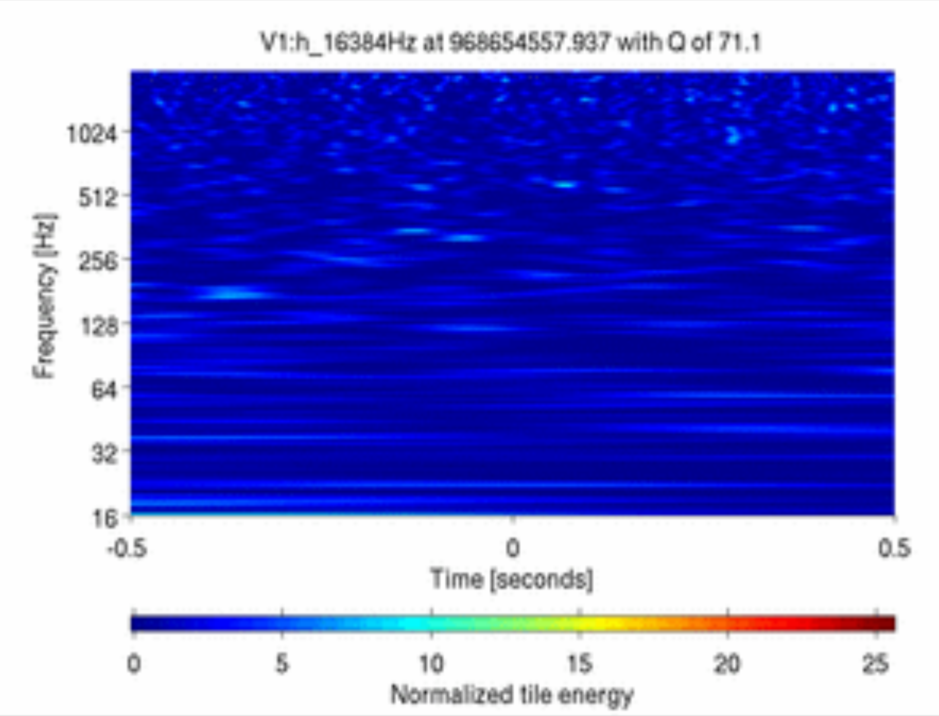

V1:h_16384Hz at 968654557.937 with Q of 71.1

GW100916, the Big Dog

- the LVC toasted with champagne before opening the envelope







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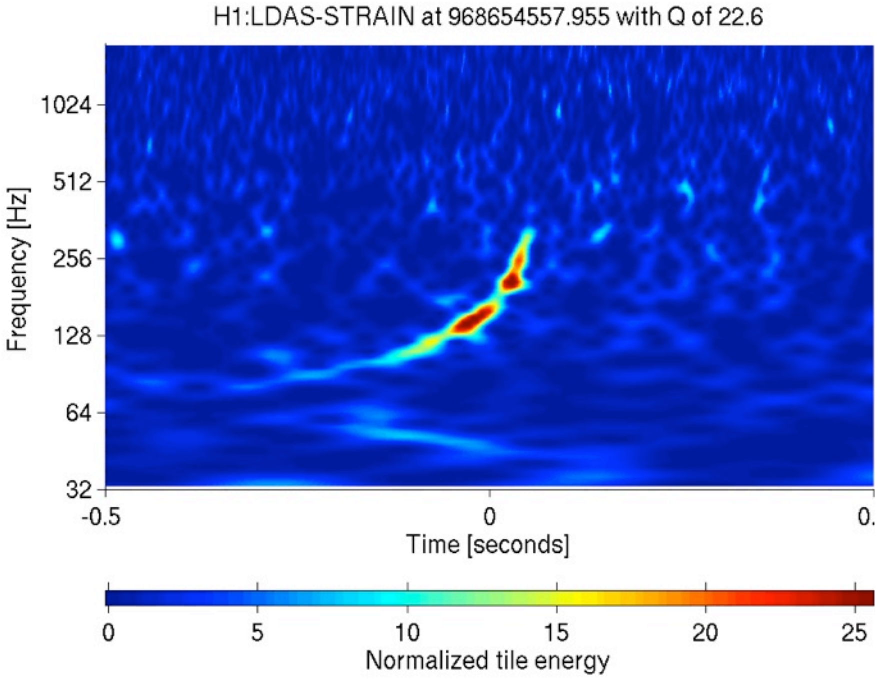
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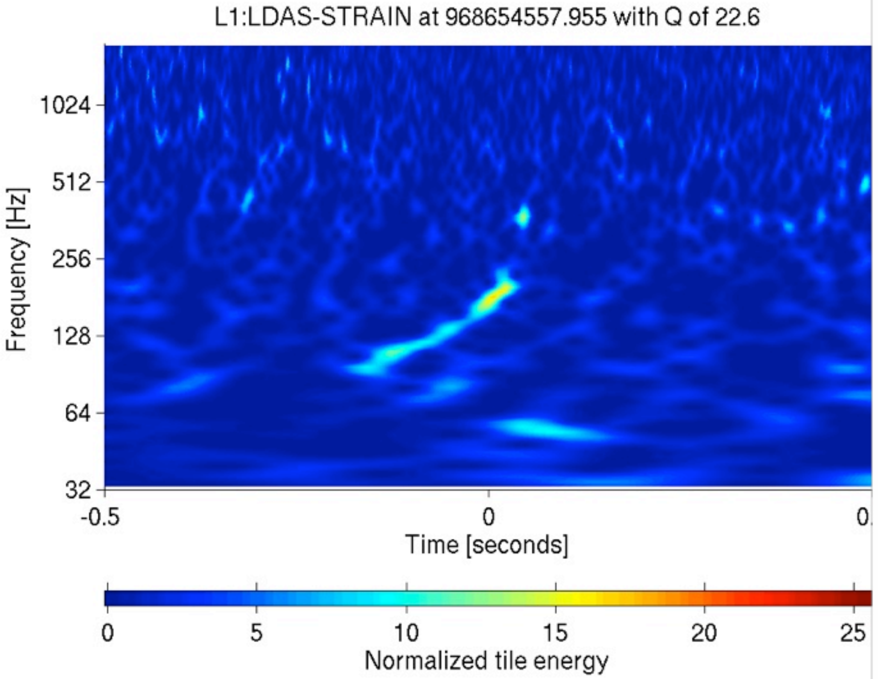
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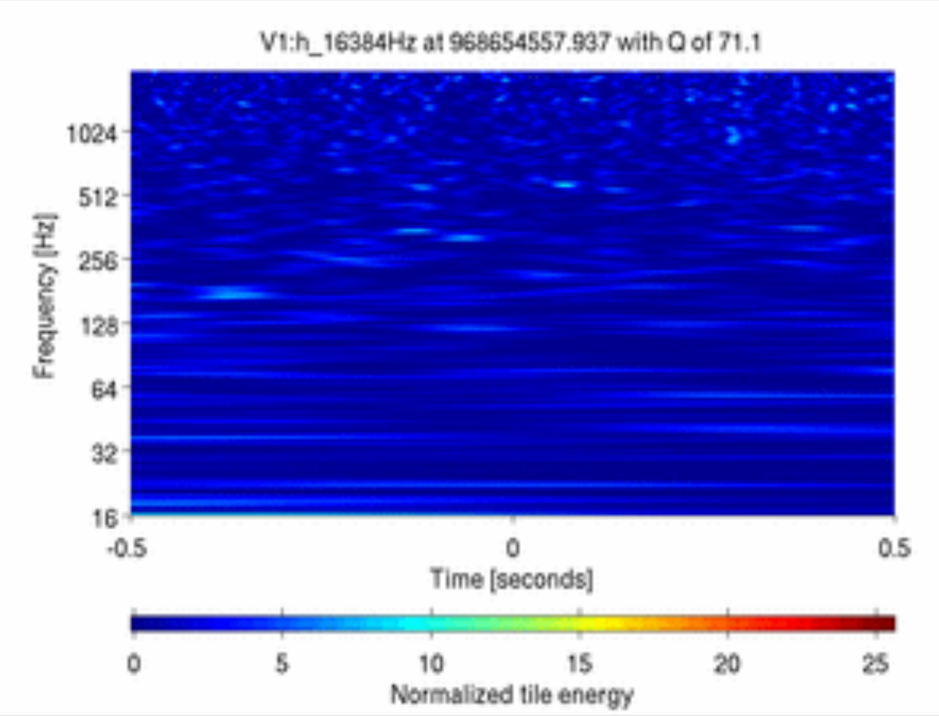
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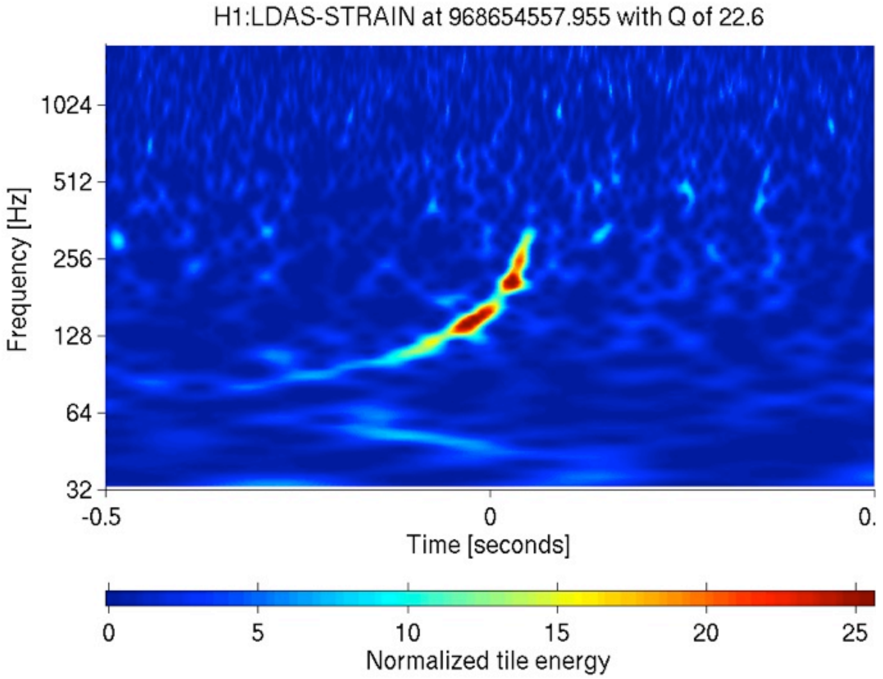

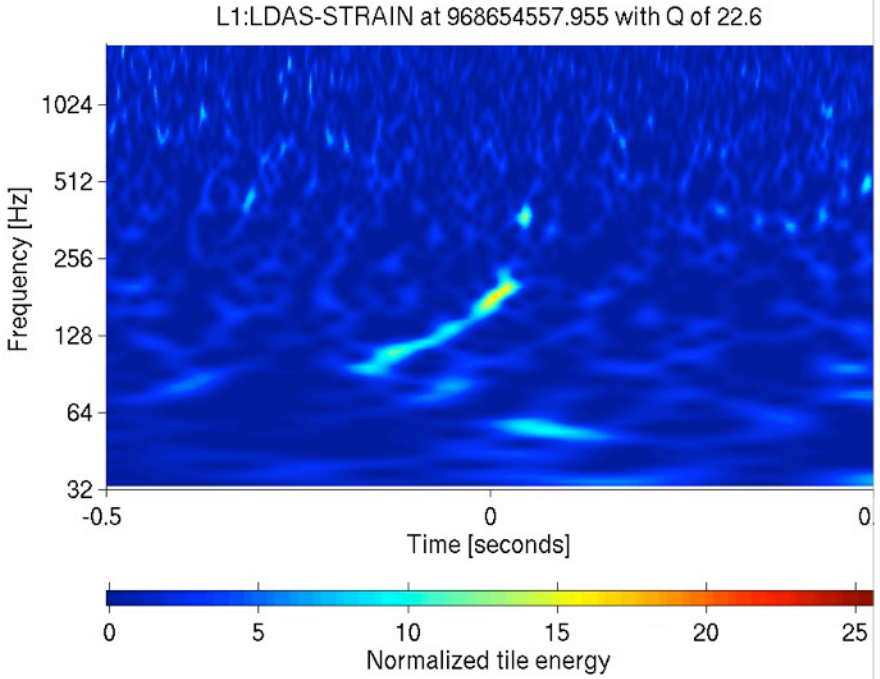

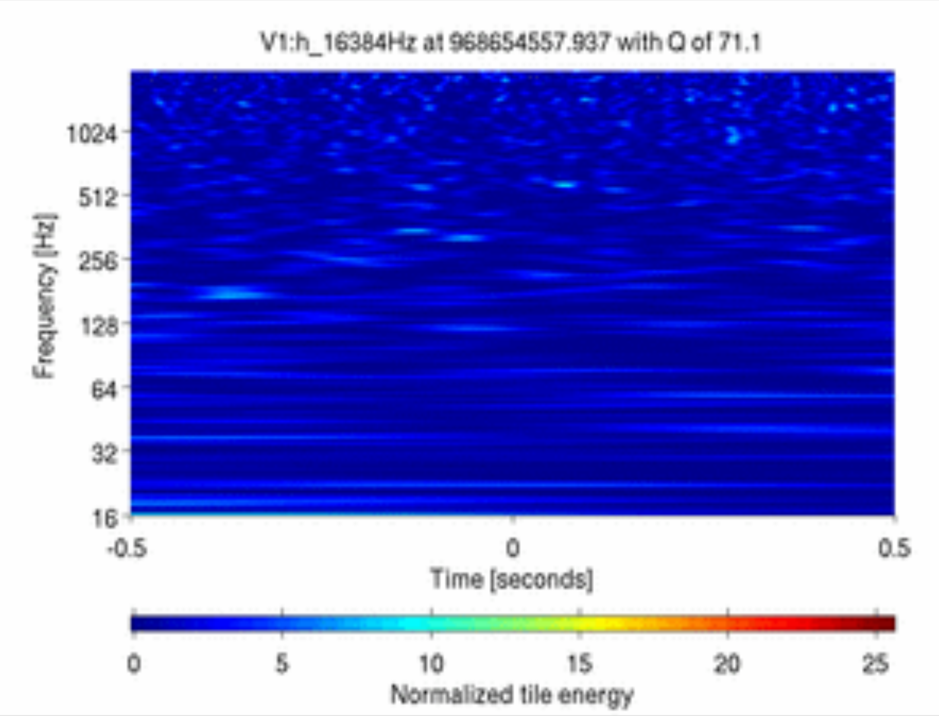

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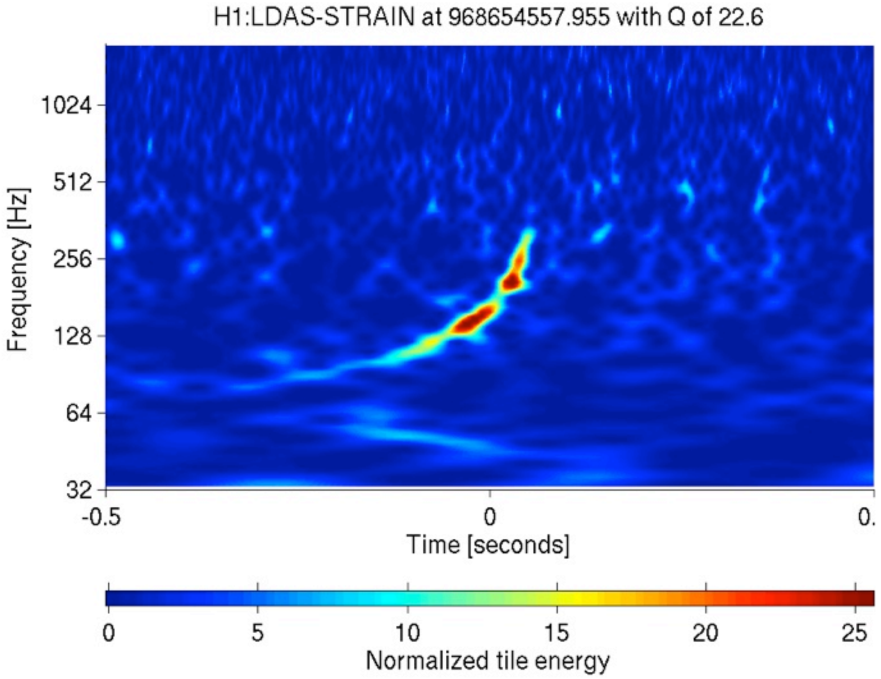

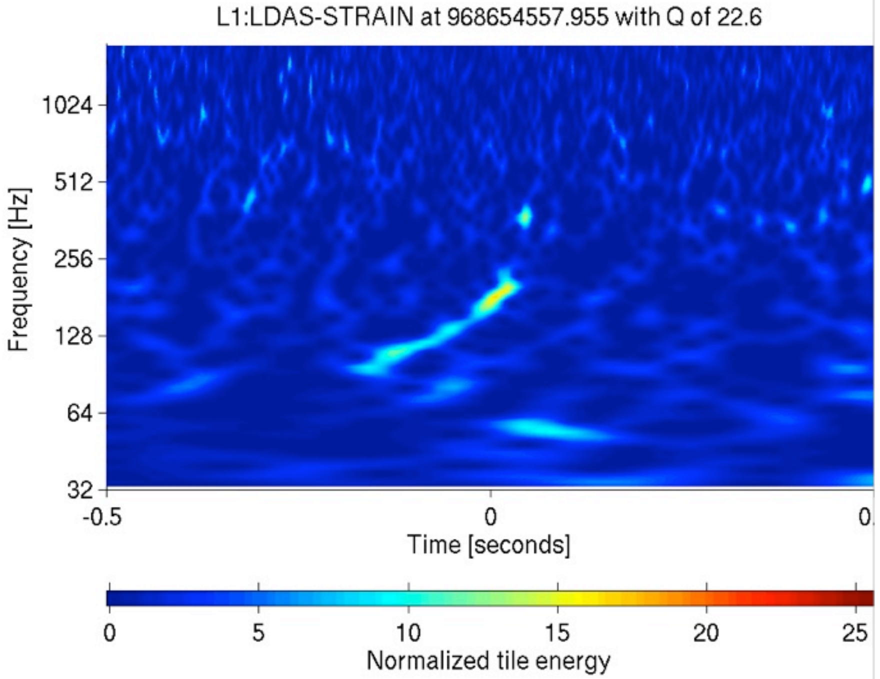

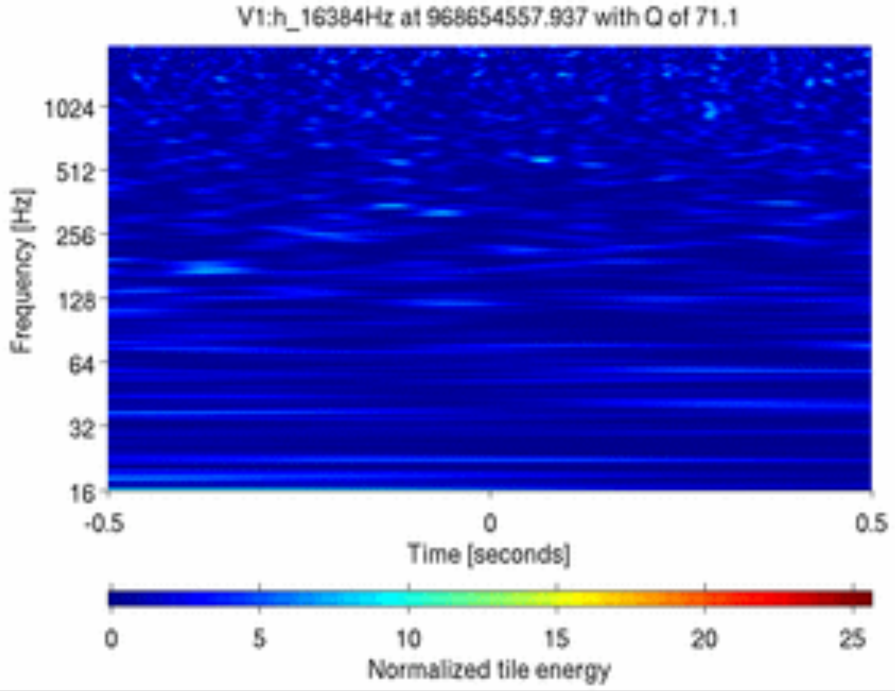

GW100916, the Big Dog

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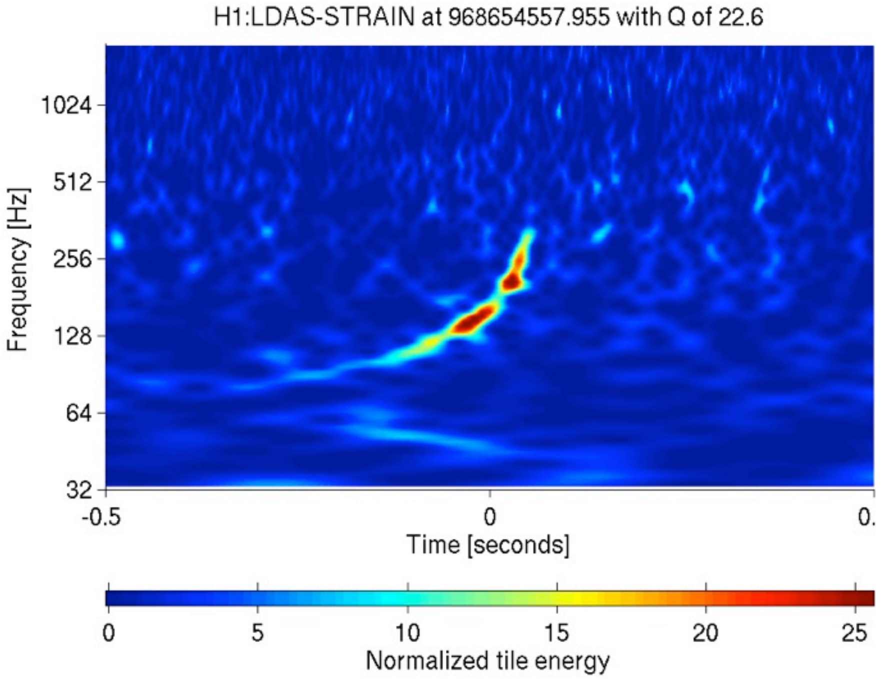
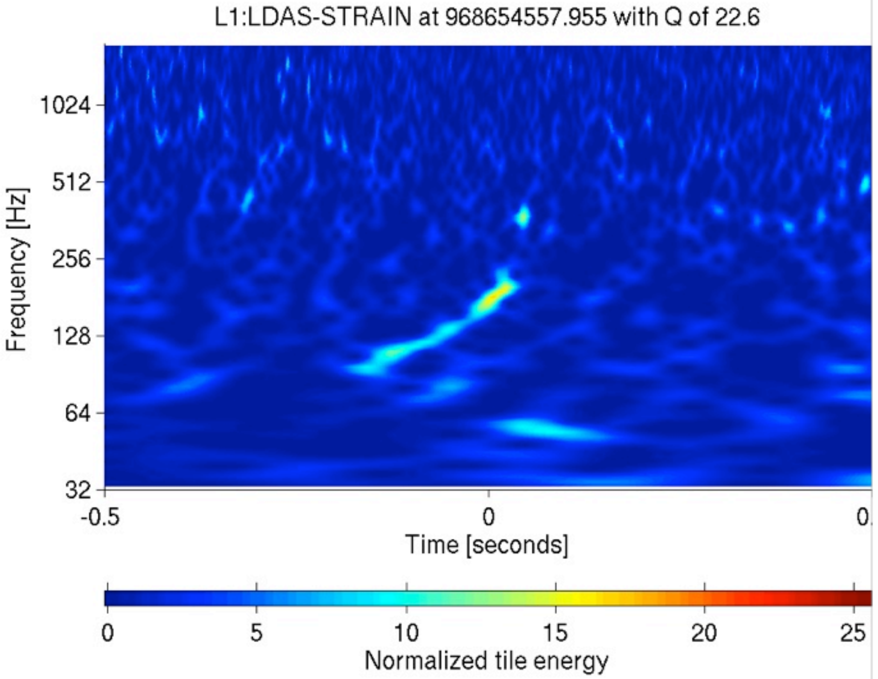
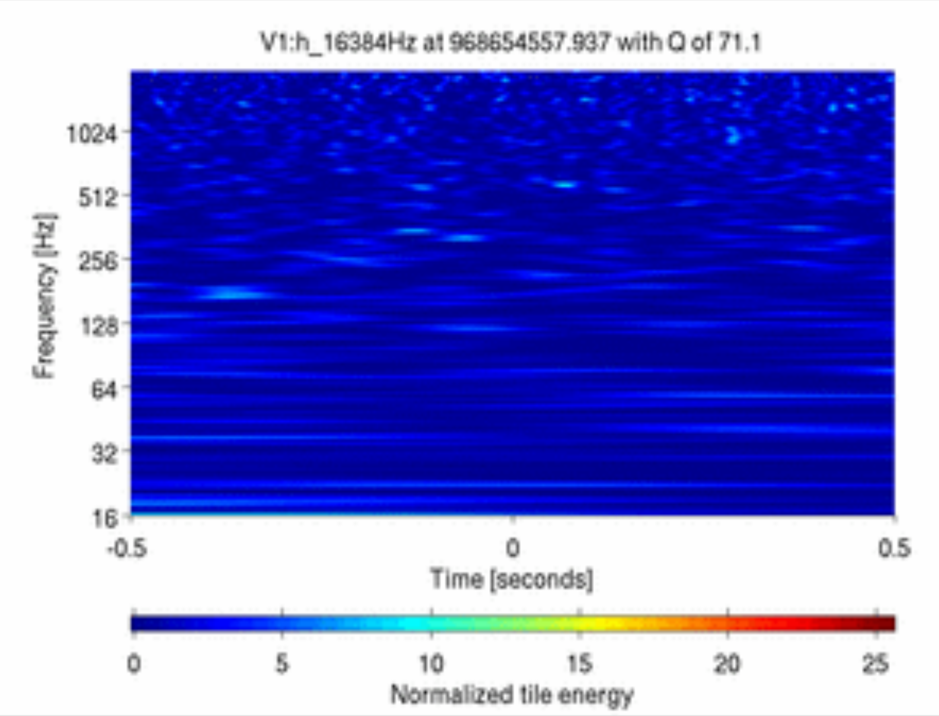
- unfortunately, it was a blind injection...
- ...but we found it!
- the process exercised methods, protocols, and people
- it showed the perils of theory, experiment, software







we design a decision scheme ("AG or GR?") with the Bayesian odds ratio $\mathcal{O}$ as the detection statistic; we set a threshold $\mathcal{O}^*$ and claim detection when $\mathcal{O} > \mathcal{O}^*$

model priors

parameter priors

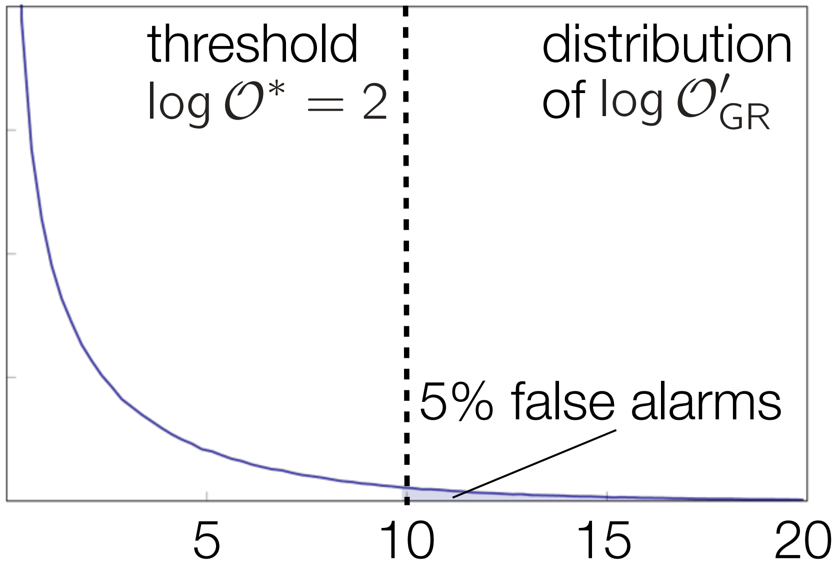
$$\mathcal{O} = \frac{P(\mathrm{AG}|s)}{P(\mathrm{GR}|s)} = \frac{P(\mathrm{AG}) \int p(s|\theta^{i,a})\, p(\theta^{i,a})\, d\theta^{i,a}}{P(\mathrm{GR}) \int p(s|\theta^{i})\, p(\theta^{i})\, d\theta^{i}}$$

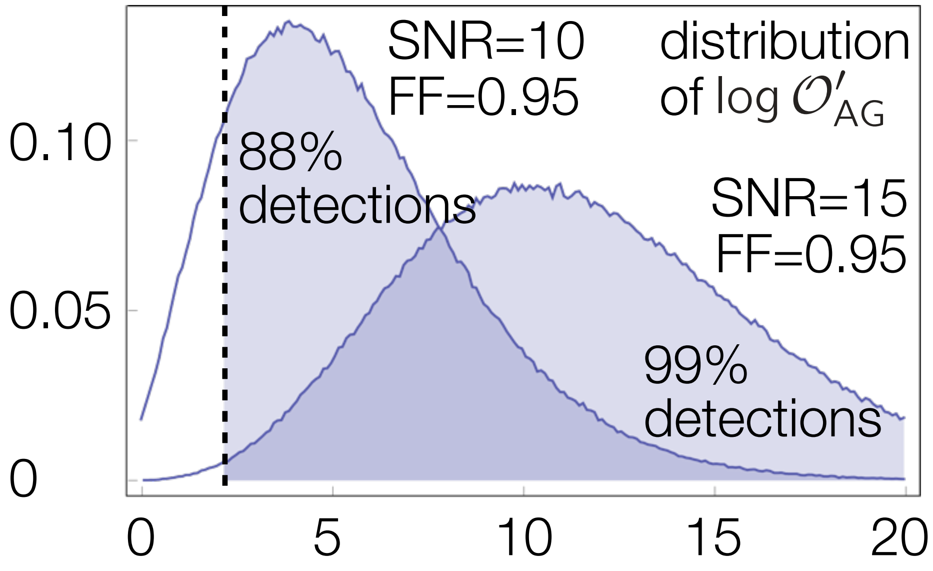
AG parameters

GR parameters

evidence (= marginal likelihood)
for AG and GR models

likelihood





background: true signal is GR

detection efficiency: true signal is AG

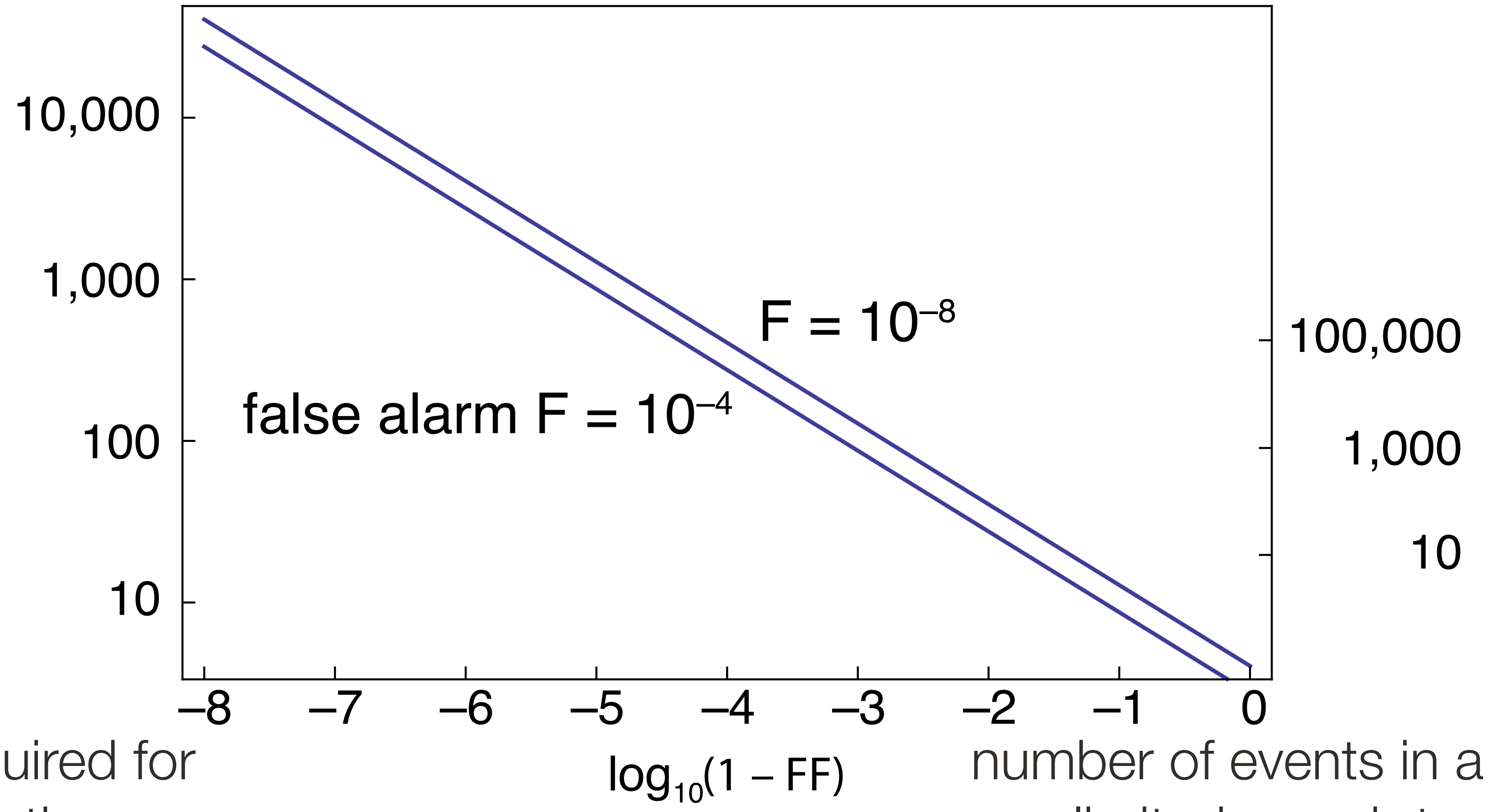
$$\mathcal{O}'_{\mathrm{GR}} = e^{x^2/2}$$

$$\mathcal{O}'_{\mathrm{AG}} = e^{x^2/2 + x\sqrt{2(1-\mathrm{FF})}\,\mathrm{SNR} + (1-\mathrm{FF})\,\mathrm{SNR}^2}$$

renormalized odds ratios (model priors
and Occam factors cancel out, see paper)

x is a normal random variable with zero mean
and unit variance (a function on noise realization)

for strong signals, $\mathcal{O}'_{\rm GR}$ and $\mathcal{O}'_{\rm AG}$ are remarkably simple functions of FF and SNR alone. For a fixed false-alarm rate, we then ask what SNR yields 50%-efficient AG detection, as a function of FF



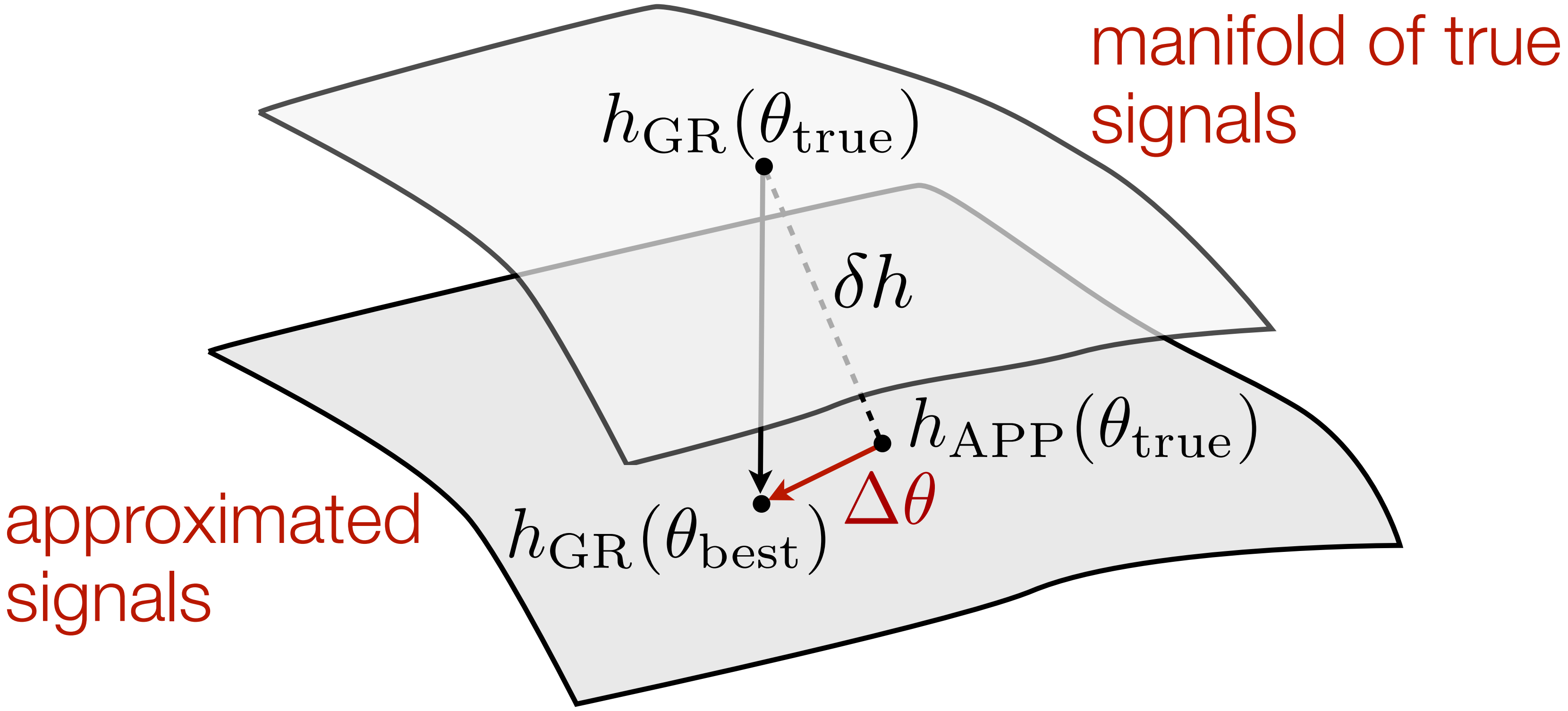
SNR required for AG detection with 50% efficiency

number of events in a volume-limited search to yield that SNR as the loudest event

only very strong AG effects (FF of 0.9–0.99) would be seen in volume-limited searches, so GR tests may have to wait for third-generation ground-based detectors, or for space detectors

an application [Vallisneri and Yunes, arXiv/1301.2627]: “fundamental” bias versus the detection of modified gravity

if model signals (GR) differ from true signals (MG) with the same parameters, the best-fitting template will be displaced by theoretical error, which is SNR-independent [see Cutler & Vallisneri 2007]


manifold of true signals
$h_{\mathrm{GR}}(\theta_{\mathrm{true}})$
δh
$h_{\mathrm{APP}}(\theta_{\mathrm{true}})$
$\Delta\theta$
approximated signals
$h_{\mathrm{GR}}(\theta_{\mathrm{best}})$

$$\delta\vec{\theta}_{\mathrm{th}} = (F_{\mathrm{bf}}^{-1})^{\alpha\beta}\big(h_{,\beta}(\vec{\theta}_{\mathrm{bf}})\big|\delta h(\vec{\theta}_{\mathrm{bf}})\big)$$

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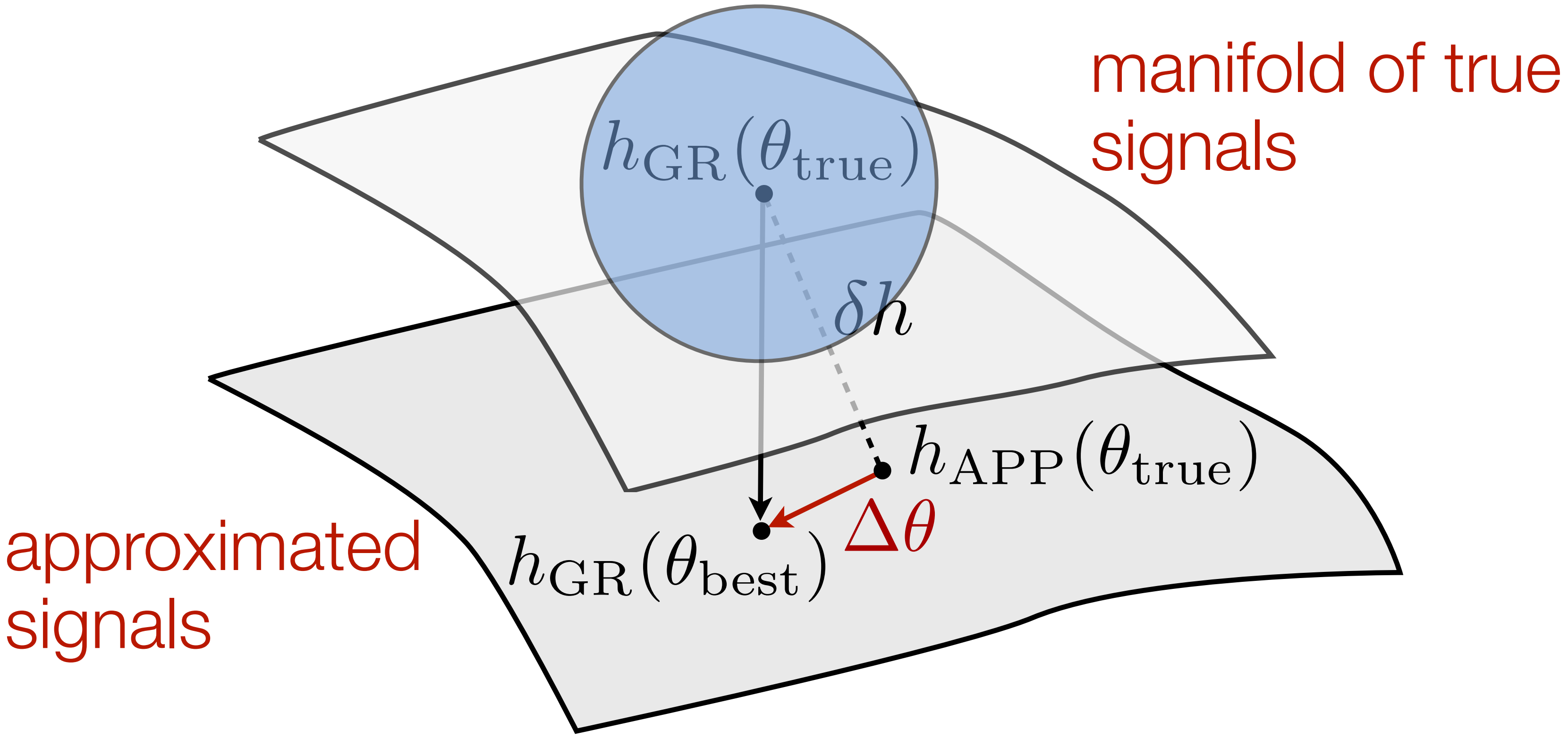
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representing modified gravity as “parametrized post-Einstein,” we compare the MG SNR$^{\text{detect}}$ with the SNR$^{\text{bias}}$ where δθ$_{\text{th}}$ > δθ$_{\text{stat}}$

$$h_{\mathrm{GR}}(f) = A_{\mathrm{GR}}(f) e^{i\Psi_{\mathrm{GR}}(f)} \quad \delta\Psi(f) = \beta\, u^b$$

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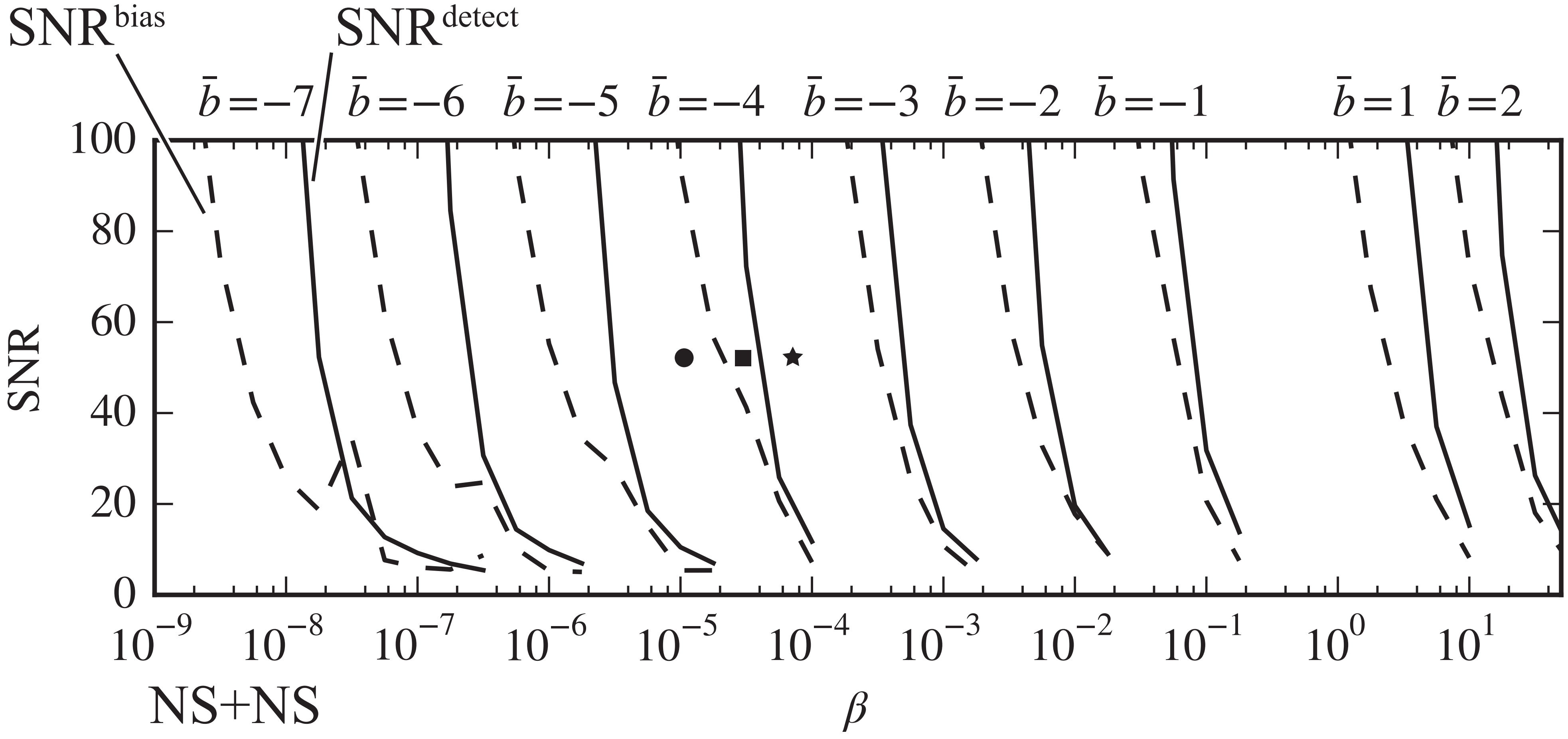

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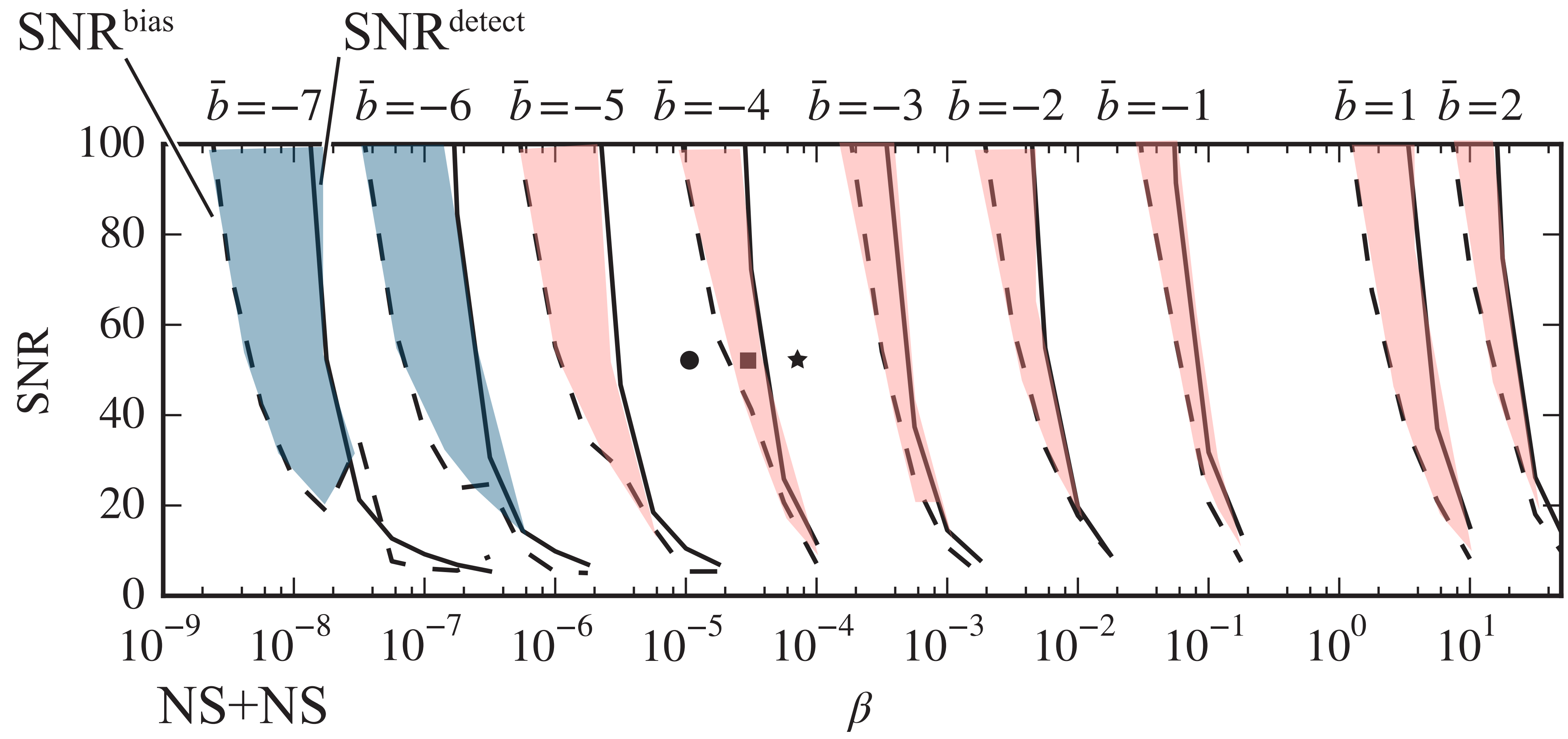
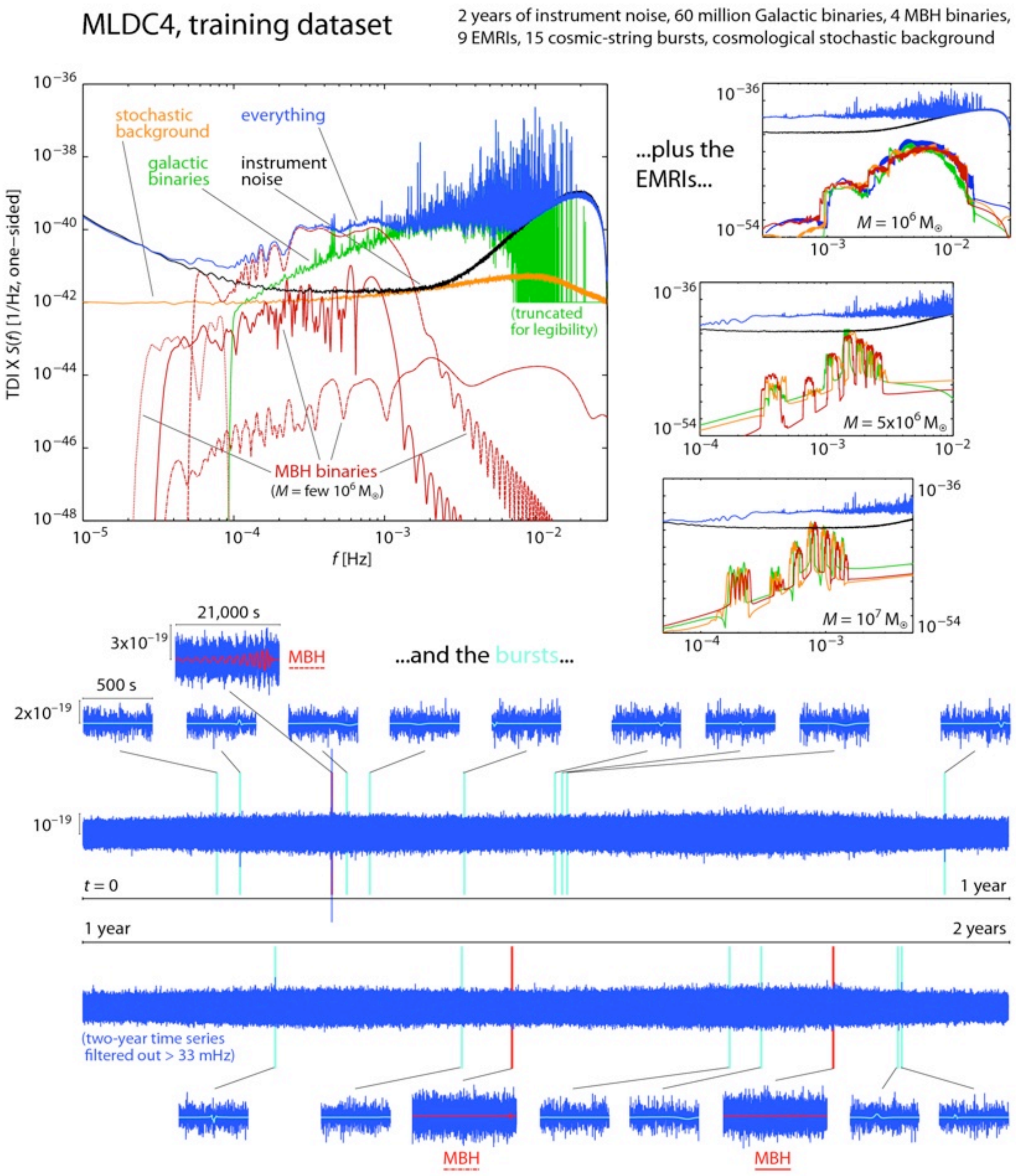


at least for simple circular inspirals, stealth bias (significant $\delta\theta_{\mathrm{th}}$, non-detectable MG) is generic!

[but see arXiv/1301.2627]

the Mock LISA Data Challenges: successfully fostering and consolidating collaborative data-analysis development



- five challenges completed between 2006 and 2011
- 70 participants, 25 institutions 30+ publications
- demonstrated the detection and parameter estimation of all major LF GW source classes, using a great variety of methods
- lisatools.googlecode.com lisasolve.googlecode.com
- acknowledged model for LISA Pathfinder and the International Pulsar-Timing Array