Bayesian model averaging for nuclear symmetry energy from effective proton-neutron chemical potential difference of neutron-rich nuclei

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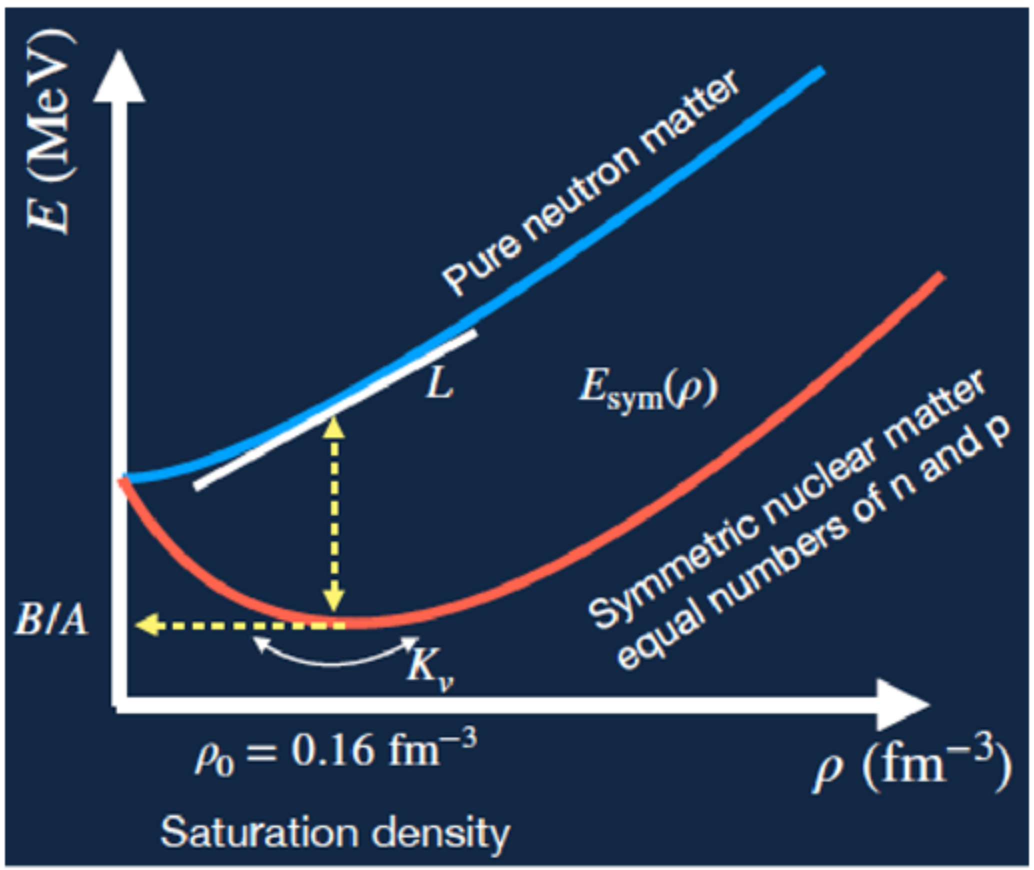
QMY, Cai, Chen, Yuan and Zhang, PLB 849 (2024) 138435

核物质状态方程(EOS)和对称能

- 核物质，是由质子和中子组成的、无限大的均匀理想系统 。
- 核物质状态方程，是描述核物质性质的关键物理参量
- 核物质状态方程对研究中子星的结构、演化以及超新星爆发有重要意义



非对称核物质每核子结合能

$$E(\rho,\delta) = E_0(\rho) + E_{\mathrm{sym}}(\rho)\delta^2 + \mathcal{O}(\delta^4)$$

$$\delta = (\rho_n - \rho_p)/\rho.$$

对称核物质状态方程

$$E_0(\rho) = E_0(\rho_0) + \frac{1}{2}K_0\chi^2 + \frac{1}{6}J_0\chi^3 + \mathcal{O}(\chi^4)$$

同位旋相关部分-对称能

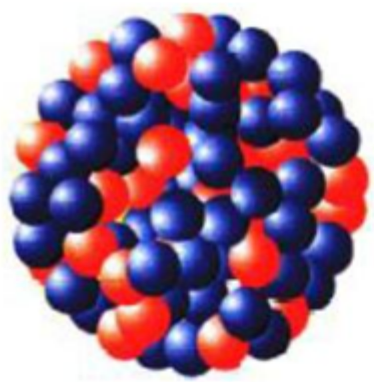
$$E_{\mathrm{sym}}(\rho) \equiv \frac{1}{2}\frac{\partial^2 E}{\partial\delta^2}\Big|_{\delta=0}$$

$$= E_{\mathrm{sym}}(\rho_0) + L(\rho_0)\chi + \frac{1}{2}K_{\mathrm{sym}}\chi^2 + \mathcal{O}(\chi^3)$$

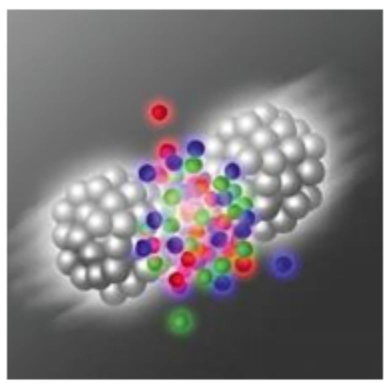
核物质状态方程(EOS)和对称能

- 核物质，是由质子和中子组成的、无限大的均匀理想系统 。有效的理论近似
- 核物质状态方程，是描述核物质性质的关键物理参量
- 核物质状态方程对研究中子星的结构、演化以及超新星爆发有重要意义

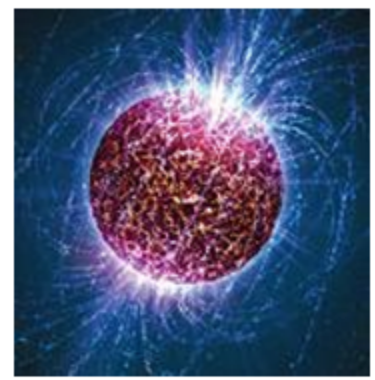
重核中心



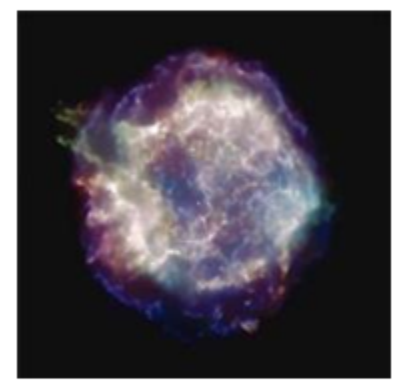
重离子碰撞



中子星内部



超新星爆发

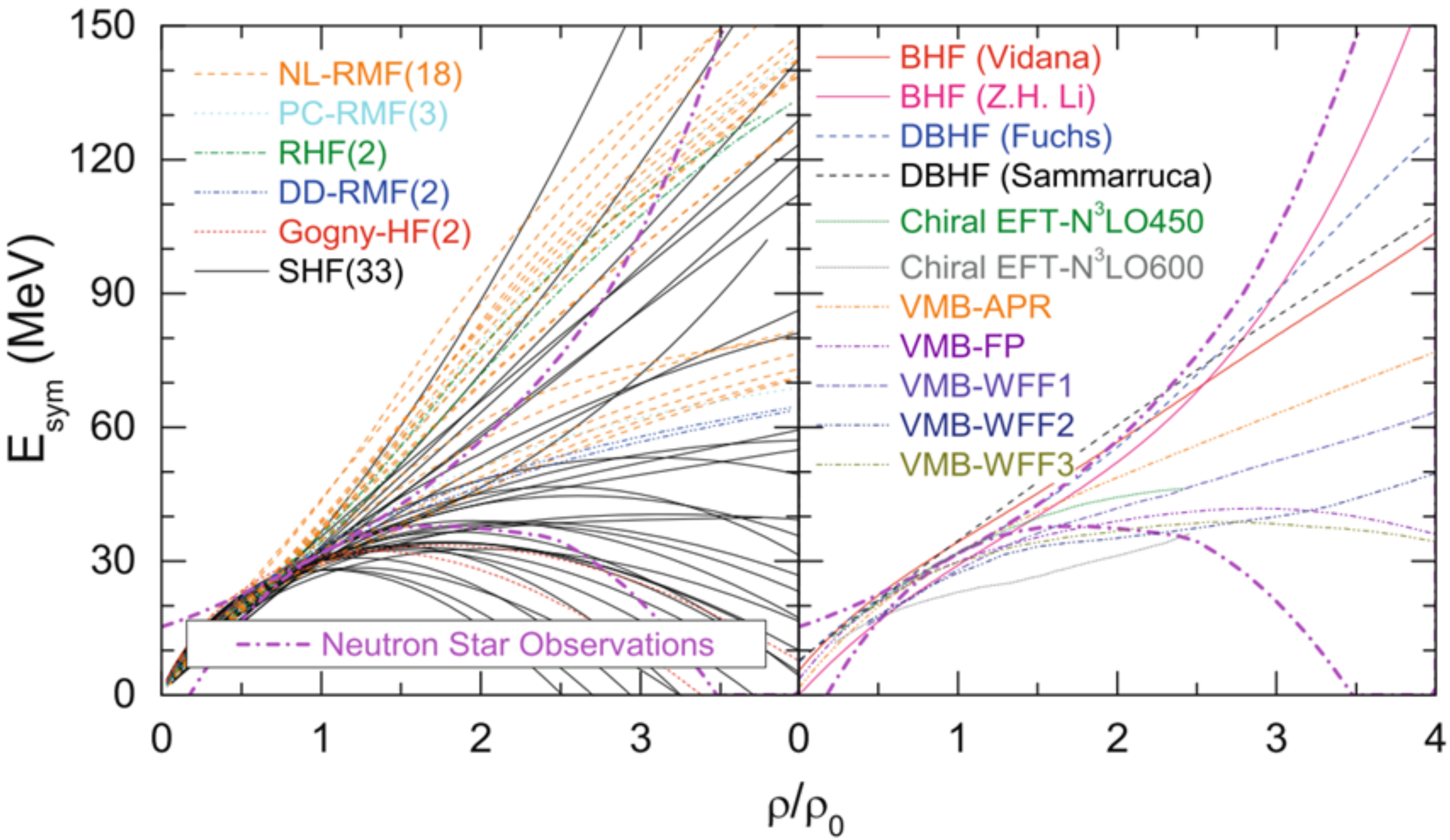


~饱和密度
Physics at fm scale
(~10 fm)

数倍饱和密度
Physics at km scale
(~10 km)

对称能的不确定性

Zhang N-B, Li B-A, The European Physical Journal A, 2019, 55(3): 39.



- 远离饱和密度处的对称能还存在很大的不确定性
- 不确定性的来源?

不确定性来源

√通常已考虑

✦ **Statistical error**

- Uncertainty propagation:

- Numerical uncertainty (e.g., Monte Carlo)

Large statistical error:

×通常未考虑

✦ **Systematic error** from imperfect modeling.

- Inter-model uncertainties and model dependence.
- Could be estimated by compare different models.

Dobaczewski, Nazarewicz and Reinhard, JPG41 (2014) 074001

Large systematic error:

如何自洽考虑两类不确定性?

贝叶斯分析-模型内不确定性

- **贝叶斯定理**：用观测量的信息更新已有的认识，得到参数的后验分布

Under model $\mathcal{M}$' s assumption

The likelihood function
of observing y given the model $\mathcal{M}$ predictions at Θ

The prior probability
of quantities of interest Θ before being confronted with the experimental measurements y

$$p(\mathcal{O}|\ \mathbf{y},\mathcal{M}) = \frac{\mathcal{L}(\mathbf{y}|\ \mathcal{O},\mathcal{M})\pi(\mathcal{O}|\ \mathcal{M})}{p(\mathbf{y}|\ \mathcal{M})}$$

The posterior probability
distribution of quantities of interest Θ given experimental measurements y

The marginal likelihood/Evidence
The probability of model $\mathcal{M}$ giving experimental measurements y

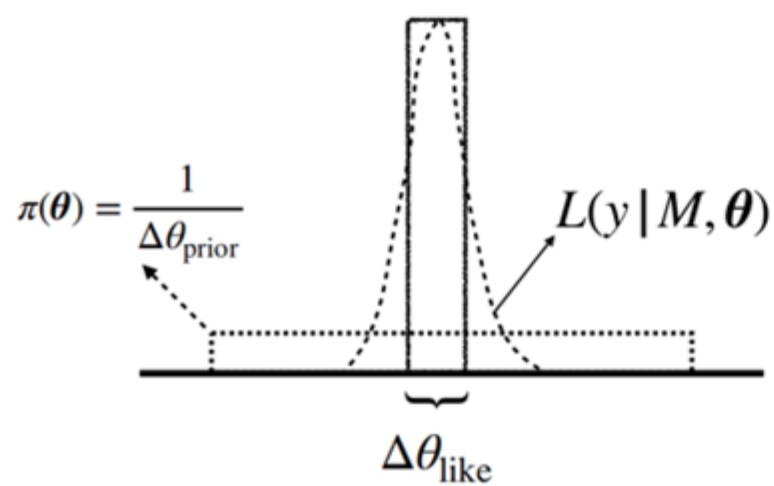
- Evidence

$$p(y \mid M) = \int d\boldsymbol{\theta} L(y \mid M, \theta)\pi(\boldsymbol{\theta})$$

$$\approx L\left(y \mid M, \theta_{\mathrm{ML}}\right)\left(\Delta\theta_{\mathrm{like}}/\Delta\theta_{\mathrm{prior}}\right)^{N_\theta}$$

Maximum likelihood

No. of parameter, model complexity



Udo von Toussaint, Rev. Mod. Phys. 83, 943 (2011)

贝叶斯模型平均(BMA)-模型间不确定性

- 模型权重=模型后验概率
- 模型后验概率包含两方面贡献：模型先验+贝叶斯证据

- Each model's contribution is weighted by its model posterior probability

$$p(\mathcal{O}|\boldsymbol{y}) = \sum_i p(\mathcal{O}|\boldsymbol{y}, \mathcal{M}_i)\, p(\mathcal{M}_i|\boldsymbol{y})$$

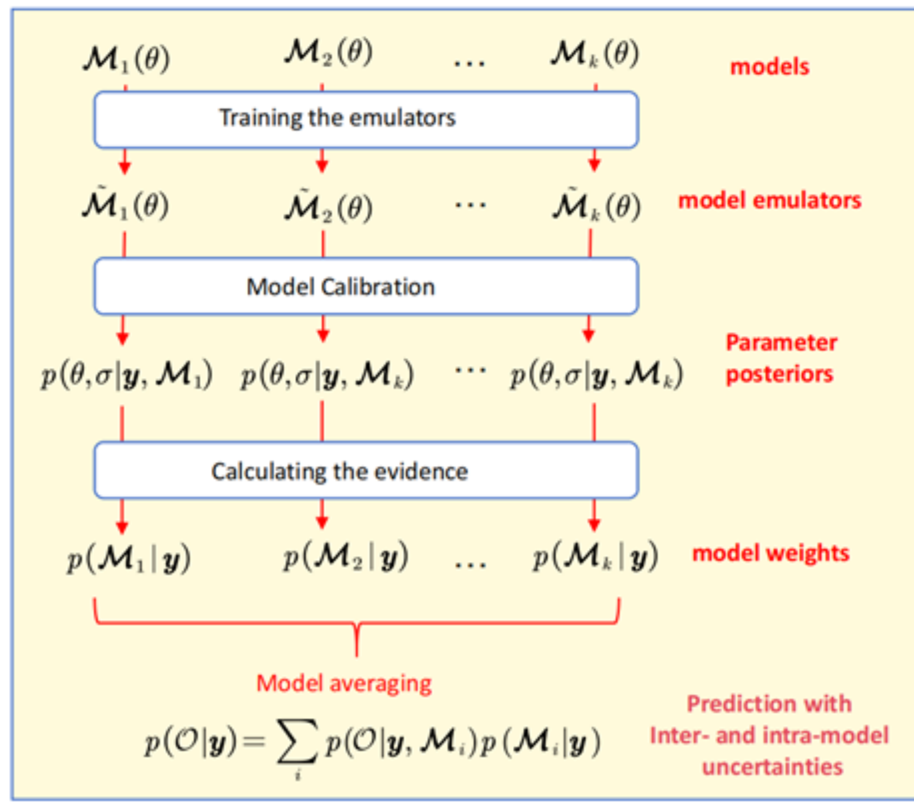
- Model posterior probability: a weighting factor

$$p(\mathcal{M}_i\,|\,\boldsymbol{y}) = \frac{p(\boldsymbol{y}\,|\,\mathcal{M}_i)\,\pi(\mathcal{M}_i)}{\sum_\ell p\,(\boldsymbol{y}\,|\,\mathcal{M}_\ell)\,\pi(\mathcal{M}_\ell)}$$

- The model prior $\pi(M_i)$ is our preference on M_i before seeing the data

- Bayesian evidence/marginal likelihood: measures the probability that the model reproduces the experimental data

$$p(\boldsymbol{y}\,|\,\mathcal{M}_i) = \int p(\boldsymbol{y}|\theta_i,\sigma_i,\mathcal{M}_i)\,\pi(\theta_i,\sigma_i|\mathcal{M}_i)\,d\theta_i d\sigma_i$$



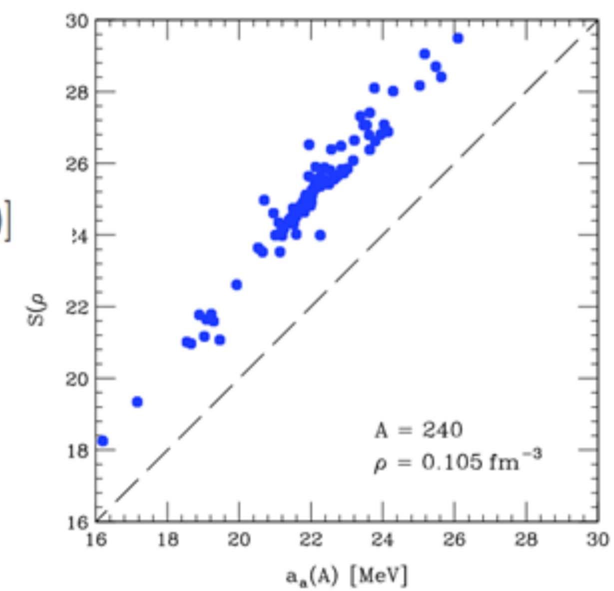
中质子有效化学势差

□ 中质子有效化学势差$\Delta\mu^*_{pn}$敏感于低密对称能

- Effective chemical potential

$$\mu_{\rm n} = \frac{\partial B(N,Z)}{\partial N} \approx \frac{B(N+2,Z)-B(N-2,Z)}{4}, \quad (1)$$
$$\mu_{\rm p} = \frac{\partial B(N,Z)}{\partial Z} \approx \frac{B(N,Z+2)-B(N,Z-2)}{4}, \quad (2)$$

Pawel Danielewicz,Jenny Lee, Nuclear Physics A 922 (2014)
M. Centelles, Phys. Rev. Lett. 102, 122502 (2009)
L.-W. Chen, Phys. Rev. C 83, 044308 (2011).
N. Wang, L. Ou, and M. Liu, Phys. Rev. C 87, 034327(2013)



- Proton-neutron chemical potential differences

$$\Delta\mu^*_{\rm pn} = \frac{1}{4}\left[B(N,Z+2)-B(N,Z-2) - B(N+2,Z)+B(N-2,Z)\right]$$

- Semi empirical mass formula

$$B(N,Z) = a_{\rm v}A - a_{\rm s}A^{2/3} - a_{\rm c}\frac{Z^2}{A^{1/3}} - a_{\rm sym}I^2A + E_{\rm mic},$$

pairing and shell effects

- Expected sensitivity

$$\Delta\mu^*_{\rm pn} \simeq a_{\rm c}\left[\frac{1-Z}{(A-2)^{1/3}} - \frac{1+Z}{(A+2)^{1/3}}\right] + a_{\rm sym}\frac{4A^2I}{A^2-4} \simeq -2a_{\rm c}\frac{Z}{A^{1/3}} + 4a_{\rm sym}I$$

$$\Delta\mu^*_{\rm pn} \propto a_{\rm sym} \approx E_{\rm sym}(\rho_r)$$

非相对论和相对论密度泛函

- **模型**：非相对论Skyrme密度泛函(EDFs)+非线性相对论平均场模型(RMF)
- **参数**：EOS宏观量-微观耦合参数
- **抽样**：50 Skyrme+50 RMF EDFs

$G_s, G_v, W_0 \quad m^*_{s,0}/m, m^*_{v,0}/m \qquad \rho_0, E_0(\rho_0), K_0 \quad E_{\rm sym}(\rho_0), L \qquad m^*_{\rm Dirac}/m, m_\sigma, c_\omega$

Analytical Transformation with pseudo-observables in nuclear matter

Standard Skyrme Hartree Fock (SHF) Model

$$
\begin{aligned}
v(\boldsymbol{r}_1, \boldsymbol{r}_2) &= t_0(1 + x_0 P_\sigma)\delta(r) \\
&+ \frac{1}{2} t_1(1 + x_1 P_\sigma)[\mathbf{k}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{k}^2] \\
&+ t_2(1 + x_2 P_\sigma)\mathbf{k}' \cdot \delta(r) k \\
&+ \frac{1}{6} t_3(1 + x_3 P_\sigma)[\rho(R)]^\alpha \delta(r) \\
&+ i W_0 \sigma \cdot [\mathbf{k}' \times \delta(\mathbf{r})\mathbf{k}]
\end{aligned}
$$

$t_0 \sim t_3, x_0 \sim x_3, \alpha, W_0$

Non-linear Relativistic Mean-Field (RMF) Model

$$
\begin{aligned}
\mathcal{L} =& \bar{\psi}\left(i\partial_\mu \gamma^\mu - m\right)\psi - e\bar{\psi}\gamma_\mu \frac{1+\tau_3}{2} A^\mu \psi - \frac{1}{4} F^{\mu\nu} F_{\mu\nu} \\
&+ g_\sigma \sigma \bar{\psi}\psi - g_\omega \omega_\mu \bar{\psi}\gamma^\mu \psi - g_\rho \vec{\rho}_\mu \bar{\psi}\gamma^\mu \vec{\tau}\psi \\
&+ \frac{1}{2}\partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{3} b_\sigma M \left(g_\sigma \sigma\right)^3 - \frac{1}{4} c_\sigma \left(g_\sigma \sigma\right)^4 \\
&- \frac{1}{4}\omega_{\mu\nu}\omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu + \frac{1}{4} c_\omega \left(g_\omega^2 \omega_\mu \omega^\mu\right)^2 \\
&- \frac{1}{4}\rho_{\mu\nu}\rho^{\mu\nu} + \frac{1}{2} m_\rho^2 \vec{\rho}_\mu \vec{\rho}^\mu + \frac{1}{2}\Lambda_V \left(g_\rho^2 \vec{\rho}_\mu \vec{\rho}^\mu\right)\left(g_\omega^2 \omega_\mu \omega^\mu\right),
\end{aligned}
$$

$g_\sigma, g_\omega, g_\rho, b_\sigma, c_\sigma, c_\omega, \Lambda_V, m_\sigma$

$\Delta\mu^*_{\rm pn}$ for doubly magic nuclei

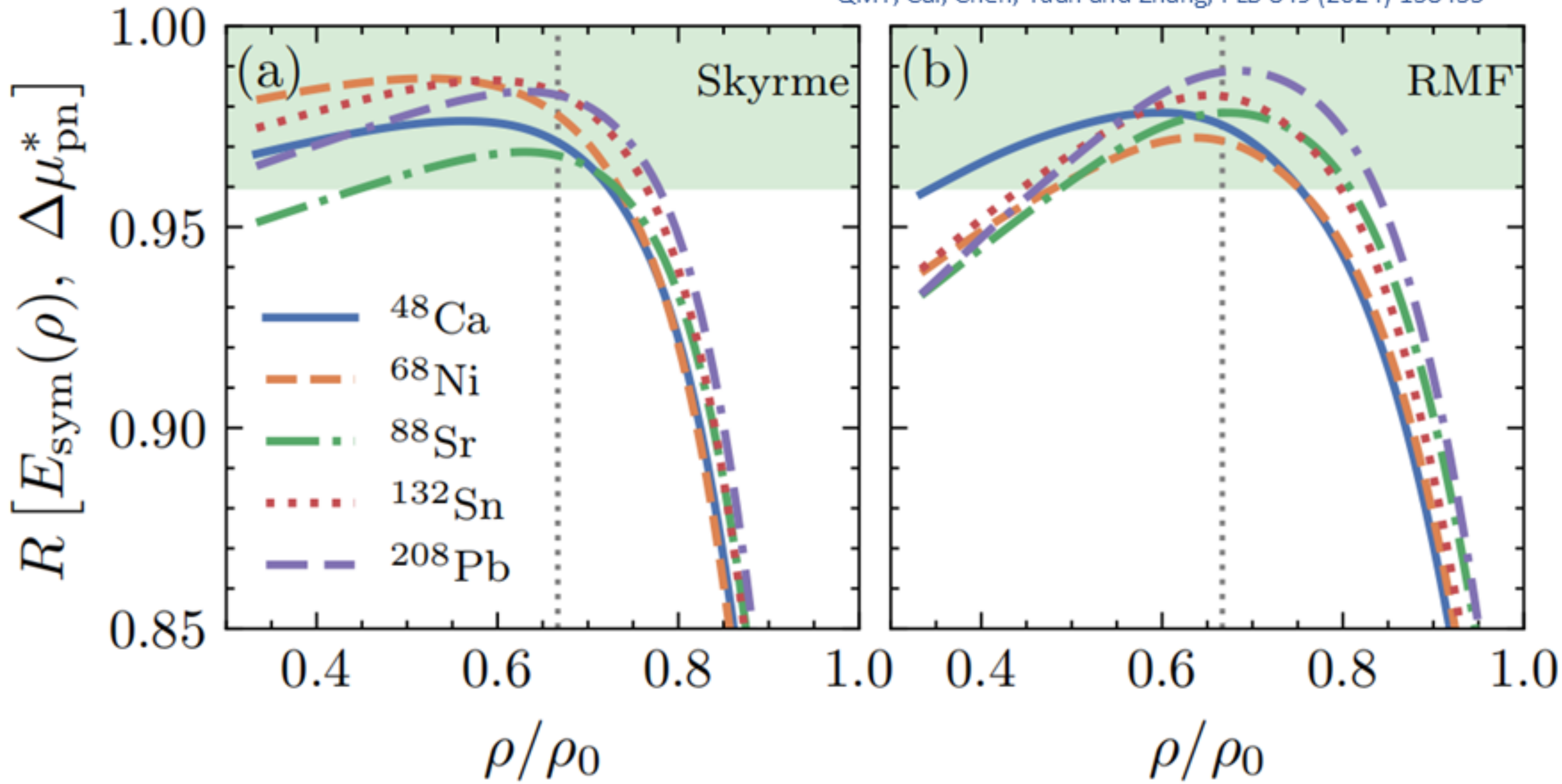
$E_{\rm sym}(\rho)$ at different densities

敏感性分析

- $\Delta\mu^*_{pn}$ 和对称能在低密处呈现强关联
- 最强关联的密度在$2\rho_0/3$左右

$$R[A,B] = \frac{\mathrm{Cov(A,B)}}{\sqrt{\mathrm{Var(A)Var(B)}}}$$

QMY, Cai, Chen, Yuan and Zhang, PLB 849 (2024) 138435

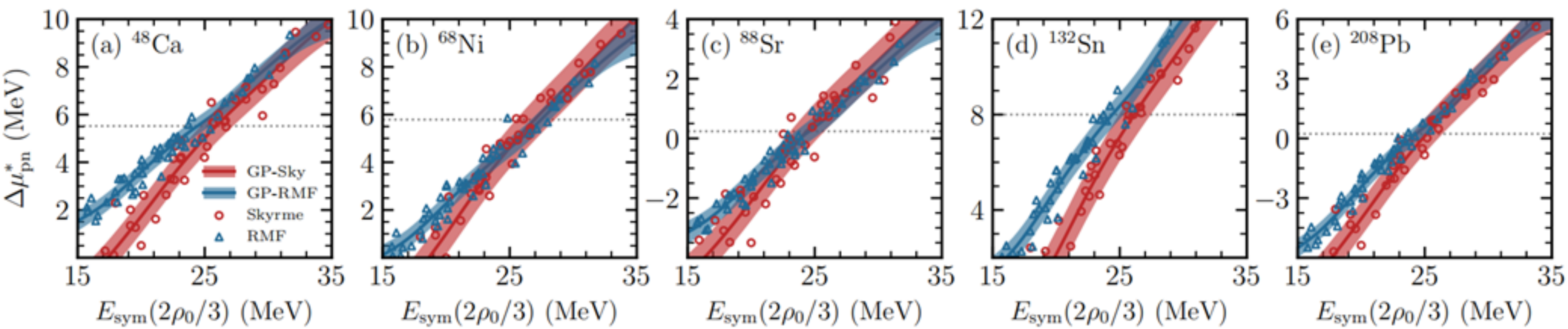


高斯过程

利用50组Skyrme密度泛函50组RMF分别构建高斯过程

M. Plumlee, O. Surer, S. M. Wild, and M. Y.-H.Chan, surmise 0.2.0, https://surmise.readthedocs.io/en/latest/

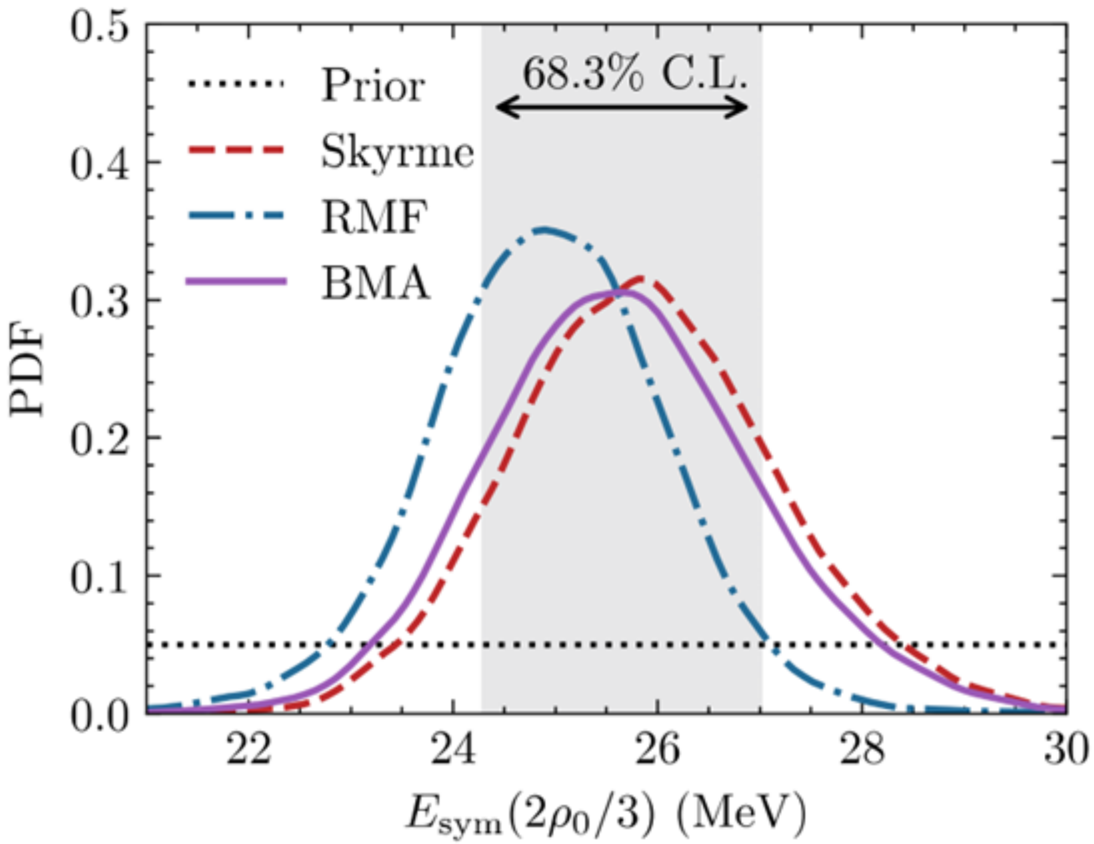
- 高斯过程给出了预测的不确定性
- Skyrme EDF和非线性相对论平均场模型间存在差异 **Model dependence!**



QMY, Cai, Chen, Yuan and Zhang, PLB 849 (2024) 138435

$2/3\rho_0$ 对称能

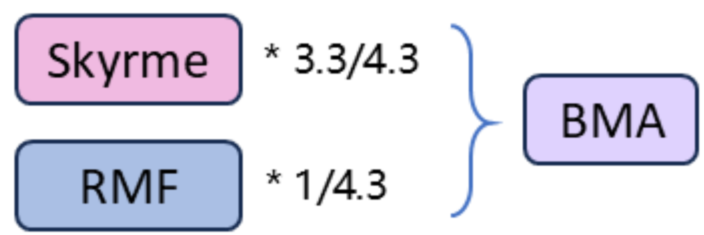
- RMF和Skyrme提取的对称能存在差异
- Skyrme EDFs描述中质子有效化学势差的能力更强
- BMA包含了**intra-model uncertainty**和**inter-model uncertainty**，给出了统计上更可靠的估计



- Model posterior probability

$$p(\mathcal{M}_i|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\mathcal{M}_i)\pi(\mathcal{M}_i)}{\sum_\ell p(\boldsymbol{y}|\mathcal{M}_\ell)\pi(\mathcal{M}_\ell)}$$

- Equal prior preference
- Evidence ratio Sky/RMF ≈ 3.3

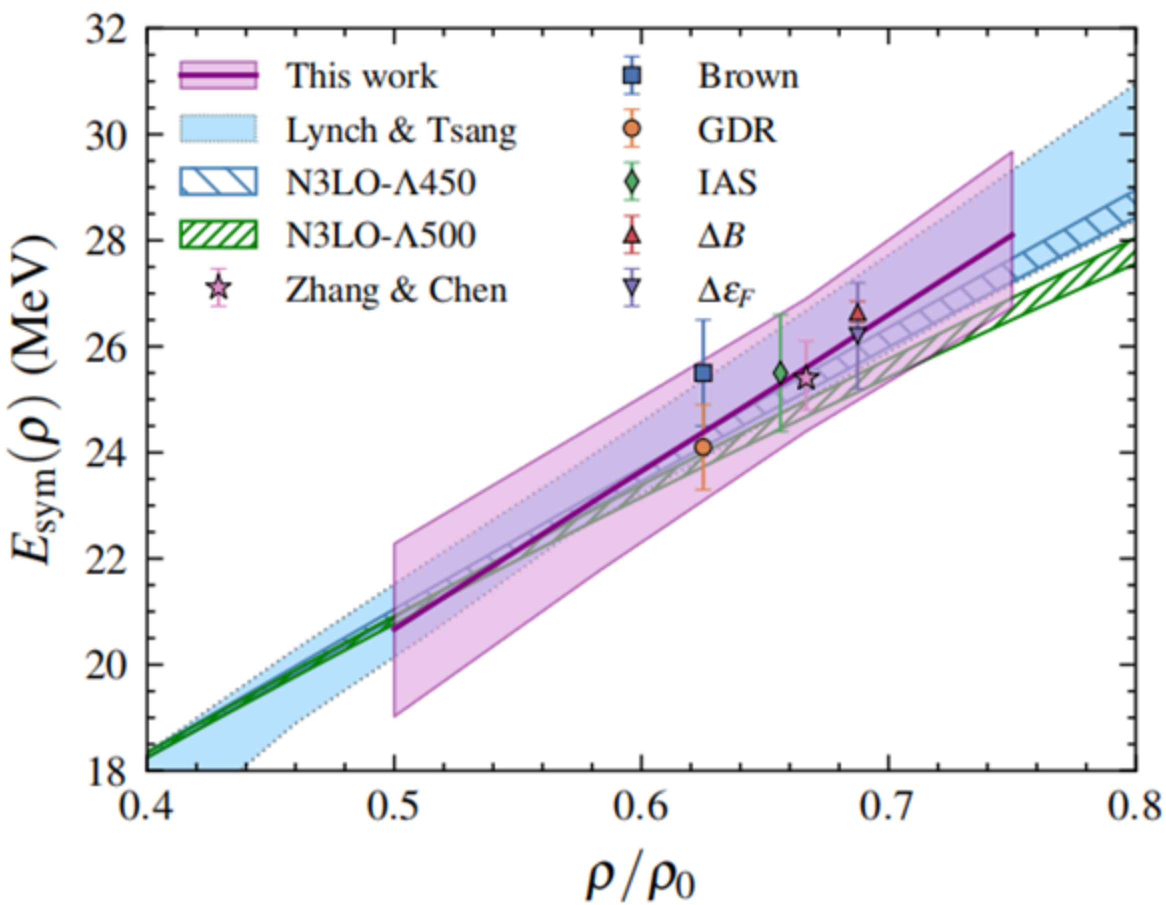


- $E_{\rm sym}(2/3\rho_0)$ is inferred to be $25.6^{+1.4}_{-1.3}$ MeV

QMY, Cai, Chen, Yuan and Zhang, PLB 849 (2024) 138435

$1/2\sim3/4\rho_0$对称能

- 利用贝叶斯平均，可提取得到$\frac{1}{2}\sim\frac{3}{4}\rho_0$低密区域的对称能
- 与微观理论计算和其他观测量的约束结果符合



- Brown: Doubly magic nuclei
  B.A.Brown, Phys. Rev. Lett. 111, 232502 (2013)
- Lynch & Tsang: various terrestrial and astrophysical constraints
  W.G.Lynch and M.B.Tsang, Phys. Lett. B. 830, 137098 (2022)
- Zhang & Chen: Doubly magic nuclei+PREX+CREX
  Z. Zhang and L.-W. Chen, Phys. Rev. C. 108, 024317 (2023)
- GDR: Giant dipole resonance
  L. Trippa *et al*, Phys. Rev. C 77, 061304 (2008)
- IAS: Isobaric analog states
  Pawel Danielewicz, Jenny Lee, Nuclear Physics A 922 (2014)
- ΔB: Isotope binding energy difference
  Z. Zhang and L.-W. Chen, Phys. Lett. B 726, 234 (2013)
- $\Delta\varepsilon_F$: Fermi energy difference
  N. Wang, L. Ou, and M. Liu, Phys. Rev. C 87, 034327(2013)

QMY, Cai, Chen, Yuan and Zhang, PLB 849 (2024) 138435

总结

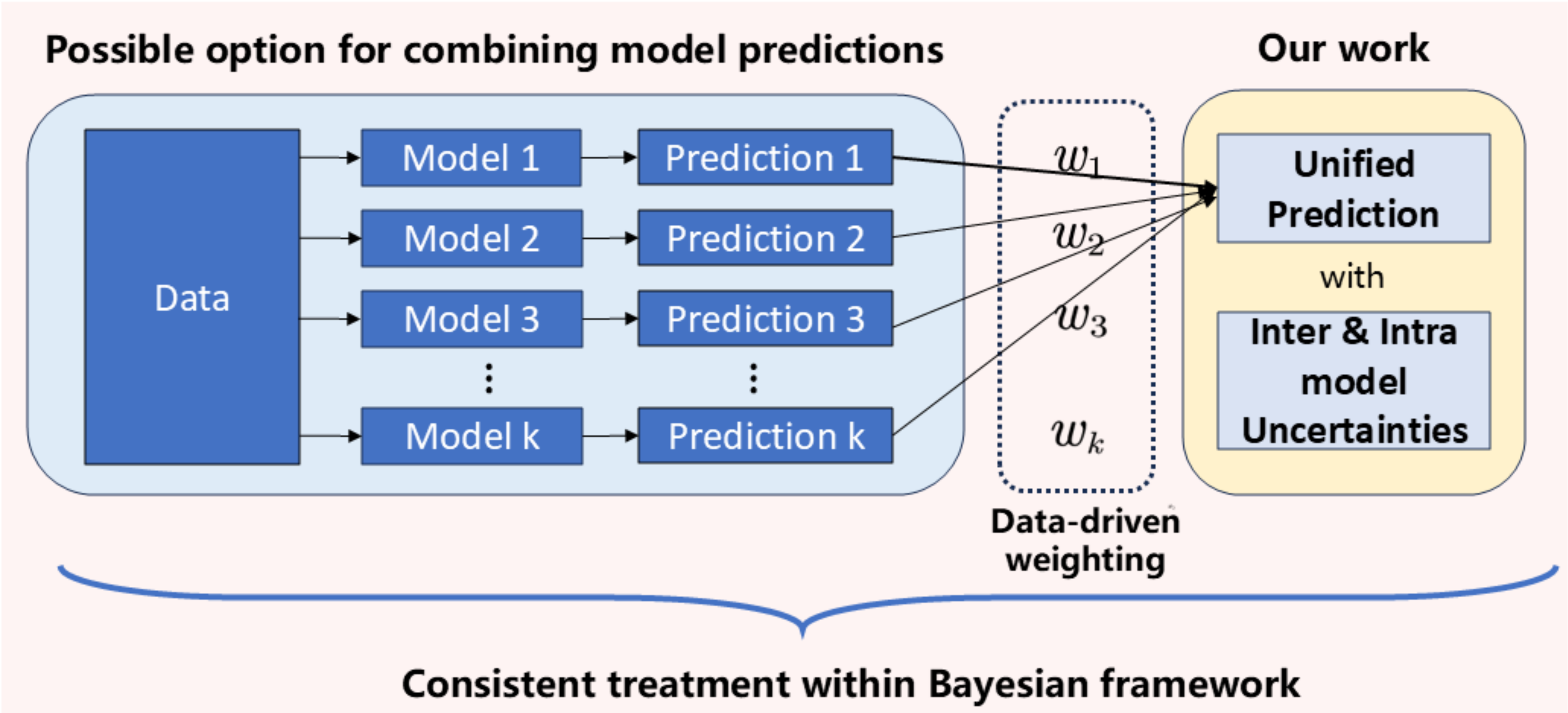
- 在非相对论Skyrme密度泛函和非线性相对论平均模型下，我们发现丰中子核的中质子有效化学势差 $\Delta\mu^*_{pn}$ 敏感于$2\rho_0/3$处的对称能
- 利用贝叶斯模型平均方法，我们提取了低密对称能 $25.6^{+1.4}_{-1.3}$ MeV
- 和微观理论计算及其他观测量的约束结果相符

- 在贝叶斯的框架下，考虑更多的实验观测量和更多的理论模型

谢谢大家！

解决途径：模型平均

- **定义**：给予每个模型一个权重，将不同模型预测结合在一起
- **要求**：模型权重由数据决定，需要反映模型描述数据的能力
- **优势**：能同时包含模型内部和模型之间的不确定性



EDFs参数经验范围

共同参数范围

$$\rho_0 = 0.155 \pm 0.01\text{fm}^{-3}; E_0(\rho_0) = -16 \pm 0.6\text{MeV};\ K_0 = 240 \pm 20\text{MeV};$$
$$E_{\text{sym}}(\rho_0) = 34 \pm 6\text{MeV};\ L = 100 \pm 100\text{MeV}$$

其他参数范围

$$\theta_{\text{RMF}} = \{\rho_0,\ E_0(\rho_0),\ K_0,\ E_{\text{sym}}(\rho_0),\ L,\ m^*_{\text{Dirac}}, m_\sigma, c_\omega\},$$

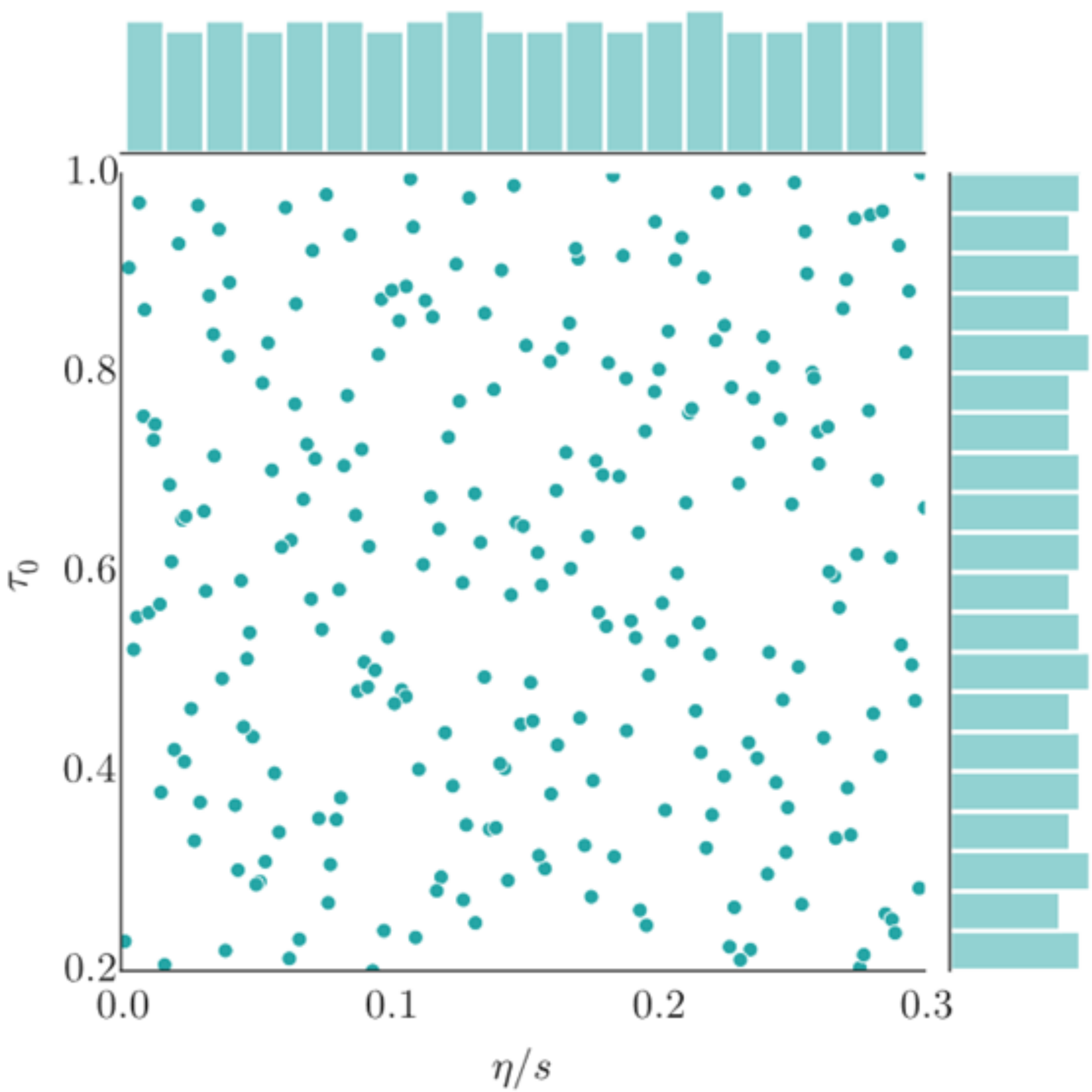
$$0.55 \le m^*_{\text{Dirac}} / m \le 0.65;$$
$$480 \le m_\sigma \le 520(\text{MeV});$$
$$0 \le c_\omega \le 0.012$$

$$\theta_{\text{Sky}} = \{\rho_0,\ E_0(\rho_0),\ K_0,\ E_{\text{sym}}(\rho_0),\ L,\ G_S,\ G_V,\ m^*_{s,0},\ m^*_{v,0}, W_0\}.$$

$$110 \le G_S \le 170(\text{MeV} \cdot \text{fm}^5);$$
$$-70 \le G_V \le 70(\text{MeV} \cdot \text{fm}^5);$$
$$90 \le W_0 \le 140(\text{MeV} \cdot \text{fm}^5);$$
$$0.7 \le m^*_{s,0} / m \le 1;$$
$$0.6 \le m^*_{v,0} / m \le 0.9;$$

拉丁超立方抽样

Jonah E. Bernhard, et al. PRC 91, 054910 (2015)



- The minimum distance between points is maximized, thus avoiding large gaps and tight clusters.
- Projections of the design into lower dimensions are uniformly distributed.

协方差矩阵

- Bayes' theorem

$$\color{red}{p(\theta,\sigma|\boldsymbol{y},\mathcal{M})} = \frac{p(\boldsymbol{y}|\theta,\sigma,\mathcal{M})\pi(\theta,\sigma|\mathcal{M})}{p(\boldsymbol{y}|\mathcal{M})} \propto p(\boldsymbol{y}|\theta,\sigma,\mathcal{M})\pi(\theta,\sigma|\mathcal{M})$$

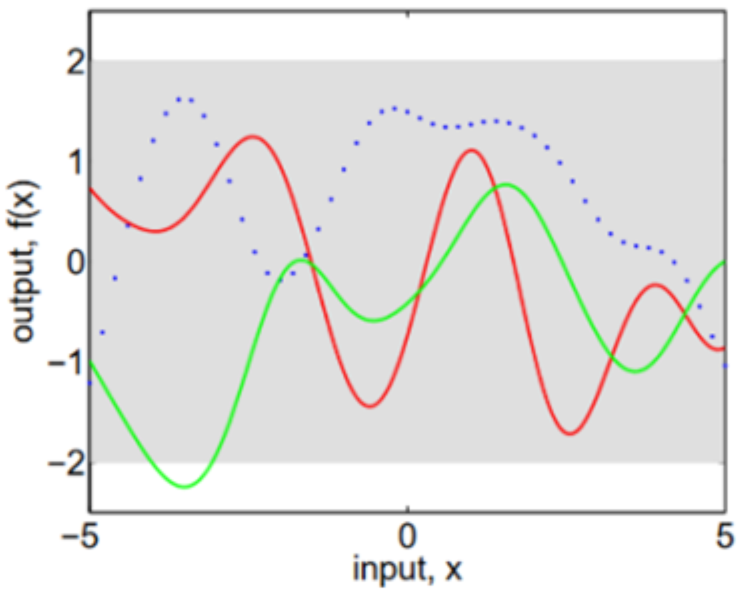
- Likelihood

$$p(\boldsymbol{y}|\theta,\sigma,\mathcal{M}) \propto \exp\left[-\frac{1}{2}(\tilde{\boldsymbol{y}}-\boldsymbol{y})^T\Sigma^{-1}(\tilde{\boldsymbol{y}}-\boldsymbol{y})\right]$$

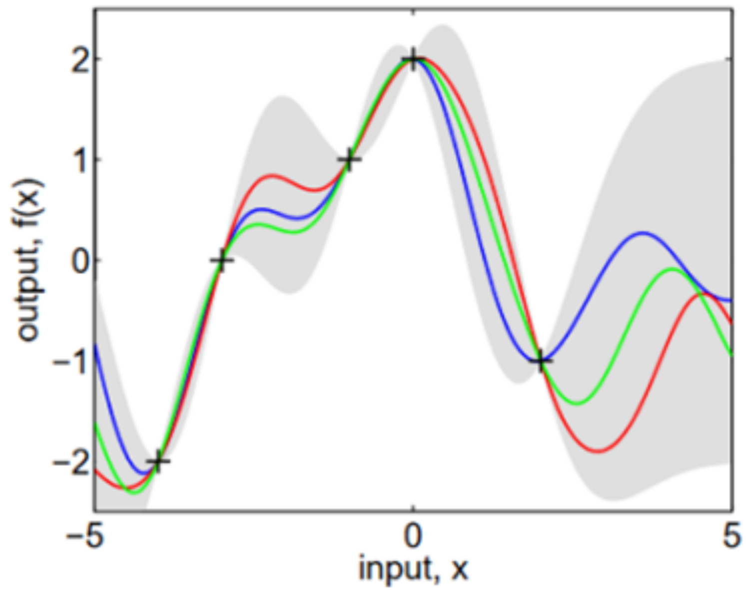
$$\Sigma = \Sigma_{\mathrm{GP}} + \mathrm{diag}(\sigma^2)$$

where σ takes into account the deficiency of theoretical models and experimental errors

高斯过程



(a), prior



(b), posterior

$$\begin{bmatrix} f(\boldsymbol{x}) \\ \boldsymbol{y}^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_f \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \Sigma_{ff} & \Sigma_{fy} \\ \Sigma_{fy}^T & \Sigma_{yy} \end{bmatrix}\right)$$

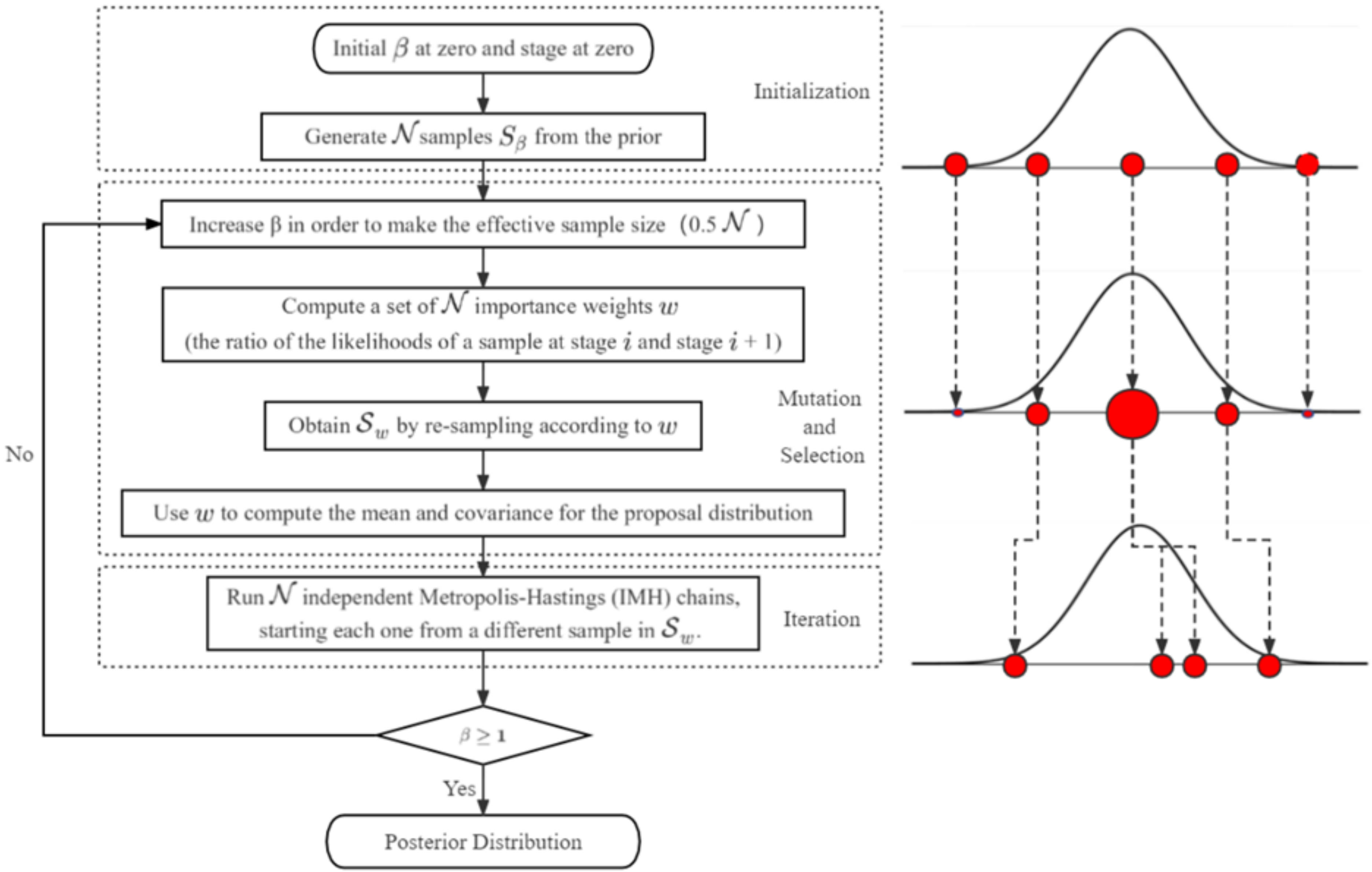
$$\Sigma = \sigma(\boldsymbol{x}, \boldsymbol{x}) = \begin{pmatrix} \sigma(x_1, x_1) & \cdots & \sigma(x_1, x_n) \\ \vdots & \ddots & \vdots \\ \sigma(x_n, x_1) & \cdots & \sigma(x_n, x_n) \end{pmatrix}$$

$$f \sim \mathcal{N}\left(\Sigma_{fy}^T \Sigma_{ff}^{-1} \boldsymbol{y} + \boldsymbol{\mu}_f, \Sigma_{yy} - \Sigma_{fy}^T \Sigma_{ff}^{-1} \Sigma_{fy}\right)$$

Prior covariance

Reduction induced by training points

SMC (Sequential Monte Carlo)



SMC (Sequential Monte Carlo)