PINNferring the Hubble function

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STRUCTURES CLUSTER OF EXCELLENCE

Overview

- Physics-informed neural networks
- Uncertainty quantification
  - Heteroscedastic
  - Repulsive ensembles
- Supernova measurements
- Hubble inference

PINNs

- Idea: machine learning can be enhanced with physics information
- Neural Networks as universal approximators
- Needs only a few labeled data points

$$\dot{\mathbf{u}}(t) = F(\mathbf{u}, t)$$
$$\mathbf{u}^i = \mathbf{g}^i$$

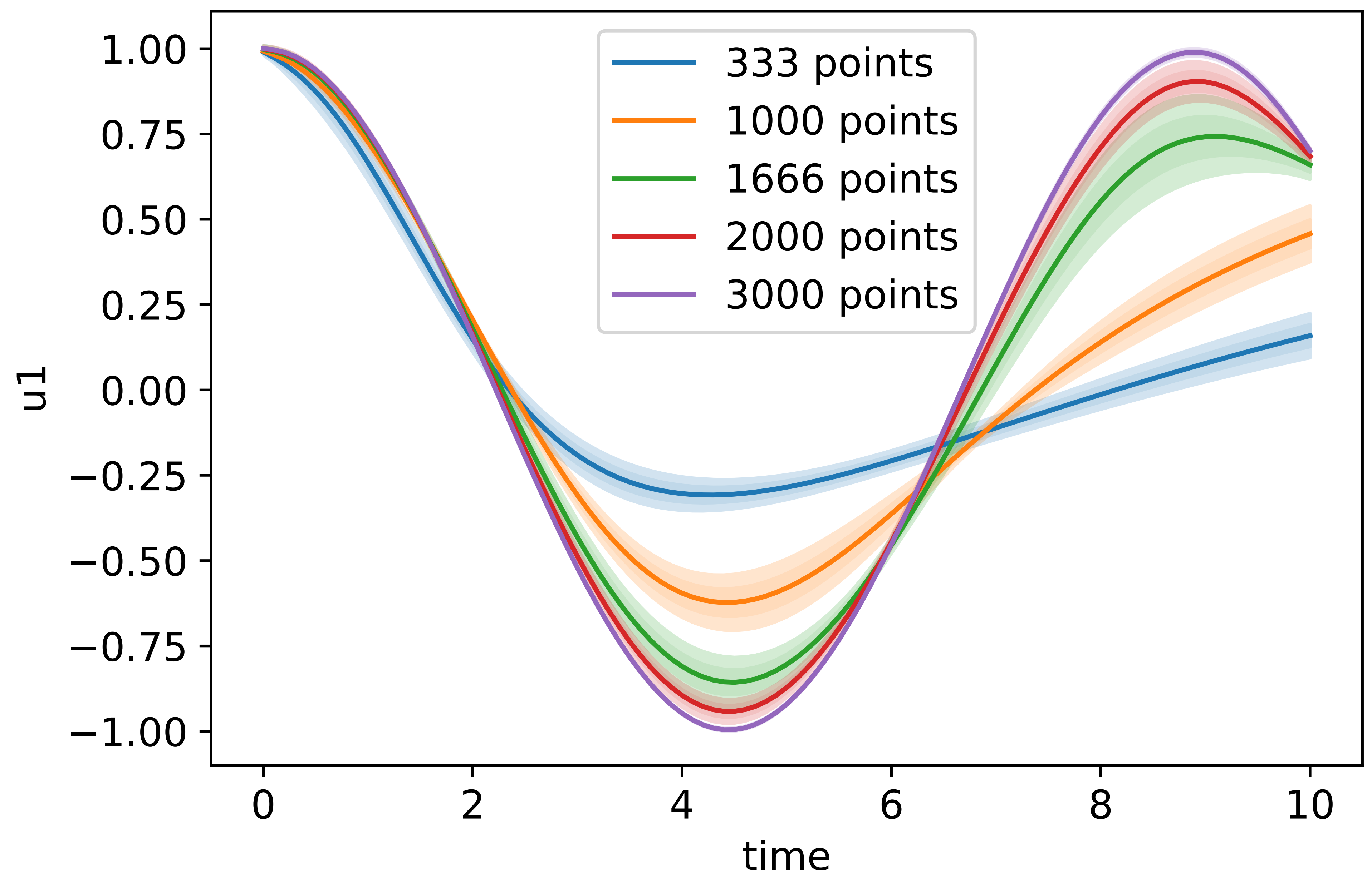
$$\mathscr{L}_{ini} = \left|\mathbf{u}_\theta^i - \mathbf{g}^i\right|^2 = \left|\mathbf{u}_\theta^i - \mathbf{u}^i\right|^2$$
$$\mathscr{L}_{\mathrm{ODE}} = \left|\dot{\mathbf{u}}_\theta(t) - F(\mathbf{u}_\theta, t)\right|^2$$
$$\mathscr{L} = (1-\alpha)\mathscr{L}_{ini} + \alpha\mathscr{L}_{\mathrm{ODE}}$$

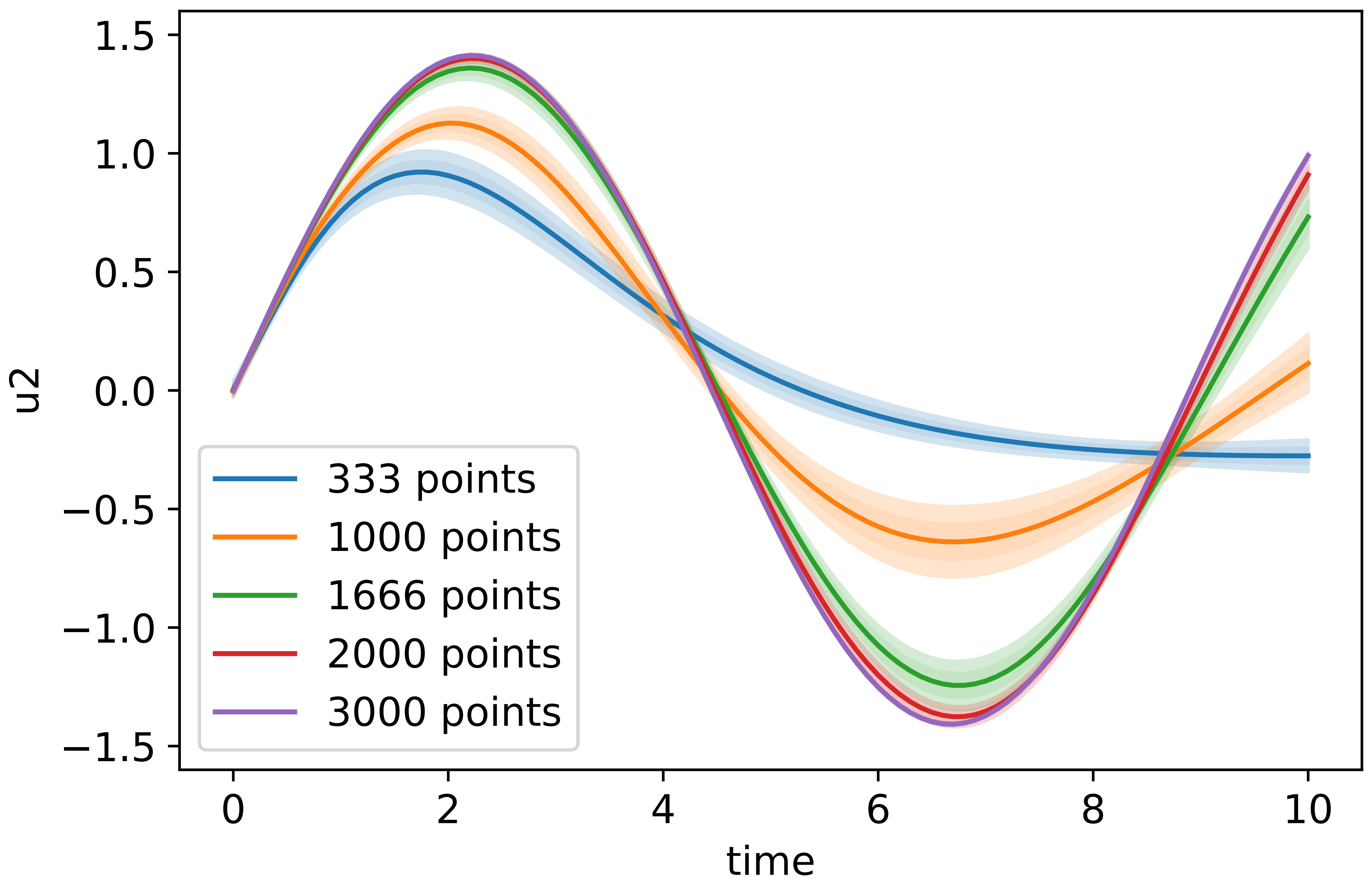
[Raissi et al., 2019,
Cuomo et al., 2022]

Harmonic oscillator

$$\ddot{u} + Au = 0, \quad u(0) = (1,0)^T, \quad \dot{u}(0) = (0,1)^T$$

$$\dot{Y} = -BY = -\begin{pmatrix} 0 & -\mathbb{I} \\ A & 0 \end{pmatrix} Y \qquad Y(t) = \exp(-Bt)\, Y(0)$$





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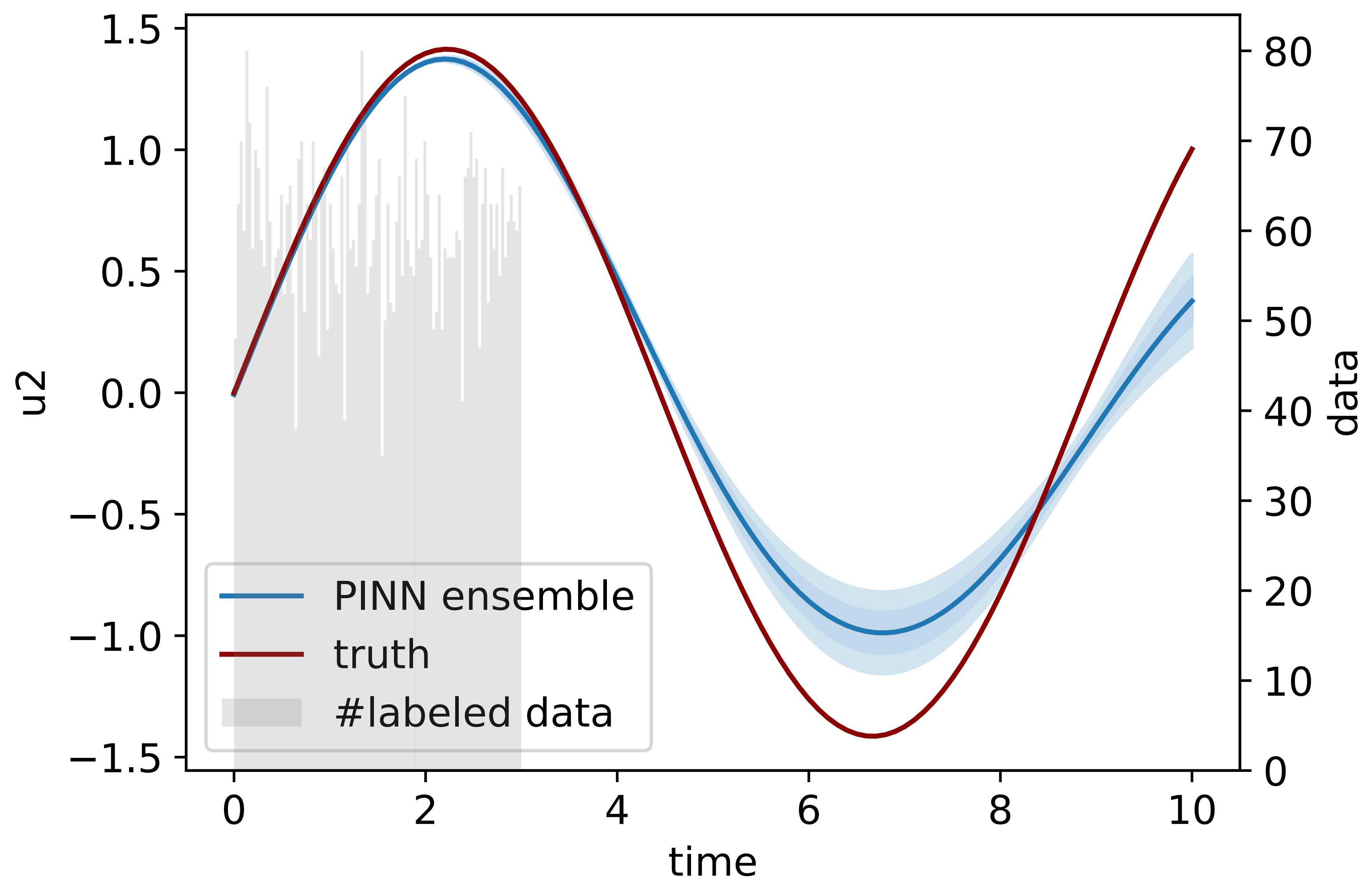

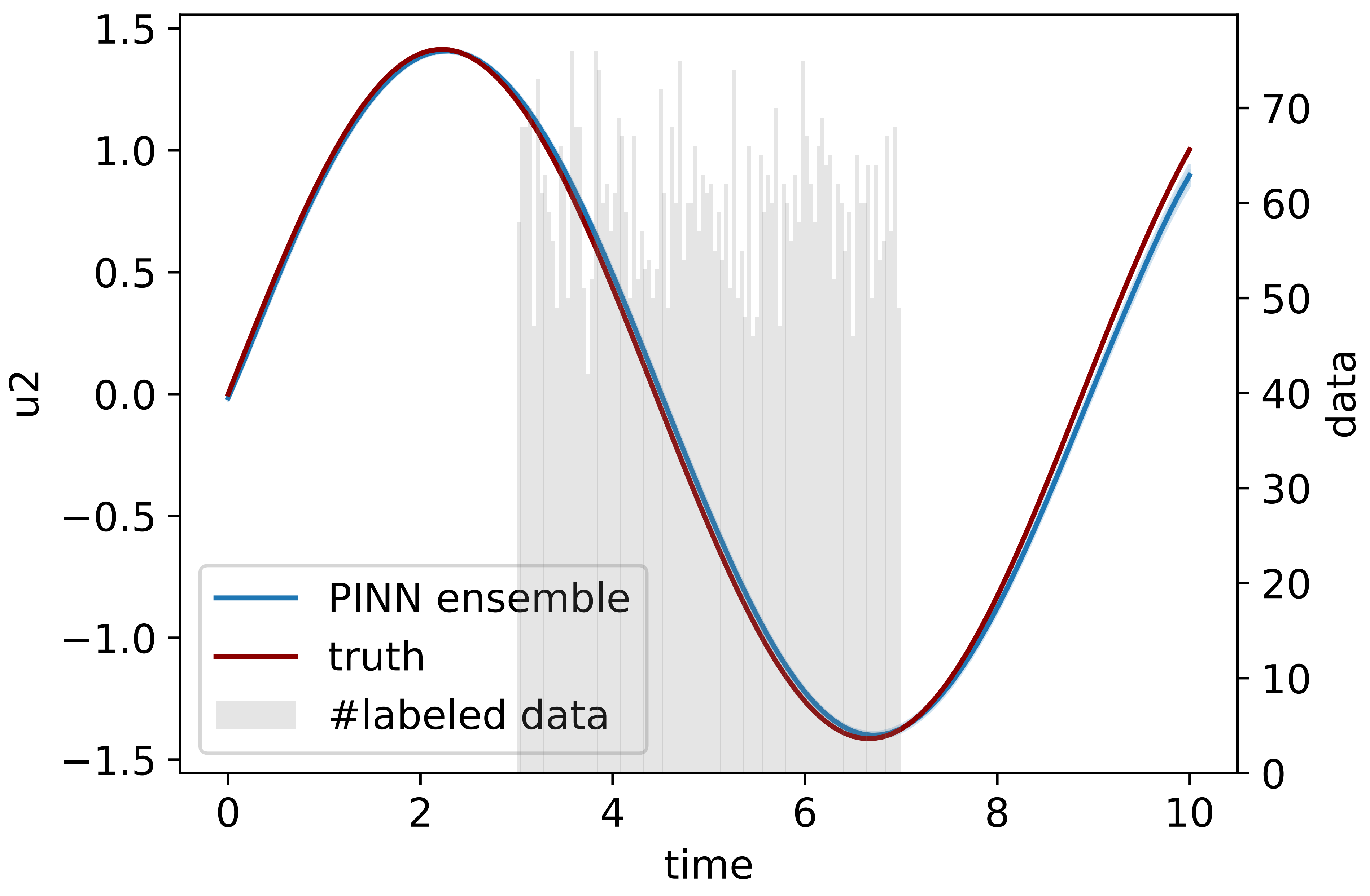

Uncertainty

- Uncertainty of the model given the data
- Construct as information of uncorrelated normal distribution

$$\mathscr{L} = \sum_{Data} - \log p(f(x_i) \,|\, f_\theta(x_i)) \qquad \mathscr{L}_{heteroscedastic} = \sum_{Data} - \log \left[\prod_{dim,k} \frac{1}{\sqrt{2\pi\sigma_\theta^k(x_i)}} \exp\left(-\frac{(f^k(x_i) - f_\theta^k(x_i))^2}{2\left(\sigma_\theta^k(x_i)\right)^2} \right) \right]$$

Uncertainty

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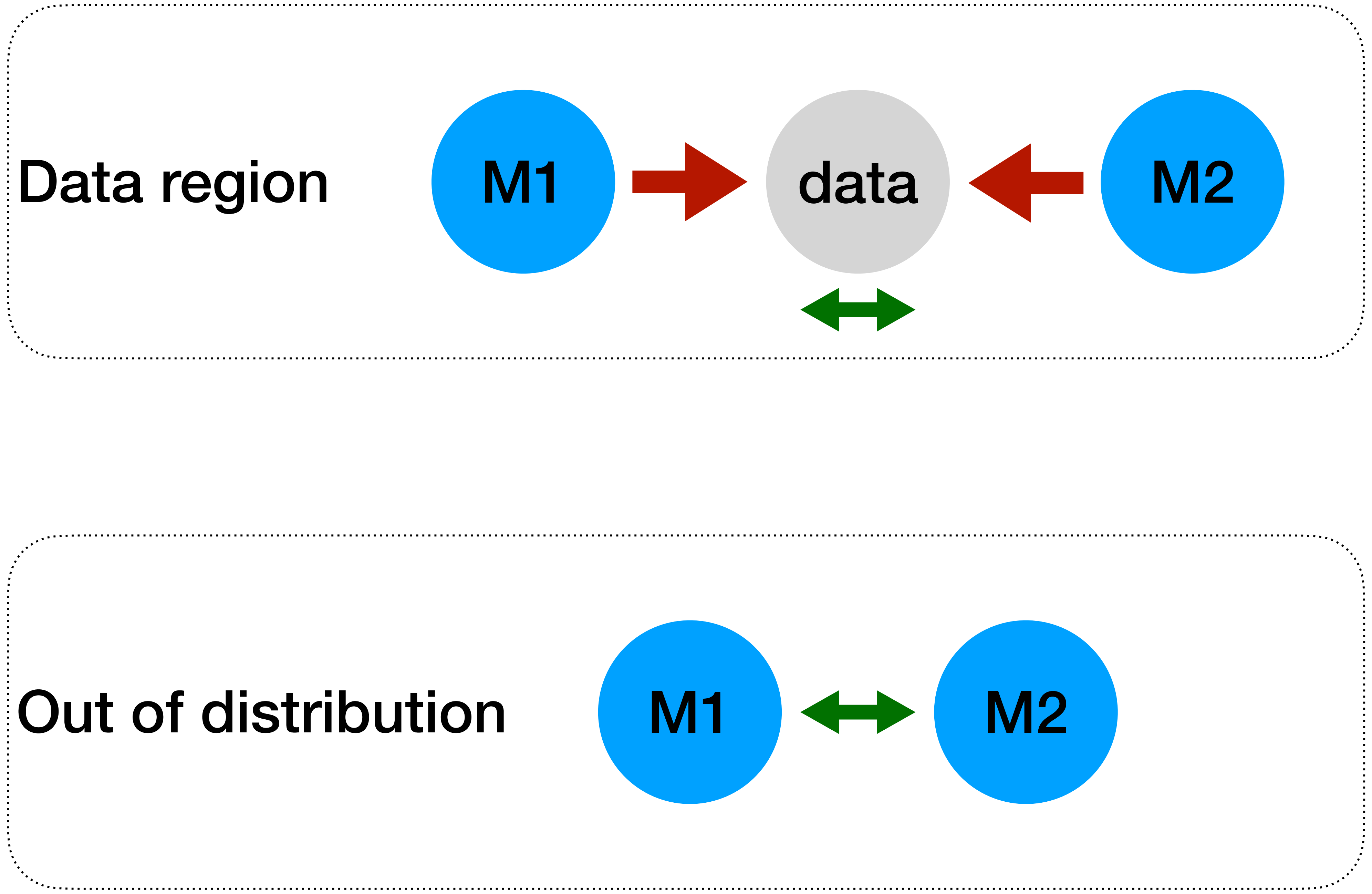
Uncertainty in PINNs

- Uncertainty as a solution to the differential equation
- Implement: double the output parameters

$$\dot{\mathbf{u}}(t) = F(\mathbf{u}, t)$$
$$\mathbf{u}^i = \mathbf{g}^i$$

$$\mathscr{L}_{he} = \sum_{Data} \left[\sum_{dim,k} \left(\frac{\left(\dot{u}_\theta^k(x_i) - F^k(u_\theta(x_i))\right)^2}{2\left(\sigma_\theta^k(x_i)\right)^2} + \log \sigma_\theta^k(x_i) \right) + \frac{n}{2} \log 2\pi \right]$$

Repulsive ensembles



$$\mathcal{L} = \sum_{i=1}^{n} \left[-\frac{1}{B} \sum_{b=1}^{B} \log p(x_b | \theta_i) + \frac{1}{N} \frac{\sum_{j=1}^{n} k(f_{\theta_i}(x), \overline{f_{\theta_j}(x)})}{\sum_{j=1}^{n} k(\overline{f_{\theta_i}(x)}, \overline{f_{\theta_j}(x)})} + \frac{|\theta_i|^2}{2N\sigma^2} \right]$$

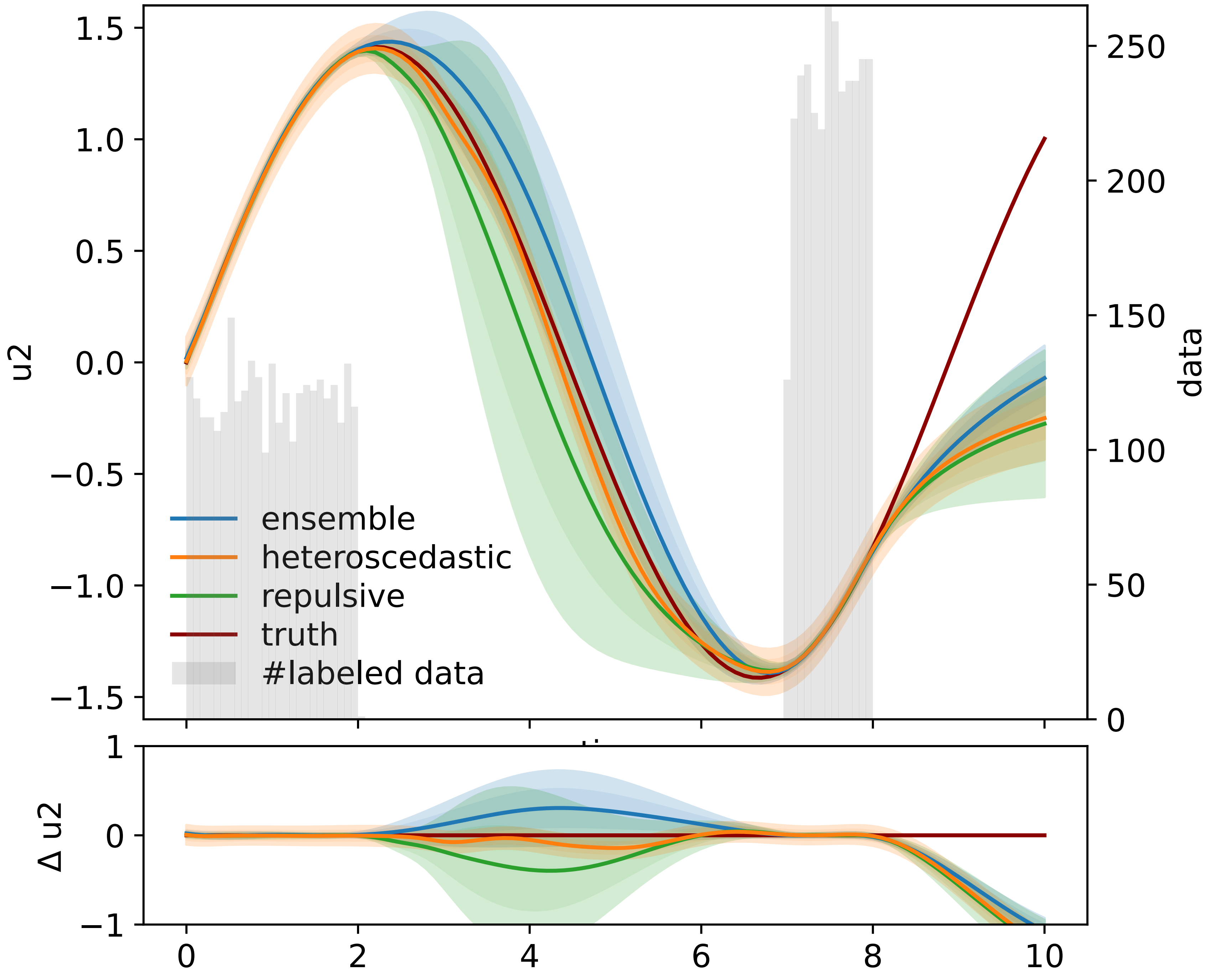
$$k(f_{\theta_i}(x), f_{\theta_j}(x)) = \prod_{b=1}^{B} \exp\left(-\frac{|f_{\theta_i}(x_b) - f_{\theta_j}(x_b)|^2}{h} \right)$$

$$h = \frac{\text{median}_{ij}\left(\sum_b |f_{\theta_i}(x_b) - f_{\theta_j}(x_b)|^2 \right)}{2\log(n+1)}$$

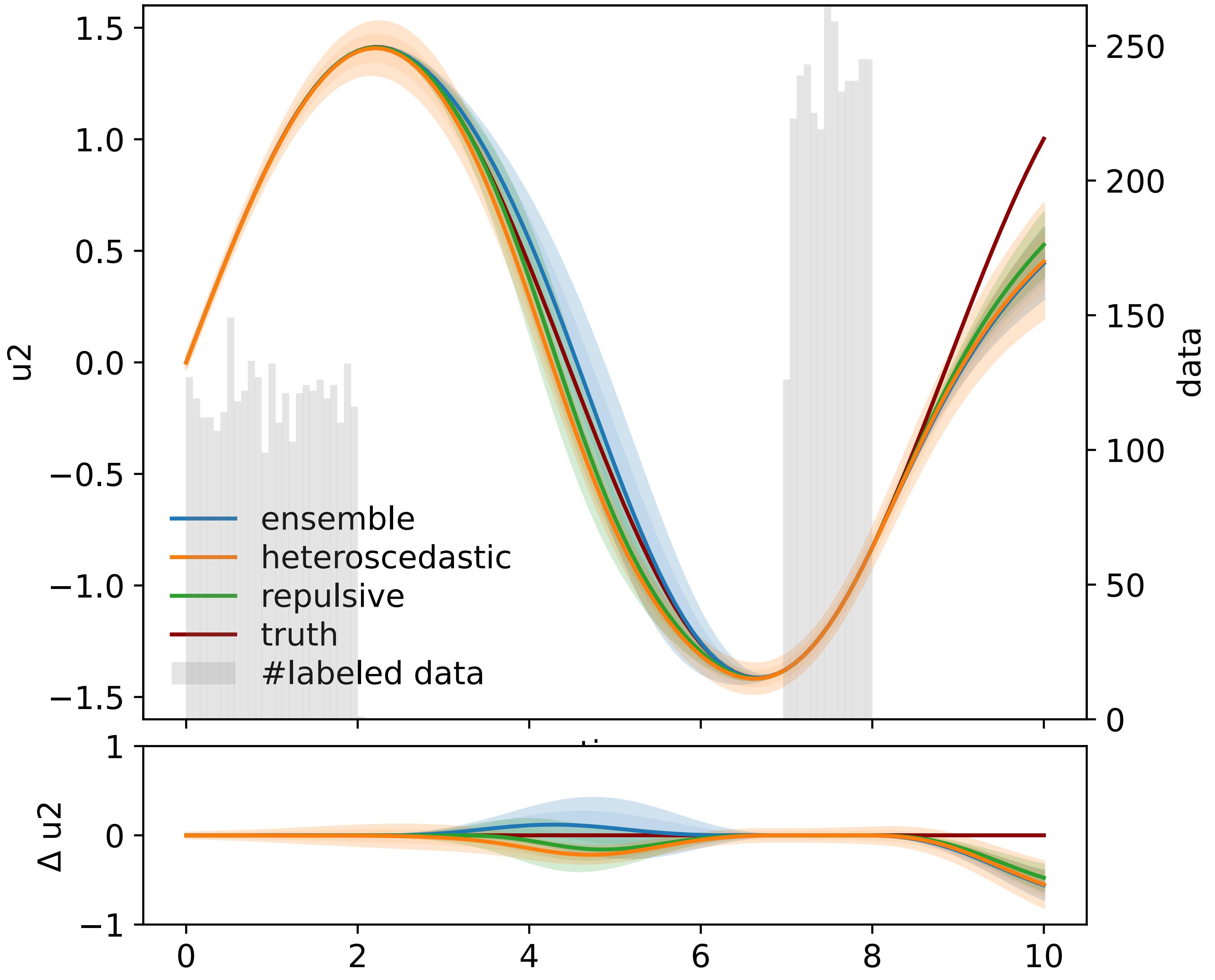
[D'Angelo, Fortuin 2021]

Harmonic oscillator

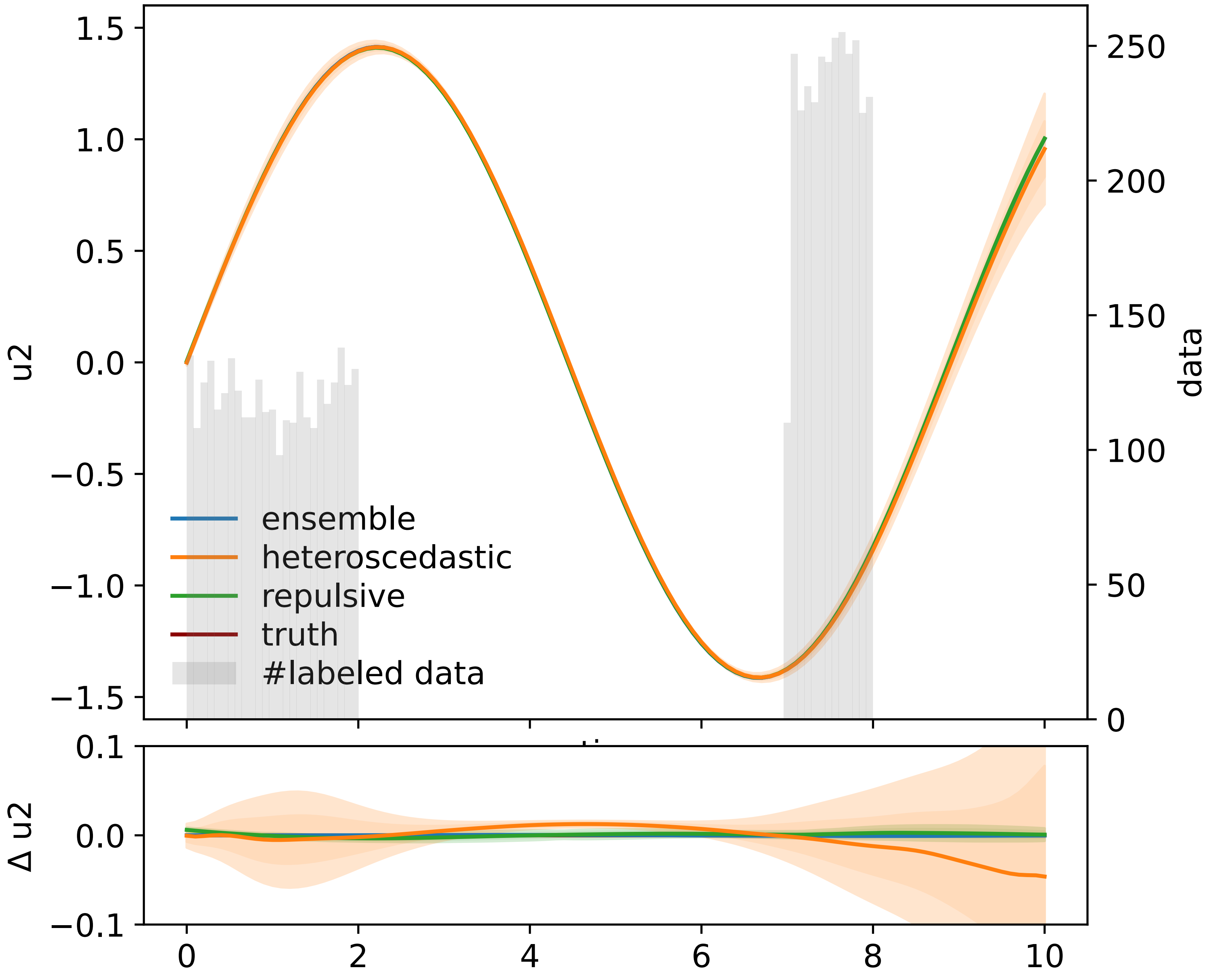
No residual points



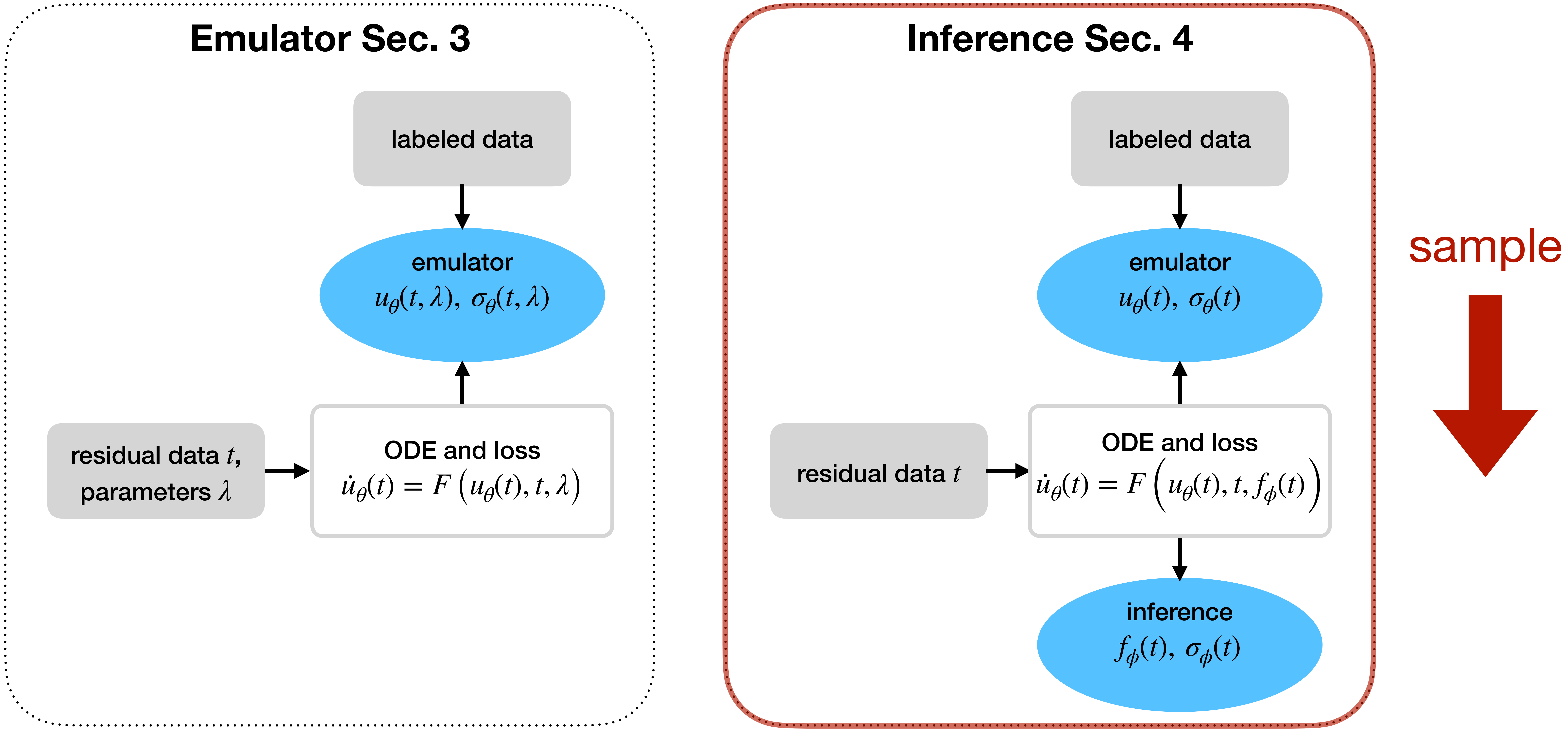
Residual points at labeled data



Residual points everywhere



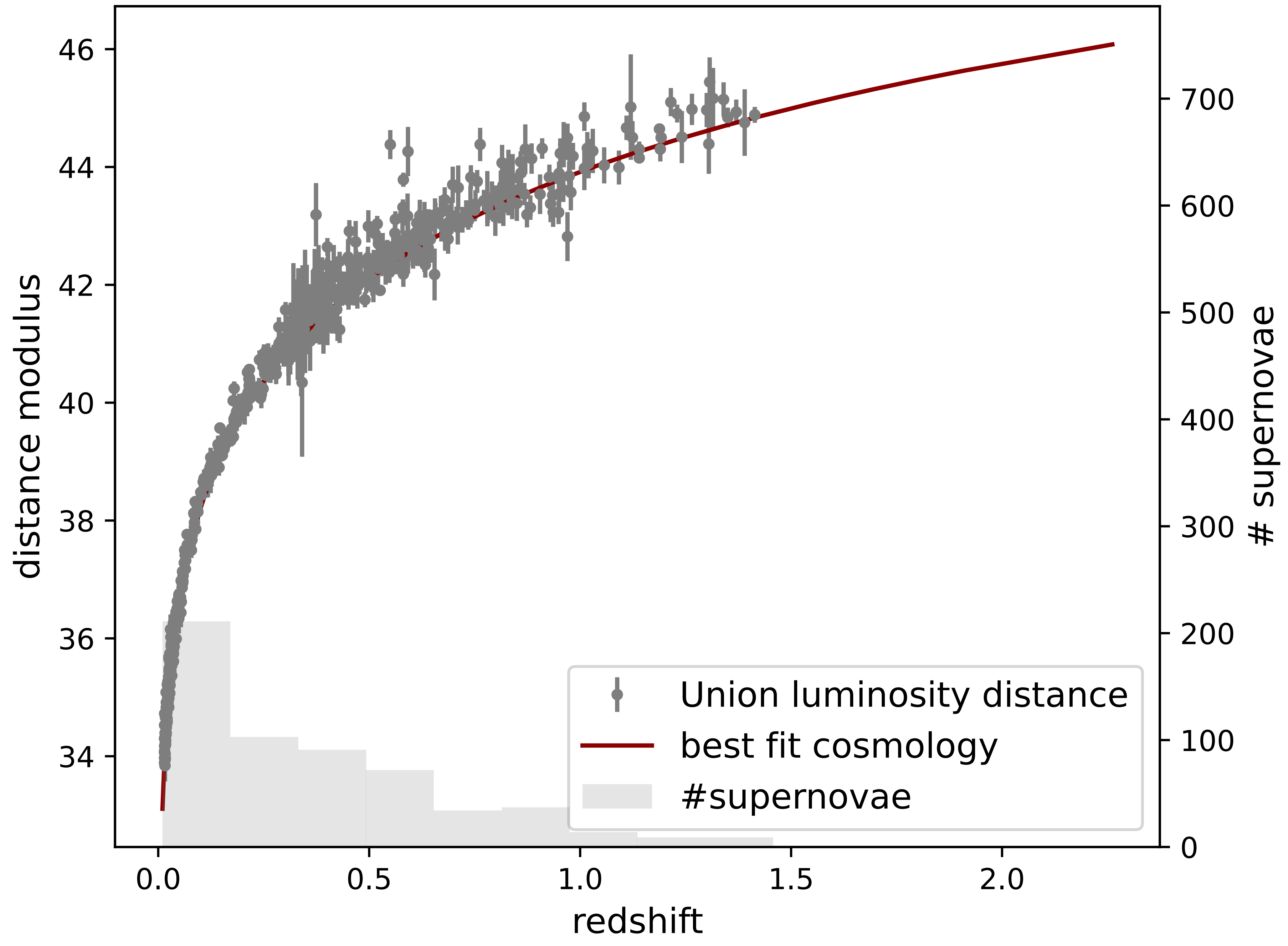
PINNference



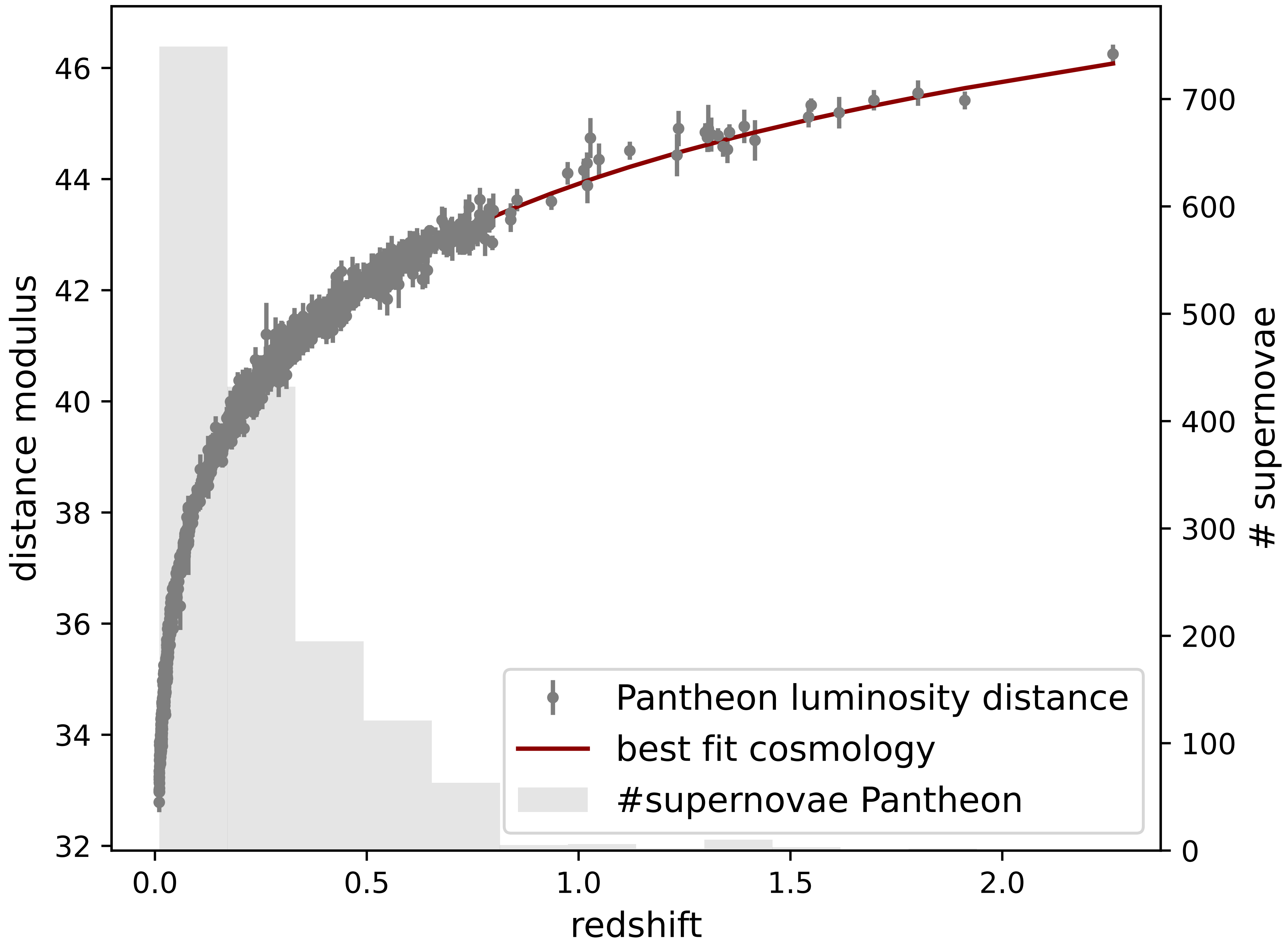
Supernovae

$$\mu = 5 \log_{10} d_L(z, \lambda) + 10$$

$$d_L(z, \lambda) = (1 + z)c \int_0^z dz' \frac{1}{H(z', \lambda)}$$



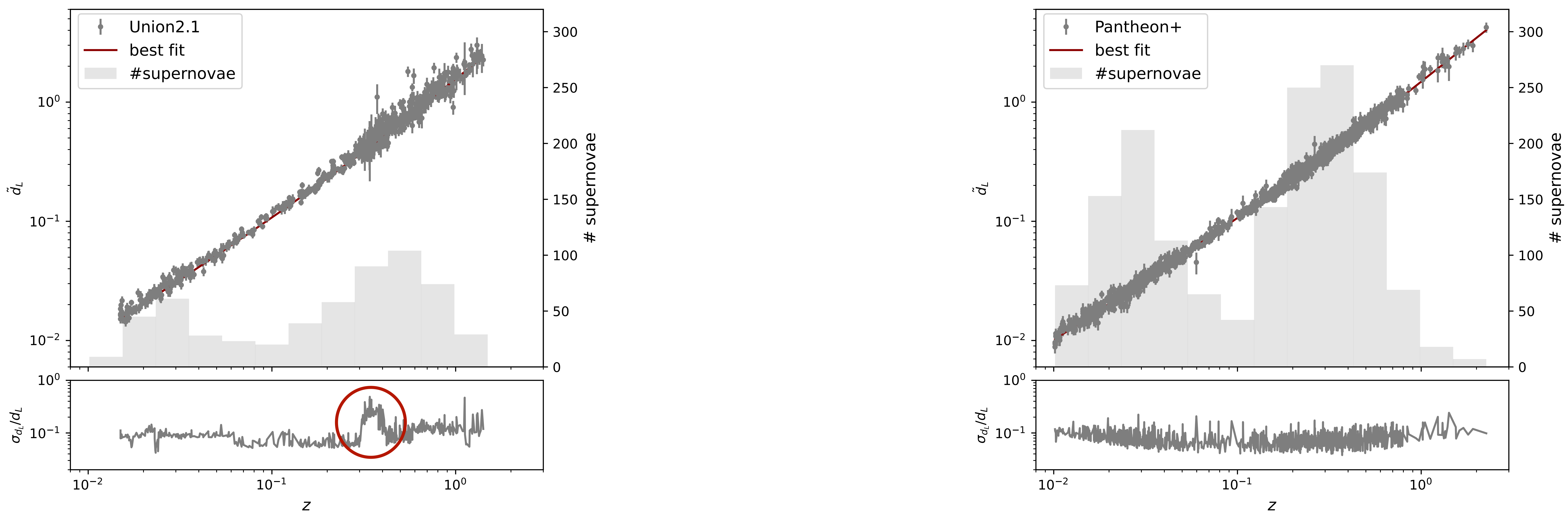
[Suzuki et al. 2011, Amanullah et al. 2010, Kowalski et al. 2008]



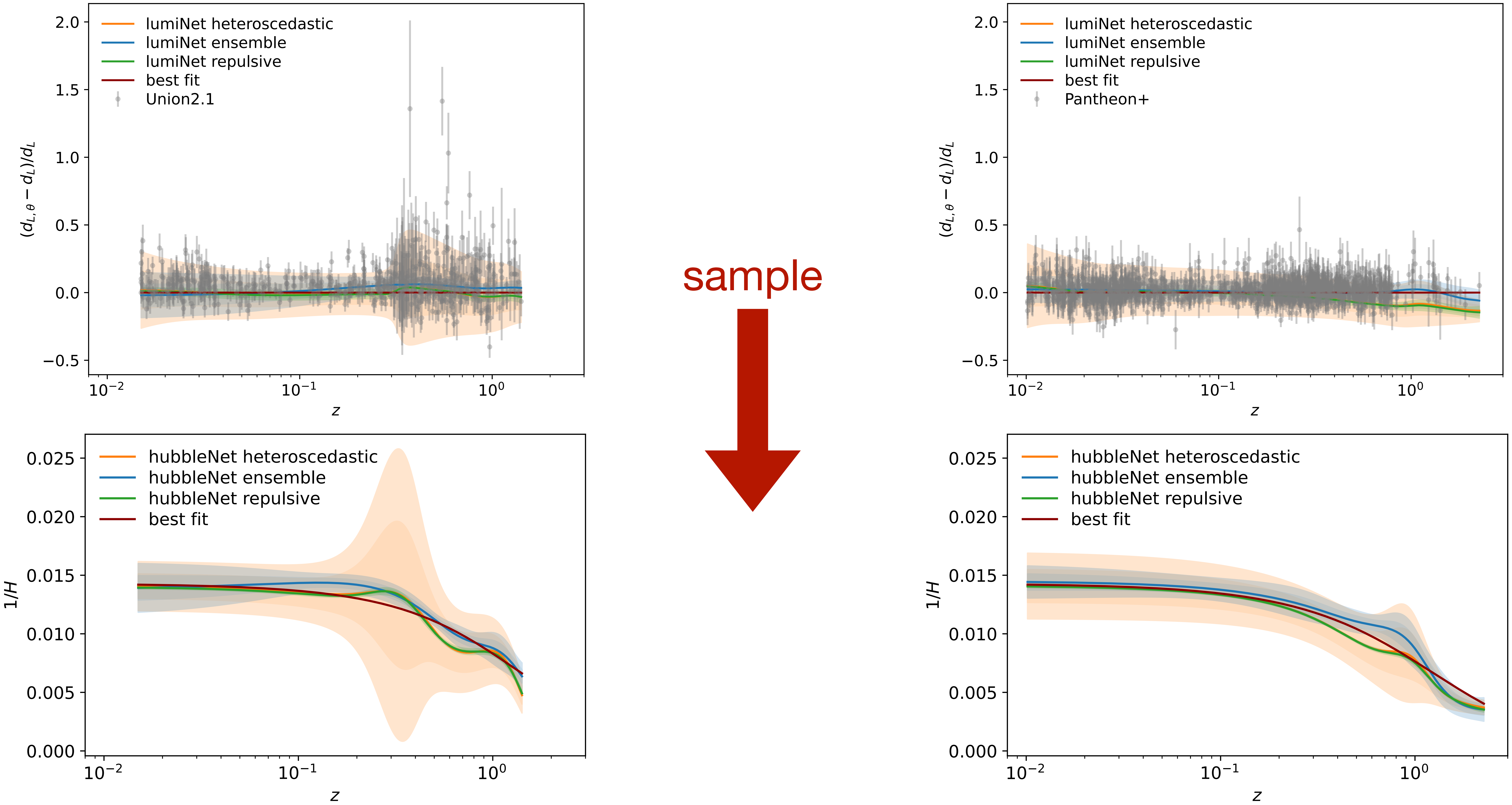
[Scolnic et al. 2022]

Supernovae

$$\frac{d\tilde{d}_{L,\theta}(z)}{dz} - \frac{\tilde{d}_{L,\theta}(z)}{1+z} - \frac{1+z}{\tilde{H}_{\phi}(z)} = 0$$



Hubble function

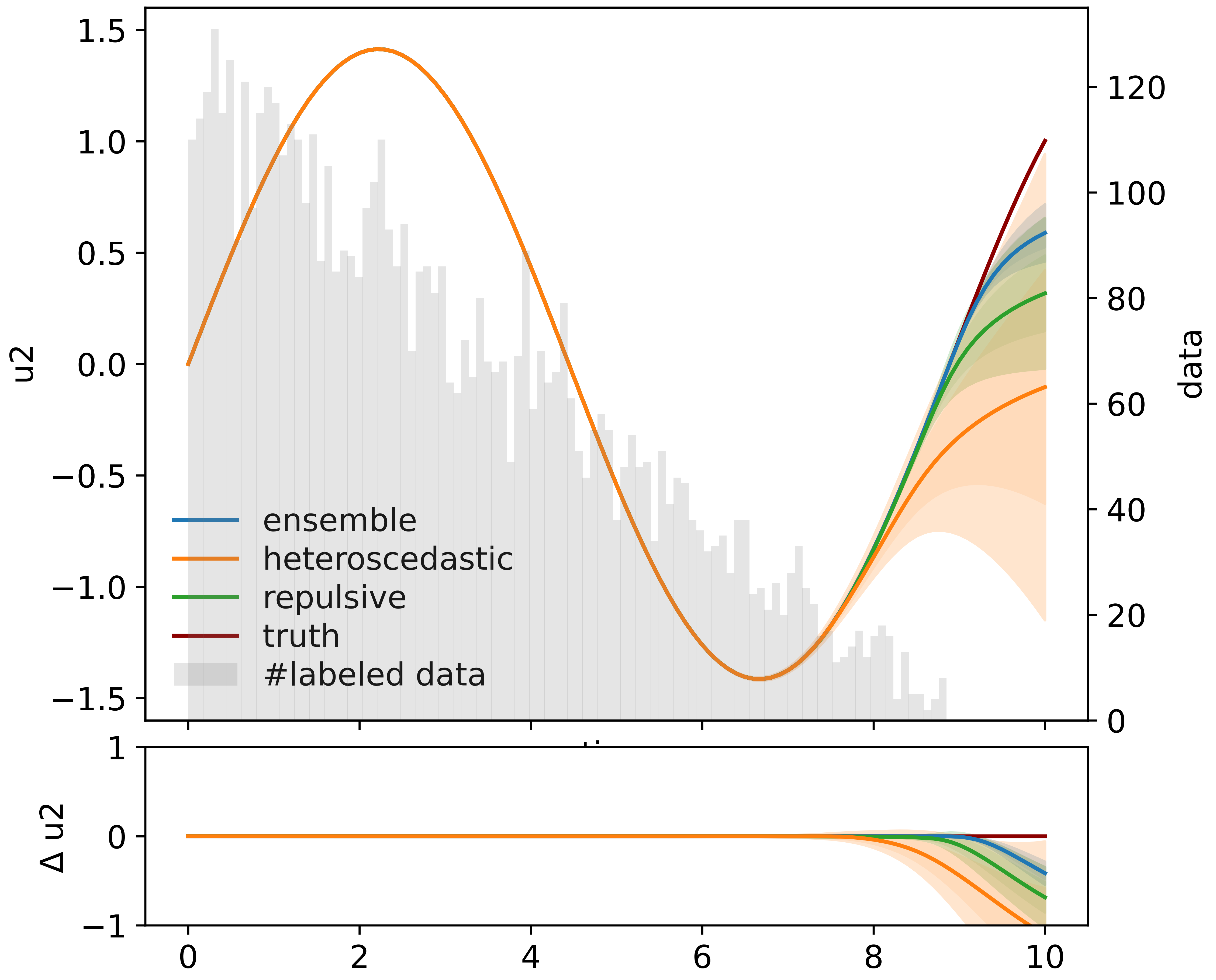


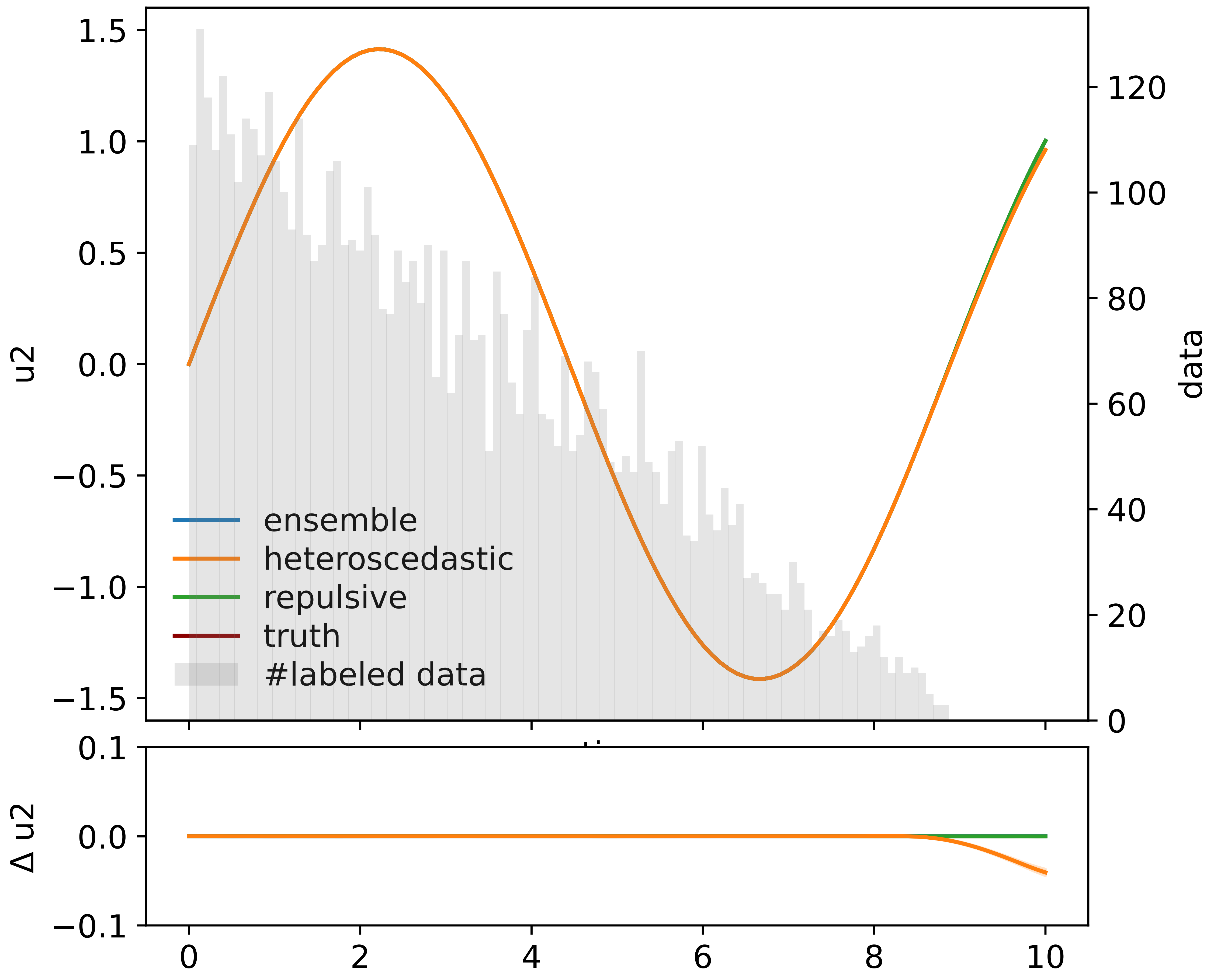
Conclusions

- PINNs learn ODE solutions locally
- ODE information can be used to construct emulators
- Model independent inference using labeled data
- Uncertainty aware inference: sample during training

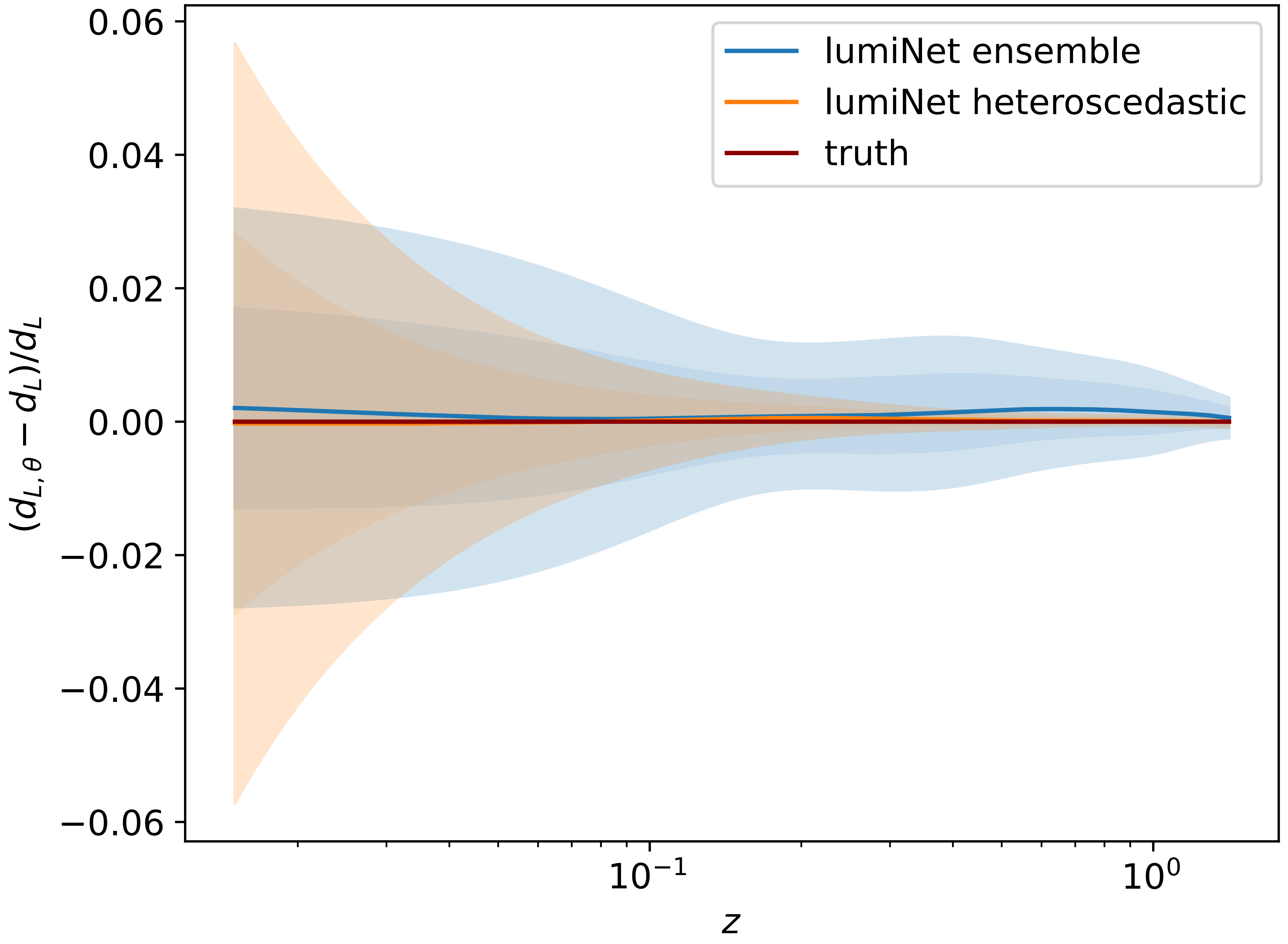
Thank you for listening!

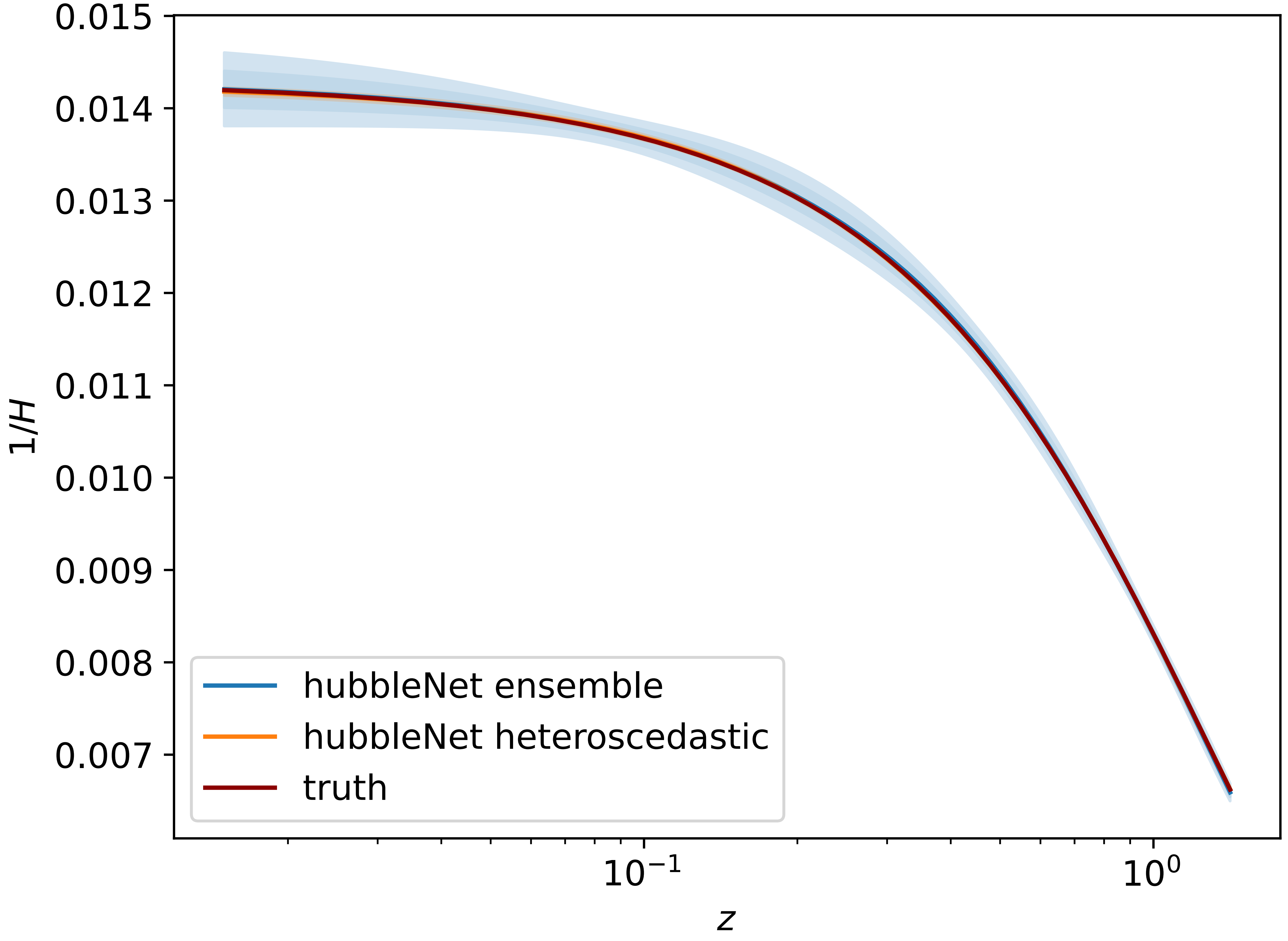
Bonus: local solution





Bonus: Hubble reconstruction





Bonus: eos reconstruction

$$w(a) = -\frac{1}{3}\frac{d}{d\log a}\log\left[\frac{H^2(a)}{H_0^2} - \frac{\Omega_m}{a^3}\right] - 1$$