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Trustworthy and Scalable Data-Driven Closure Models

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Computational simulations often require constitutive/closure models

$$\frac{\partial \boldsymbol{u}}{\partial t} = R(\boldsymbol{u}, Q) \qquad\qquad Q \approx \hat{Q}(\boldsymbol{u}; \boldsymbol{\theta})$$

- represent unresolved phenomena
- enhance computational efficiency
- correct model-form error

Closure and constitutive models arise in a variety of application areas

Nonlinear structural dynamics

$$\ddot{u} + 0.3\,\dot{u} - u + Q(u) = F(t)$$

Learn a nonlinear spring force

Epidemiological modeling

$$\frac{dS}{dt} = -\frac{\beta IS}{N_{pop}}$$

$$\frac{dI}{dt} = \frac{\beta IS}{N_{pop}} - \gamma I - \xi(S, I, R)I$$

$$\frac{dQ}{dt} = \xi(S, I, R)I - \delta Q$$

$$\frac{dR}{dt} = \gamma I + \delta Q$$

Learn a state-dependent transition rate into quarantine

Data-driven methods are a promising new direction for developing constitutive and closure models

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Constitutive artificial neural networks: A fast and general approach to predictive data-driven constitutive modeling by deep learning

Kevin Linka[a,*], Markus Hillgärtner[b], Kian P. Abdolazizi[a,b], Roland C. Aydin[c], Mikhail Itskov[b], Christian J. Cyron[a,c]

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RESEARCH ARTICLE

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A mechanics-informed artificial neural network approach in data-driven constitutive modeling

Faisal As'ad[1] | Philip Avery[1] | Charbel Farhat[1,2,3]

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Deep neural networks for data-driven LES closure models

Andrea Beck*, David Flad, Claus-Dieter Munz

SIAM J. Applied Dynamical Systems
Vol. 17, No. 4, pp. 2381–2413

Data-Driven Discovery of Closure Models*

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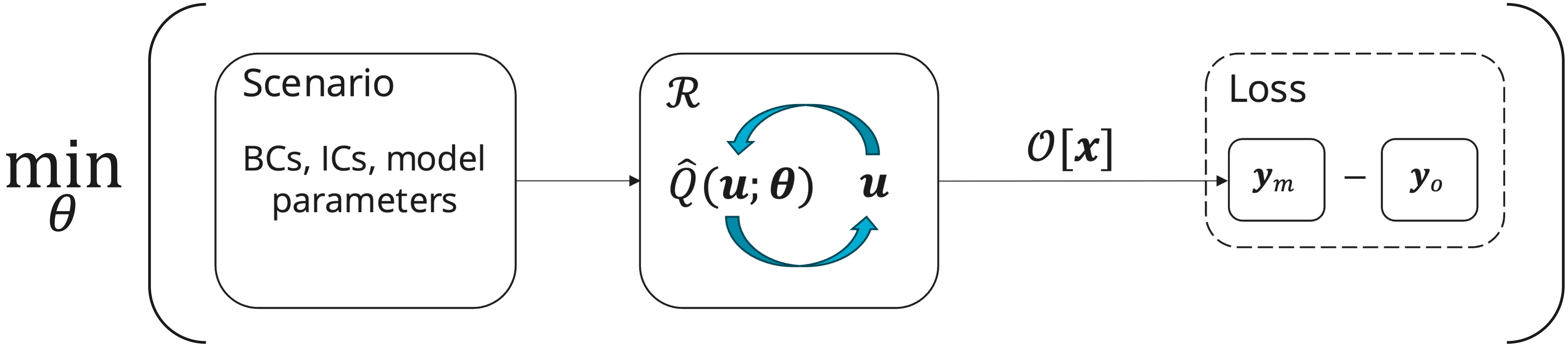
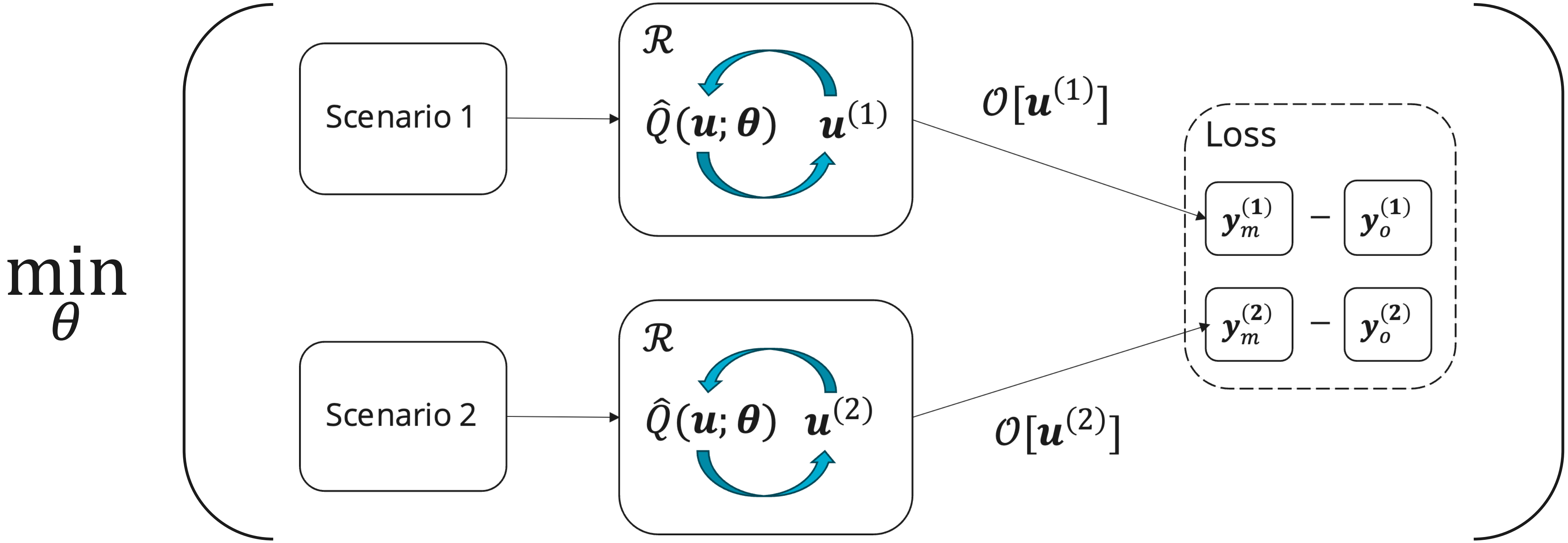
Training data-driven closures within complex dynamical system models is computationally prohibitive



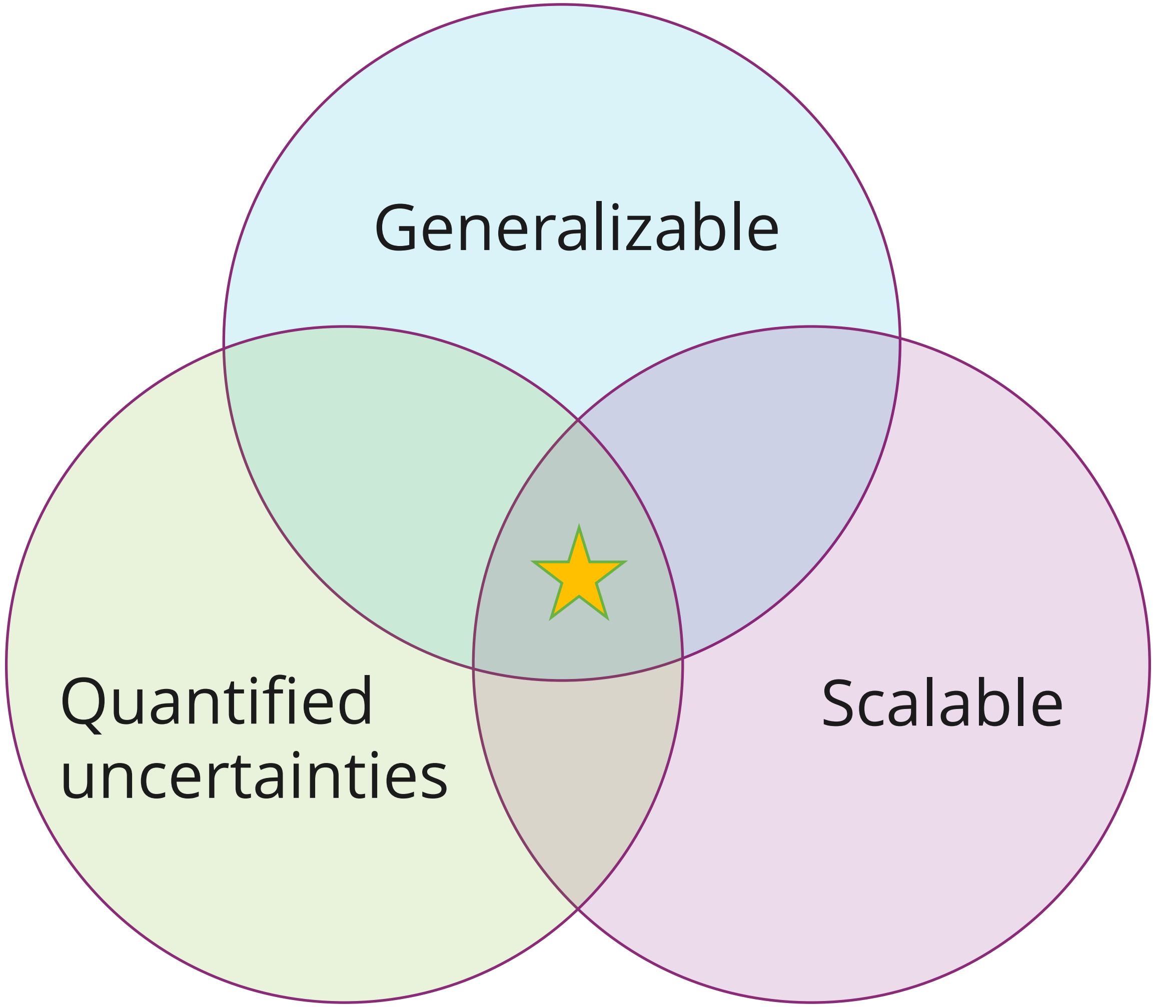
- Gradient-based training requires differentiation through governing equations
- Each training step requires solving complex dynamical system model
- **High cost limits data-driven model exploration**

Multiple scenarios for generalizability exacerbates this issue



Multiple scenarios requires multiple costly model solves per training step.

How can we ***practically*** develop data-driven closure models that are generalizable and scalable with quantified uncertainties?



Idea: decouple the costly model-based inference from data-driven closure formulation and training

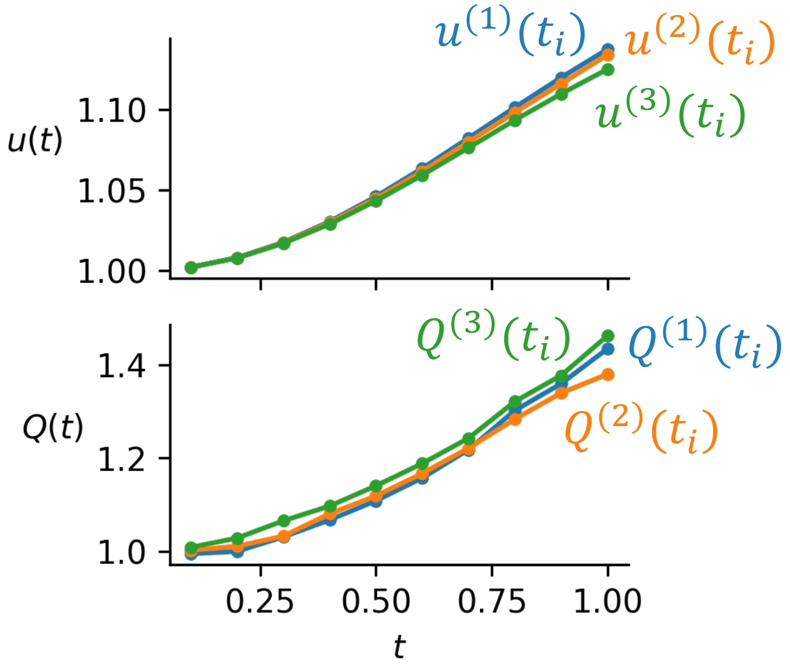
Model-based inference

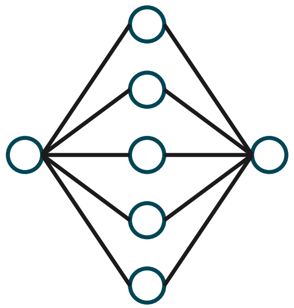
Get $\boldsymbol{u}(\boldsymbol{t}), Q(\boldsymbol{t})$ pairs using data assimilation

→

Closure-model training

Learn data-driven closure for Q as operator acting on $\boldsymbol{u}$





$$u^{(j)}(t_i) \rightarrow \quad \rightarrow \hat{Q}\left(u^{(j)}(t_i); \boldsymbol{\theta}\right) = \hat{Q}_{ij}(\boldsymbol{\theta})$$

$$\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) \propto \sum_{ij} \left\| \hat{Q}_{ij}(\boldsymbol{\theta}) - Q^{(j)}(t_i) \right\|$$

Idea: decouple the costly model-based inference from data-driven closure formulation and training

Model-based inference

Get $\boldsymbol{u}(\boldsymbol{t}), Q(\boldsymbol{t})$ pairs using data assimilation

→

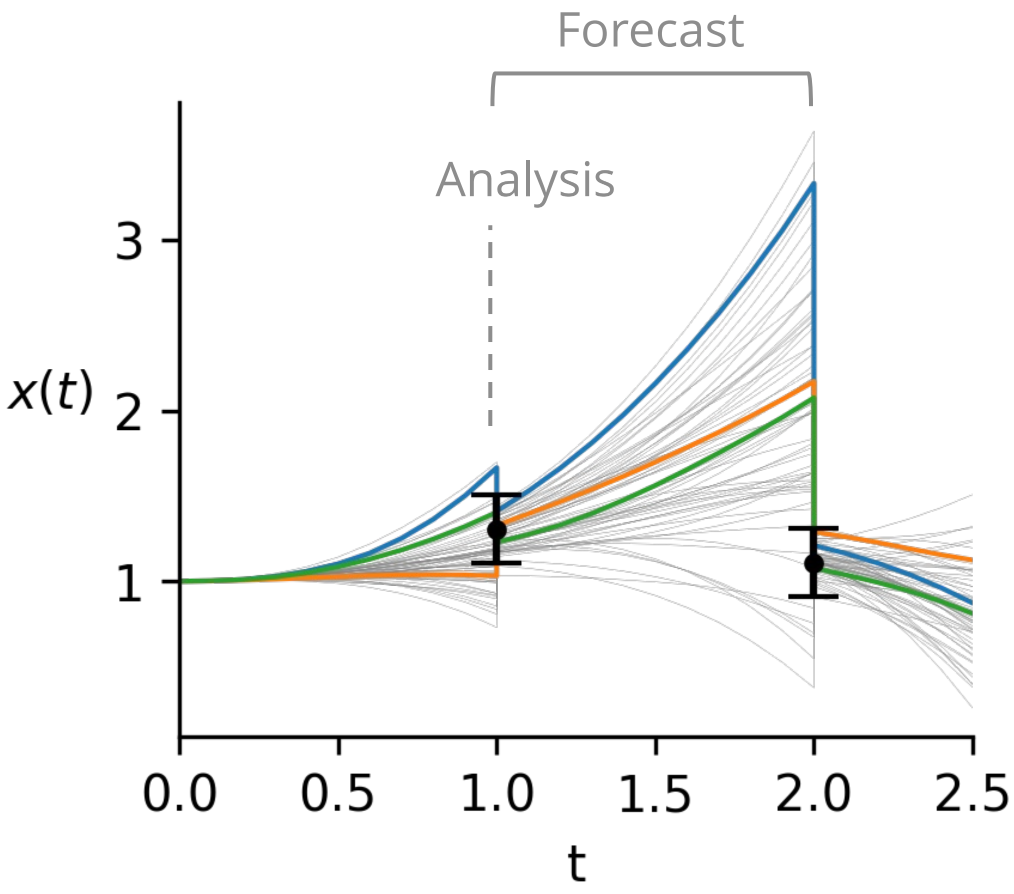
Closure-model training

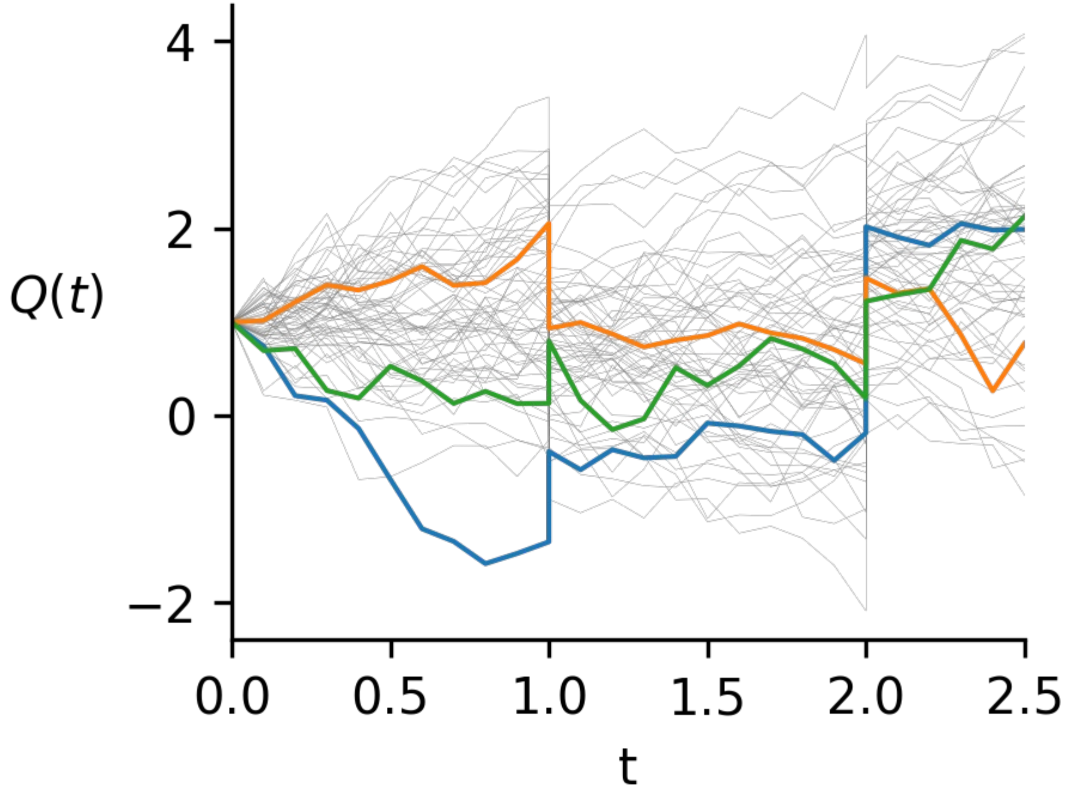
Learn data-driven closure for Q as operator acting on $\boldsymbol{u}$

- Incur costly model-based calibration once
- Data-driven closure model formulation & training now a straightforward (much cheaper) regression problem
  - **Enables greater model exploration and uncertainty quantification**

Bayesian data assimilation generates approximate posterior samples

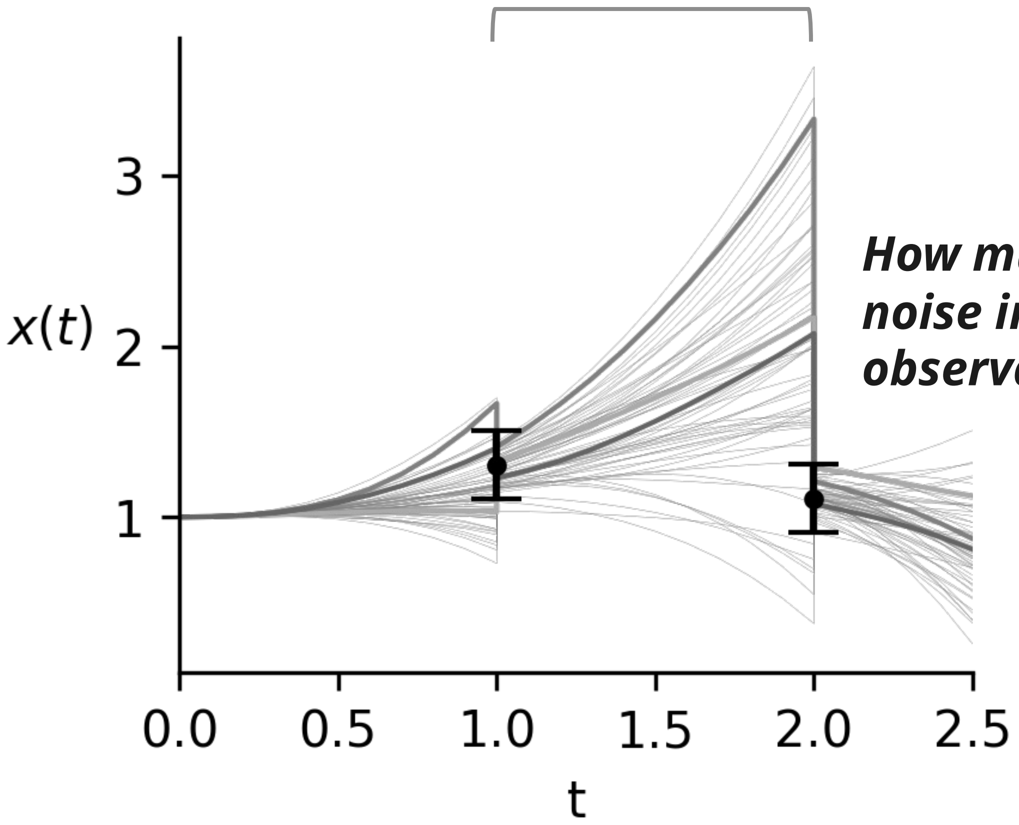
- x, Q samples are time-marched together
- "Synthetic dynamics" (e.g., Brownian motion) are assumed for Q



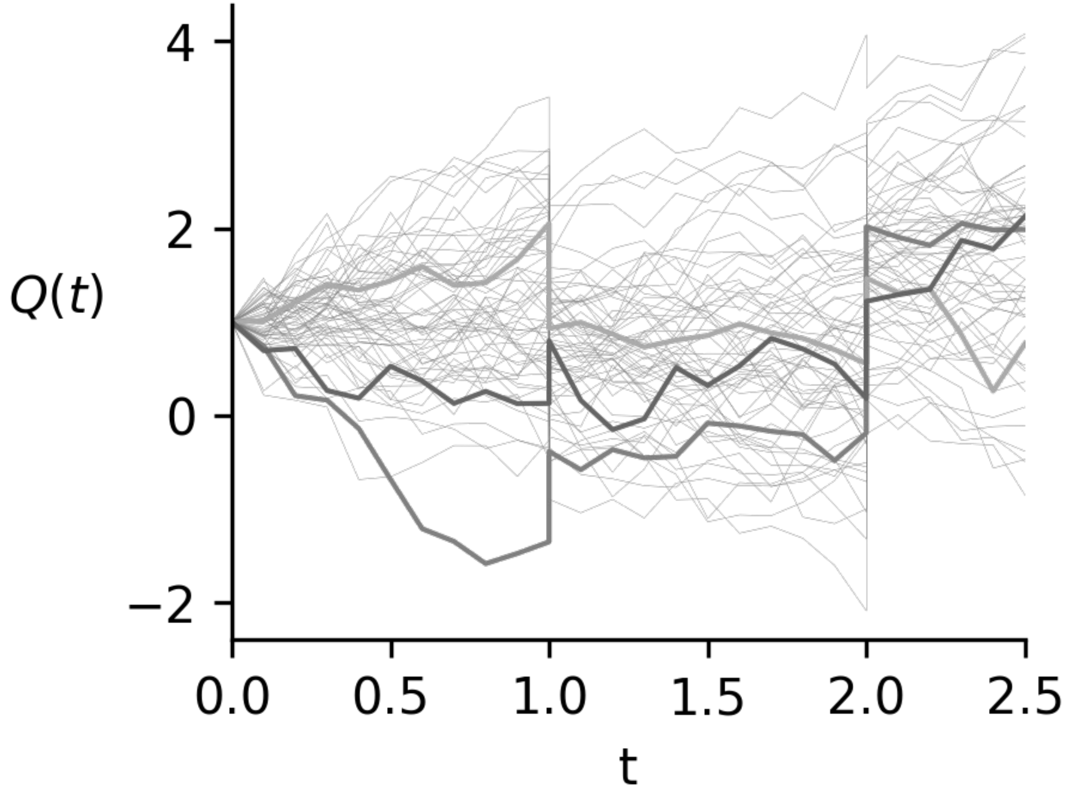


When will data assimilation be successful?

How much time between observations?

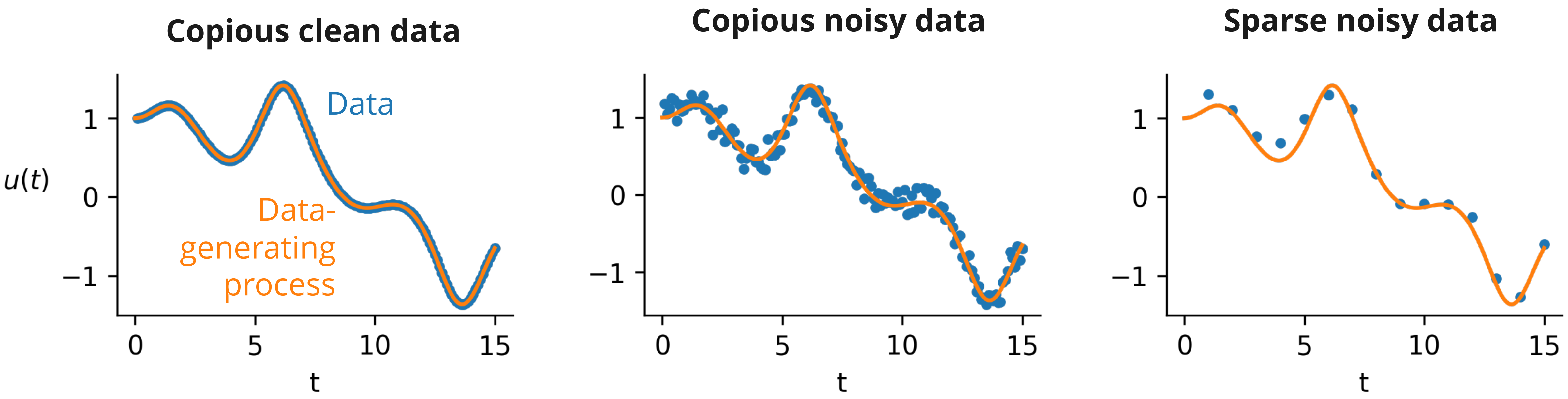


How much noise in observations?



We investigated these questions in the context of the Duffing oscillator

$$\ddot{u} + 0.3\,\dot{u} - u + Q(u) = F(t) \qquad \text{True } Q(u) = u^{2.8}$$

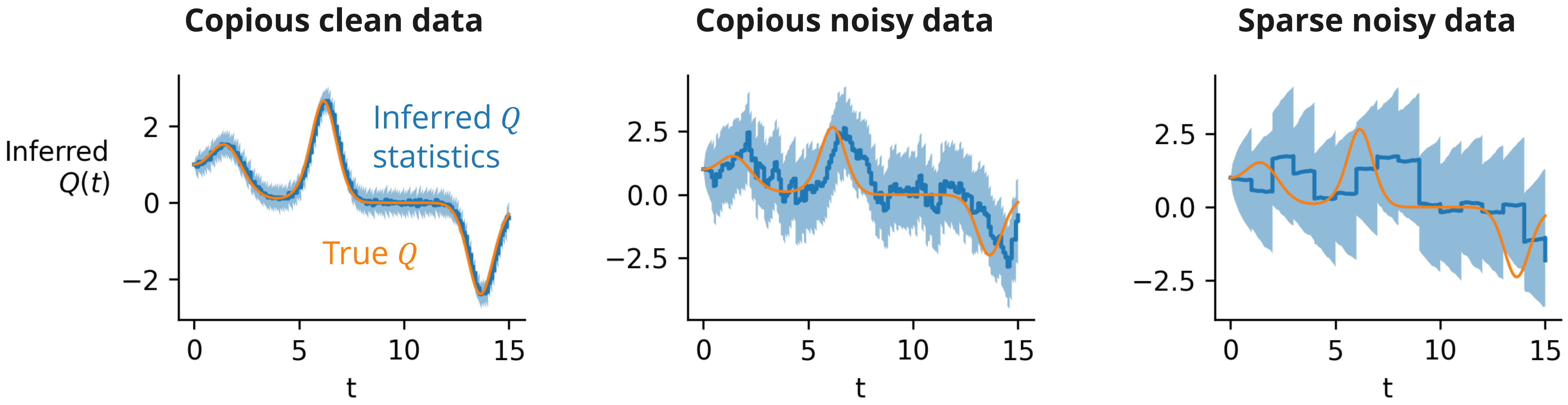


Can we obtain accurate estimates of Q?

Can we get better estimates using assumed dynamics for Q?

Q estimates degrade with noisier sparser data if no dynamics for Q are assumed

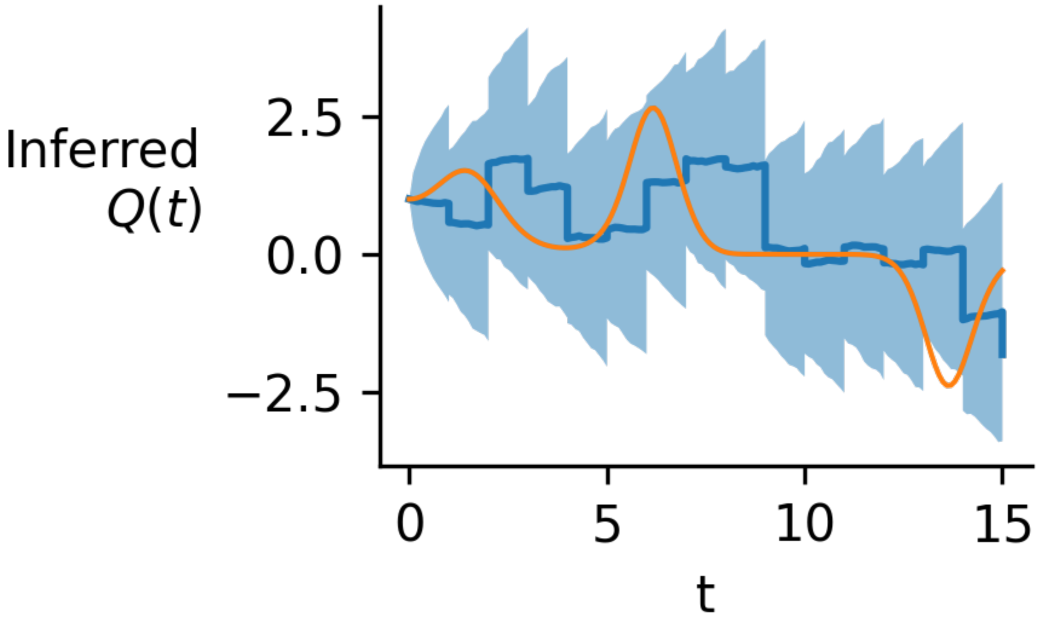
$$dQ_t = \sigma_Q dW_t$$



Sparse, noisy data can produce good Q estimates if good baseline dynamics are assumed

No prior information on Q dynamics

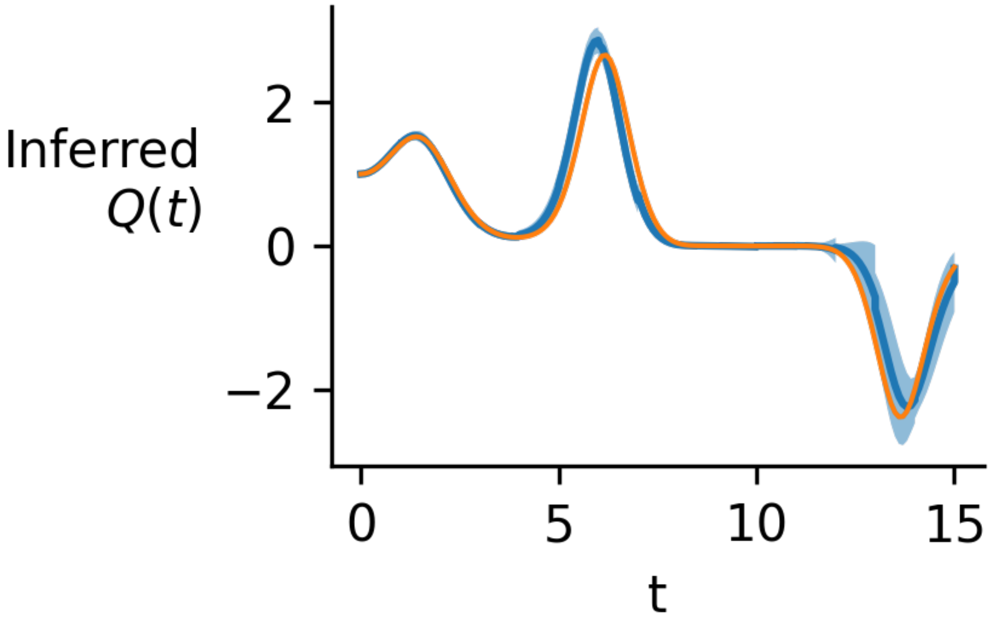
$$dQ_t = \sigma_Q dW_t$$



Close but not perfect dynamics assumed for Q

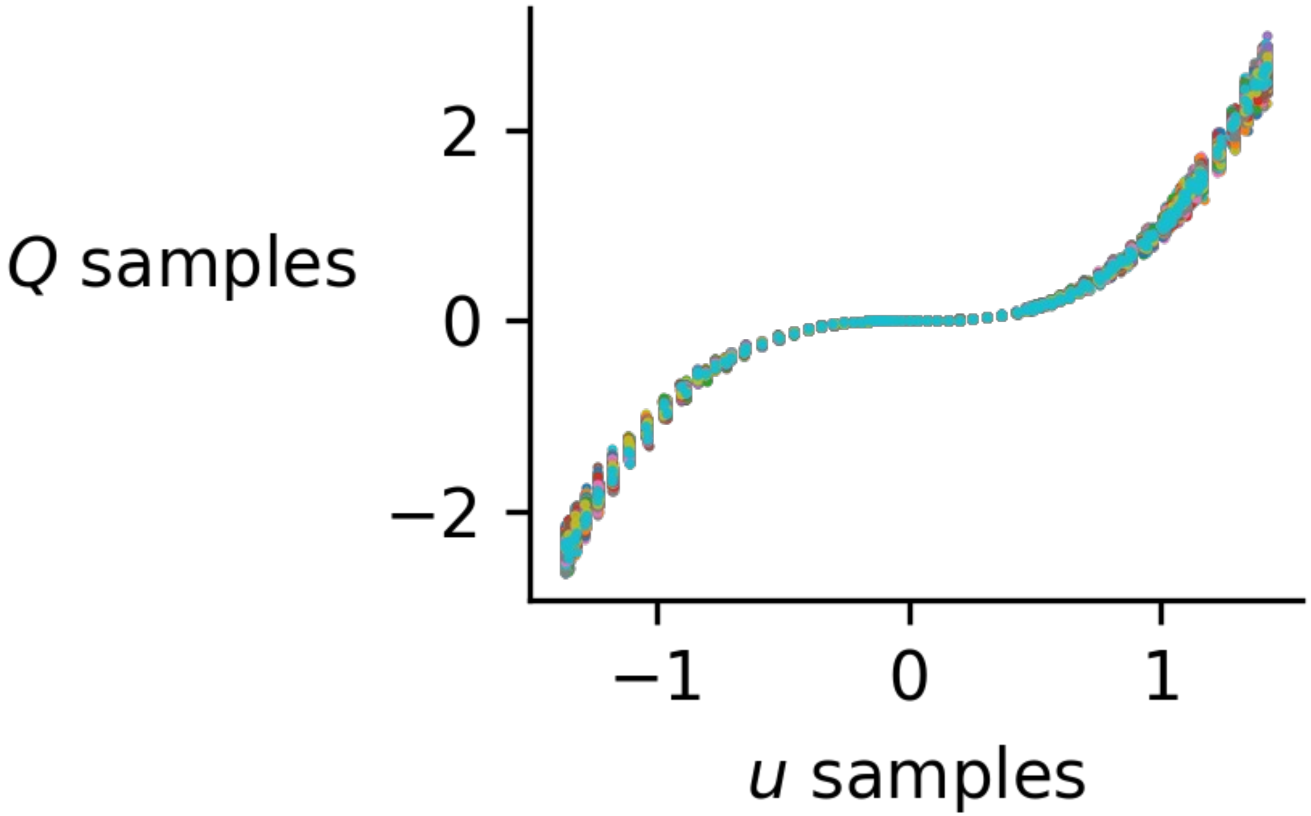
$$Q_t = cu^3,$$
$$dc_t = \sigma_c dW_t$$

True $Q(u) = u^{2.8}$



Could use previously developed closure/constitutive models as baseline dynamics.

Using inferred Q to develop a data-driven closure/constitutive model



We can now explore many formulations for Q with ***no further dynamical system model evaluations***.

- Neural nets
- GPs
- Polynomials
- …

Different colors represent different sample time series.

Conclusions and future work

- Data-driven closure models (DDCMs) can significantly advance beyond current state of the art in many application areas.
- Trustworthy DDCMs must be scalable and generalizable with quantified uncertainties.
- Our approach achieves these goals by decoupling costly dynamical-system based inference from DDCM formulation and training.
- We have investigated when this approach can be successful and methods to address sparse and noisy data.
- Next steps:
  - ML models with quantified input and output uncertainties
  - Out-of-distribution detection for quantified regions of applicability