Beyond Generalised Bayes: Prediction-Centric Alternatives

Chris. J. Oates

`https://postbayes.github.io/seminar/`

March 2025

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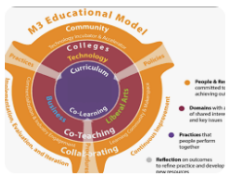
Growth Engineering
Essential Learning Models ...



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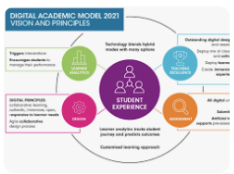
M3 Educational Model Overview ...



The University of Law
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St John the Baptist Cat...
St John the Baptist C...

Abu Hanifah Foundation
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The Proposed Teachin...

David White
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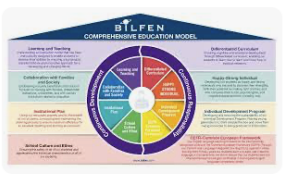
Disciplinary and Interdisciplinary Scie...
Modeling competence in science ...



Bilfen
Bilfen Compherensive Education Model

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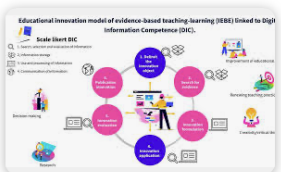
Digital education mode...

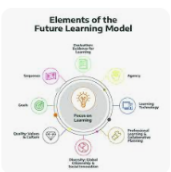

Child and Adolescent Psychiatry and Mental ...
child mental health among K-12 students...

MDPI
Sustainable Teaching Model ...

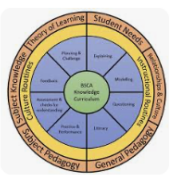
Growth Engineering
Essential Learning Mod...



MDPI
Evidence-Based Educational Innovation ...



SEK Education Group
Modelo educativo | SEK



Bolton St Catherine's Aca...
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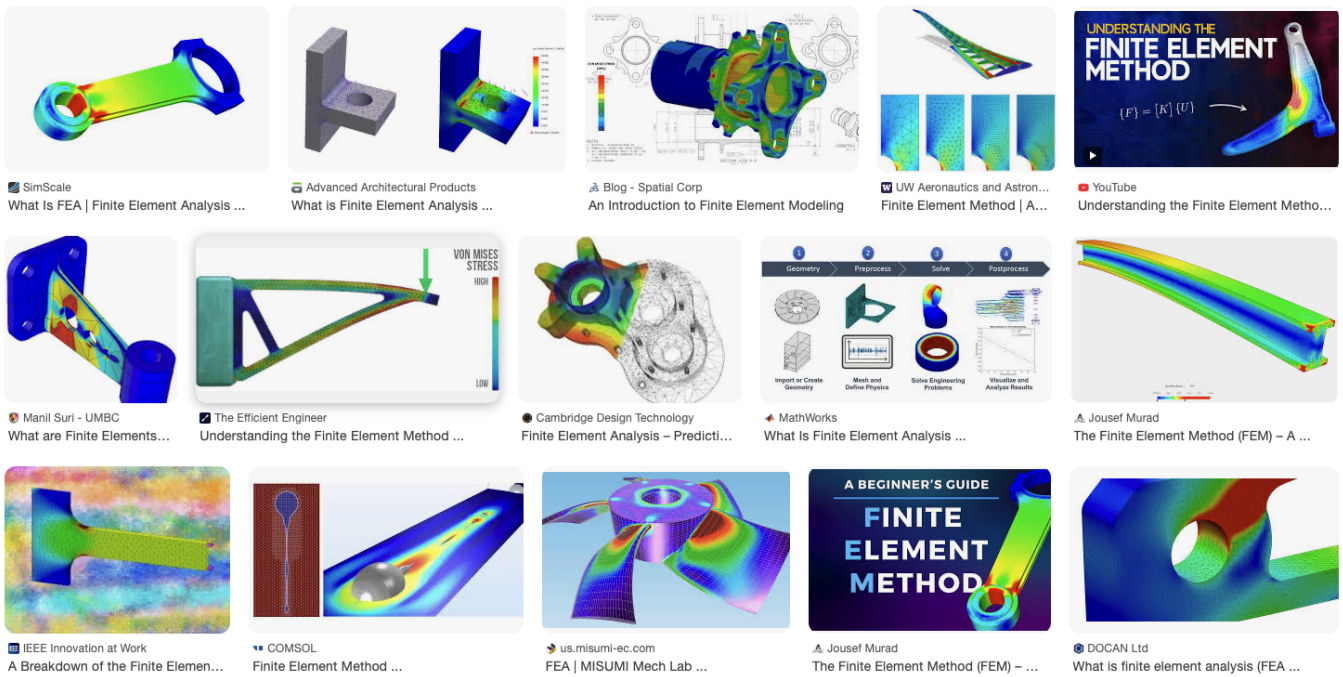

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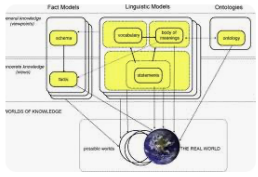
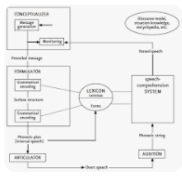


E ScienceDirect.com
Linguistic Model - an overview ...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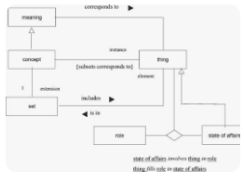
Model/Models in linguistics



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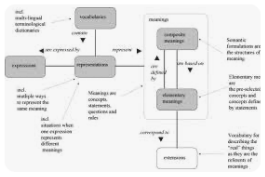
Linguistic modeling appli...

W Wikipedia
Logico-linguistic mod...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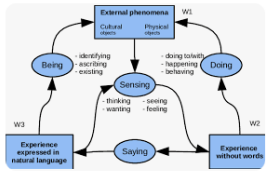

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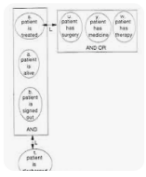
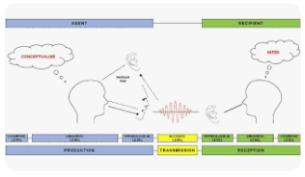
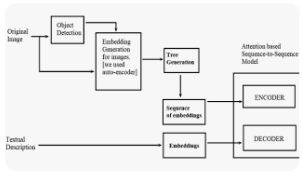
Data flow diagram of a linguistic model ...


Wikipedia
Logico-linguistic m...


SLT info
Communication Model



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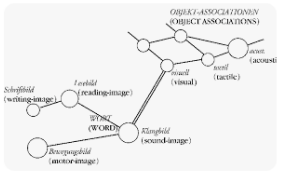
Visual Linguistic Model and Its ...



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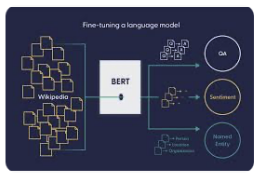
1891) linguistic model: "The word ...



Deepset
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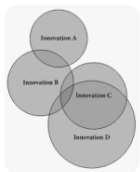
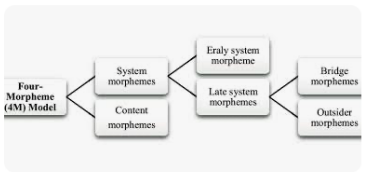


Wikipedia
Wave model - Wiki...



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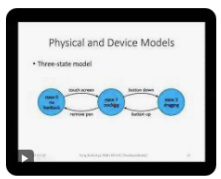
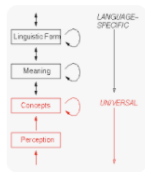
4-M model for linguistic analysis ...



YouTube
Linguistic Model, Backus–Naur ...



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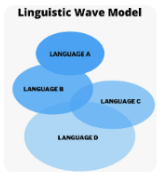
Models of Languag...



Globe Language
Wave Model - Globe ...

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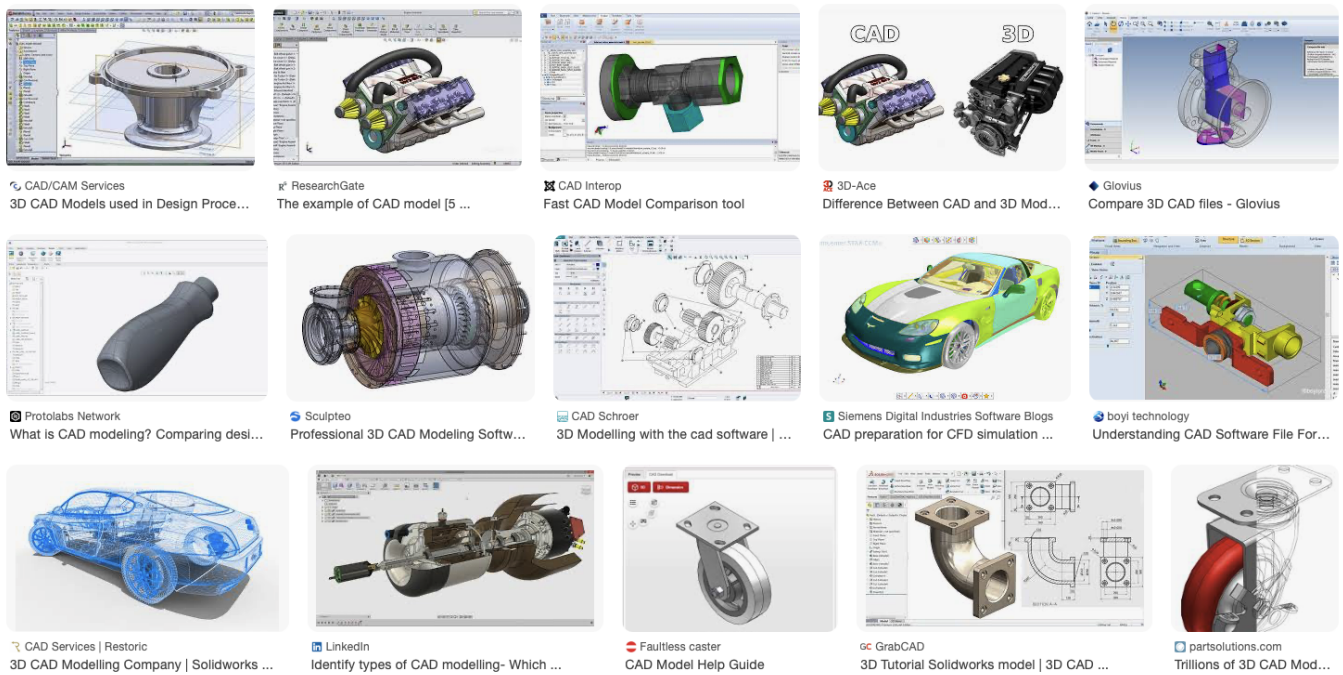

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Focus on deterministic models

$$M_\theta : \mathcal{X} \to \mathcal{Y}$$

with parameters denoted $\theta \in \Theta$.

Challenge: How to use such a "model" for statistical inference and (causal) prediction?

Usual Solution: Turn the "model" M_θ into a "statistical model"

$$P_\theta : \qquad y_i = M_\theta(x_i) + \epsilon_i, \qquad \epsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2 I)$$

using knowledge of the equipment used to make the measurement.

Unfortunately a good "model" can lead to a misspecified "statistical model"...

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Model Misspecification in Cell Signalling

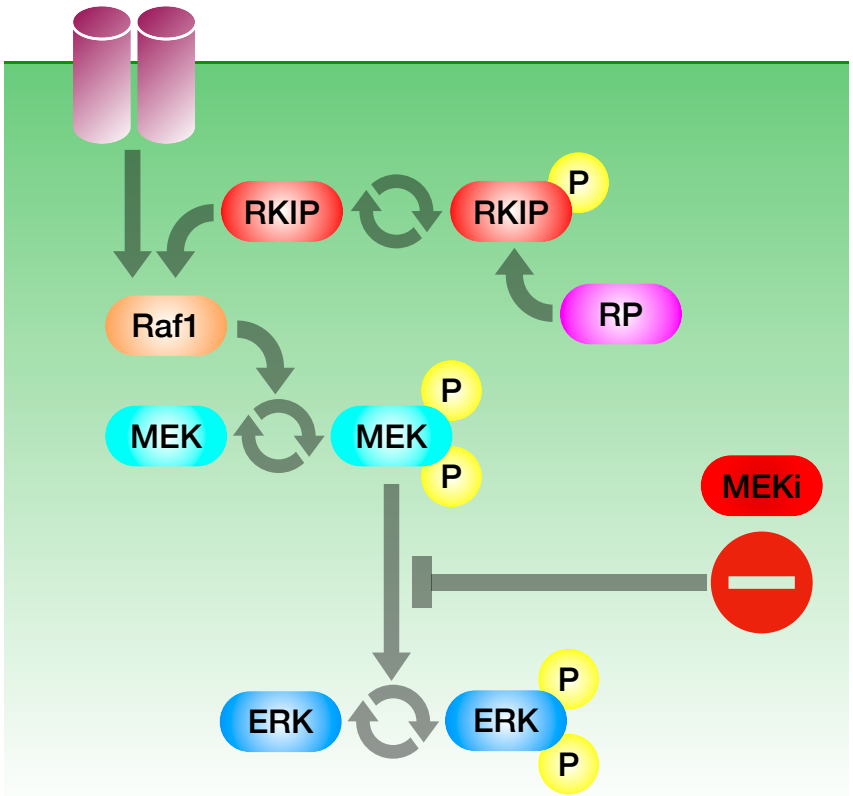

Figure: ERK signalling model.

Systems biology has invested decades of effort into the design of detailed ODE descriptions of cellular signalling pathways, with thousands of models hosted on repositories such as `BioModels` [Malik-Sheriff et al., 2020].

e.g. ERK signalling is modelled as

$$\frac{\mathrm{d}u}{\mathrm{d}x} = f_\theta(x, u), \qquad \theta \in \mathbb{R}^{11}$$

Data are (reasonably, as far as this talk is concerned) treated as noisy observations of molecular concentrations $u(x)$ at discrete times $x_{1:n}$.

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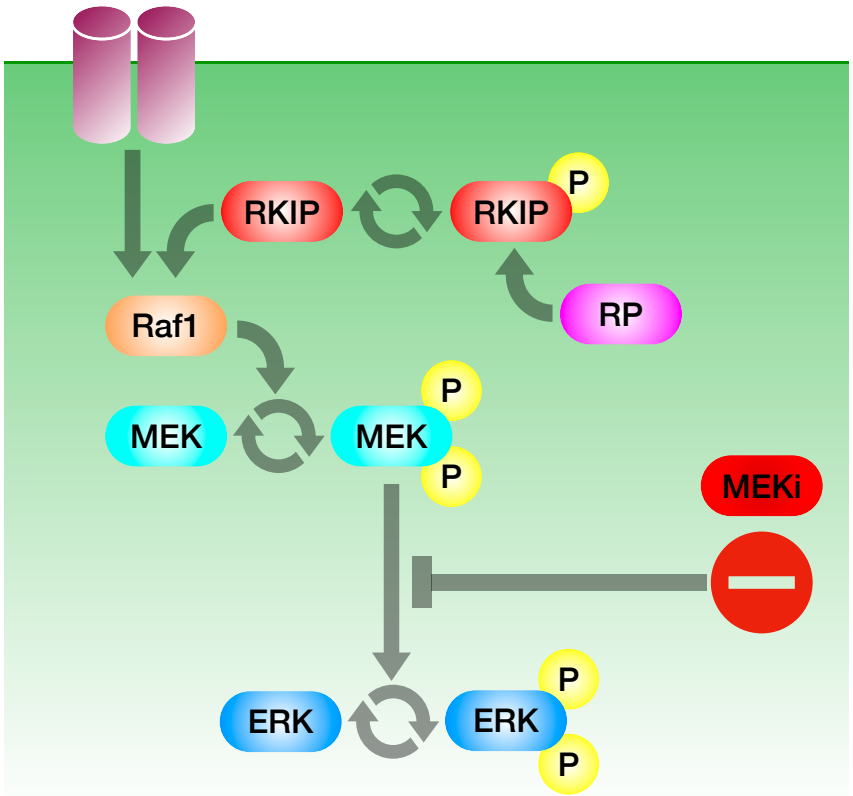

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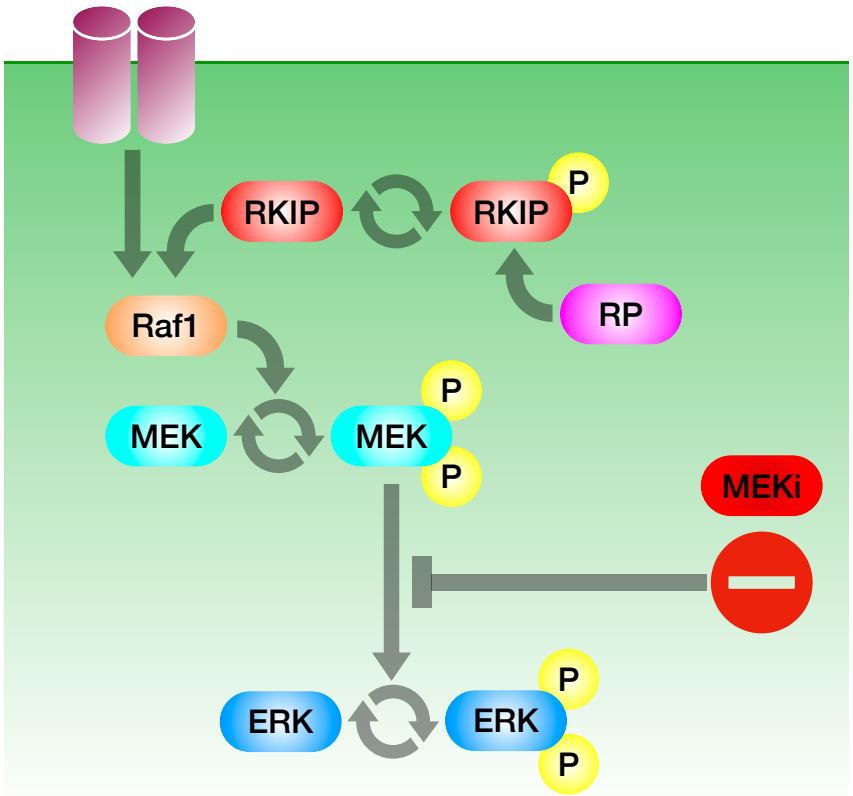

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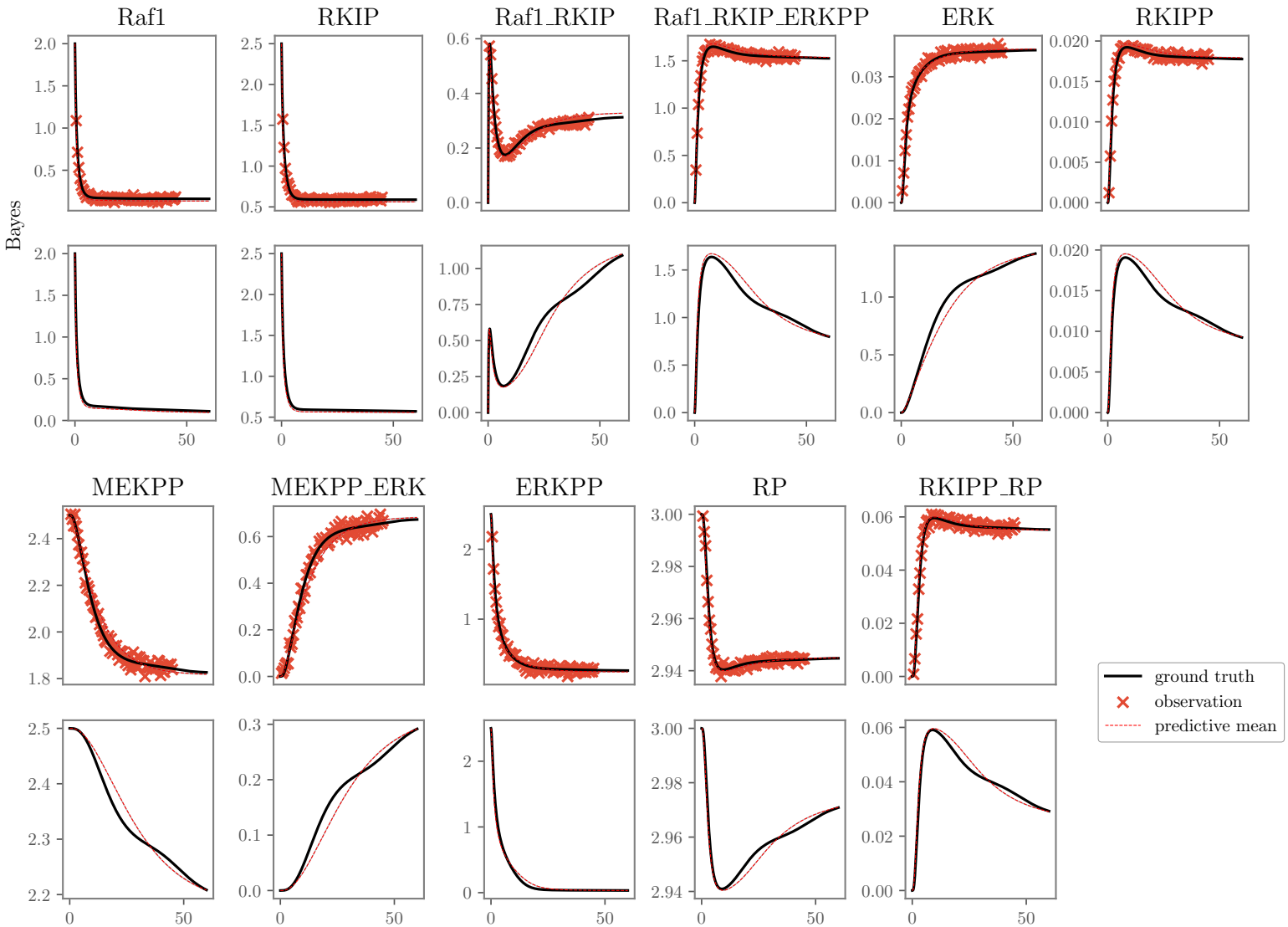

Figure: Posterior predictive for the ERK signalling model.

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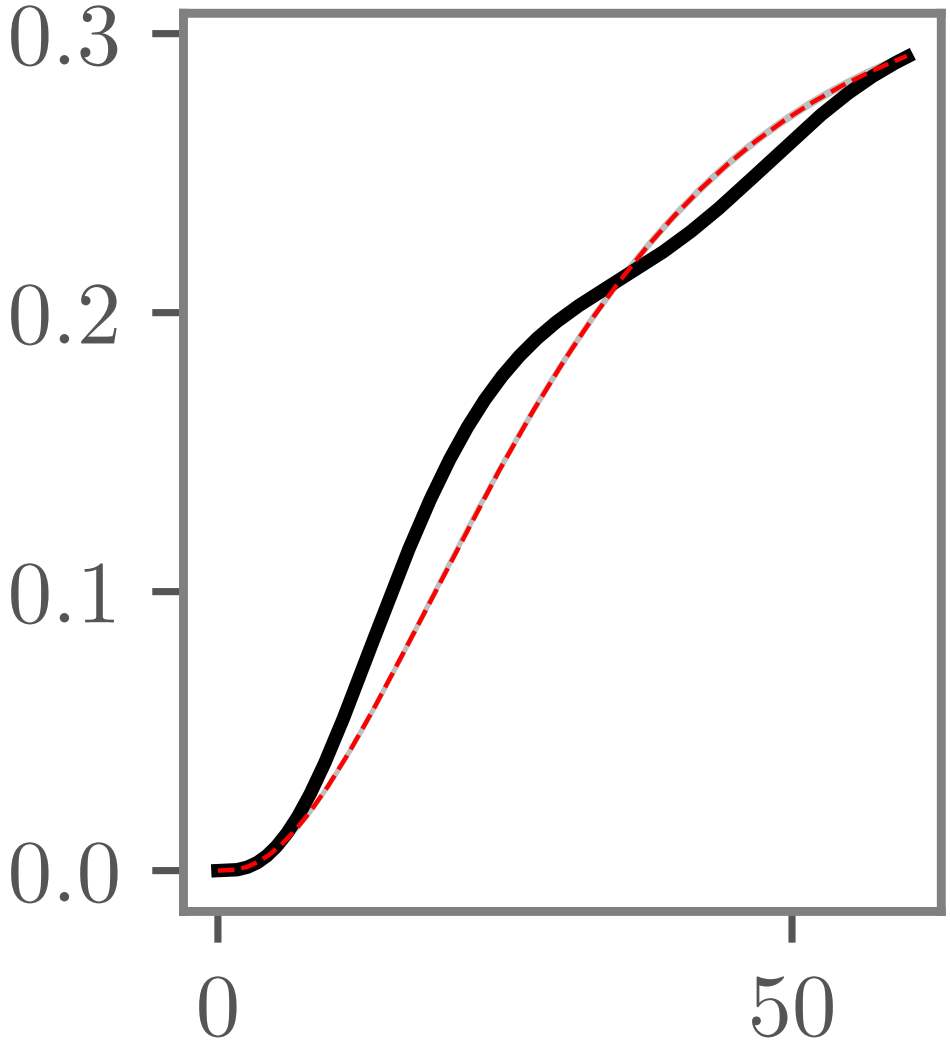

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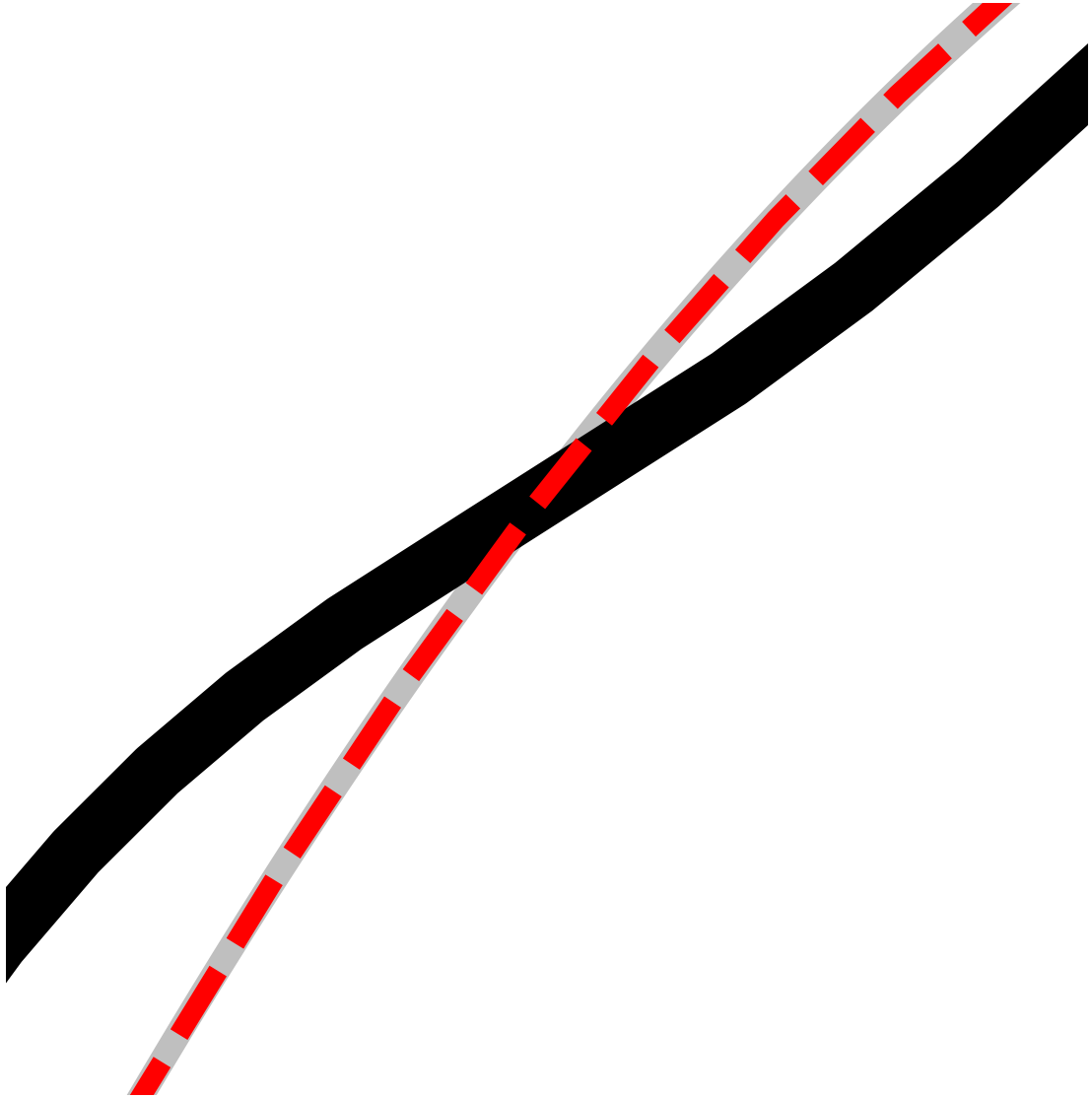

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Bayesian inference for misspecified models has been widely studied.

e.g. Kennedy and O'Hagan [2001]:

- parameter $\theta \in \Theta$
- IID data $y_{1:n} = (y_1, \ldots, y_n) \in \mathcal{Y}^n$
- misspecified model $M_\theta : \mathcal{X} \to \mathcal{Y}$
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Limitations

- high data requirement to learn the residual R;
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Limitations

- high data requirement to learn the residual R;
- **causal prediction impossible in this framework**.

TL/DR: Better Bayesian Inference Does Not Help

Bayesian inference for misspecified models has been widely studied.

e.g. Kennedy and O'Hagan [2001]:

- parameter $\theta \in \Theta$
- IID data $y_{1:n} = (y_1, \ldots, y_n) \in \mathcal{Y}^n$
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Other Choices of L_n and λ_n
For various other choices of L_n and λ_n, generalised Bayesian methods can produce robust posteriors suitable for dealing with certain forms of statistical model misspecification [see Hooker and Vidyashankar, 2014, Ghosh and Basu, 2016, Knoblauch et al., 2018, Schmon et al., 2020, Chérief-Abdellatif and Alquier, 2020, Dellaporta et al., 2022, Husain and Knoblauch, 2022, Altamirano et al., 2023, 2024, Duran-Martin et al., 2024].

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Concentration of Generalised Posterior
For convenient choices of L_n and λ_n, the magnitude of the data-fit term generally increases with n. As a result, $Q_n^\dagger \to \delta_{\theta^\dagger}$ [Miller, 2021].

So need to tune the learning rate...

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Tuning the Learning Rate
Several ideas have been proposed to select the learning rate λ_n - c.f. Ryan Martin's talk. But these involve approximations and/or can be computationally demanding.

Tuning the learning rate is complicated - seek alternative to generalised Bayes...?

Prediction-Centric Alternatives

Setting Given a model P_θ that is useful (e.g. for causal prediction) but misspecified.

Step 1: Mitigate Misspecification Form a mixture model

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Step 2: Learn Q For example, by matching the predictive distribution of P_Q to the dataset.

Example: Nonparametric Maximum Likelihood
This approach solves

$$\arg\min_{Q \in \mathcal{P}(\Theta)} -\frac{1}{n} \sum_{i=1}^{n} \log p_Q(y_i)$$

where p_Q is a density for the mixture model P_Q [see Chapter 5 of Lindsay, 1995].

- approximates $\mathrm{KL}(P_\star, P_Q)$ when $y_{1:n}$ is a collection of n independent samples from $P_\star \in \mathcal{P}(\mathcal{Y})$
- lack of regularisation causes computational difficulties and non-identifiability [see e.g. Laird, 1978], as the minimising measure will generally be fully atomic, see Lindsay [1995, e.g. Theorem 21 in Chapter 5] and Jordan-Squire [2015].

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Lai and Yao [2024] considered

$$\arg\min_{Q \in \mathcal{Q}} \underbrace{-\frac{1}{n}\sum_{i=1}^{n} \log p_Q(y_i)}_{\text{predictive fit}} + \underbrace{\lambda_n \mathrm{KL}(Q, Q_n^\dagger)}_{\text{regularisation}}$$

where

- predictive fit assessed using log-predictive density (or any proper scoring rule)
- regularisation is toward the standard Bayesian posterior $Q_n^\dagger$
- for computation, parametric VI is used.

Prediction-Centric Alternatives

Setting Given a model P_θ that is useful (e.g. for causal prediction) but misspecified.

Step 1: Mitigate Misspecification Form a mixture model

$$P_Q = \int P_\theta \, \mathrm{d}Q(\theta) \in \mathcal{P}(\mathcal{Y}).$$

Step 2: Learn Q For example, by matching the predictive distribution of P_Q to the dataset.

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Prediction-Centric Uncertainty Quantification

Our Take: *Prediction-Centric Uncertainty Quantification* (PCUQ).

Joint work with Zheyang Shen (Newcastle), Jeremias Knoblauch (UCL), and Sam Power (Bristol)

- (for now) IID data $y_{1:n} = (y_1, \ldots, y_n) \in \mathcal{Y}^n$
- empirical measure of the dataset $P_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{y_i}$
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- prediction-centric posterior

$$Q_n = \underset{Q \in \mathcal{P}(\Theta)}{\arg\min} \; \frac{1}{2} \underbrace{\mathrm{MMD}^2(P_n, P_Q)}_{\text{predictive fit}} + \underbrace{\lambda_n \, \mathrm{KL}(Q, Q_0)}_{\text{regularisation}}$$

Measuring Predictive Fit

The use of *maximum mean discrepancy* (MMD) [see e.g. Gretton et al., 2012], as opposed to other statistical divergences, confers outlier-robustness to PCUQ, which may be valuable in the misspecified context, and carries computational advantages, enabling the use of powerful emerging sampling methods based on gradient flows [Wild et al., 2023].

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Regularisation Target

Q_0 acts on Q_n in essentially the same way that Q_0 acts on Gibbs measures like $Q_n^\dagger$, as a reference measure in a Radon–Nikodym derivative [Bissiri et al., 2016, Knoblauch et al., 2022]. That is, once can reason about 'updating belief distributions' using PCUQ.

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Learning Rate

Compared to generalised Bayes, **PCUQ depends less critically on the learning rate** λ_n. i.e. support of Q_n is not a singleton set when $\lambda_n \to 0$.

Model Misspecification in Cell Signalling

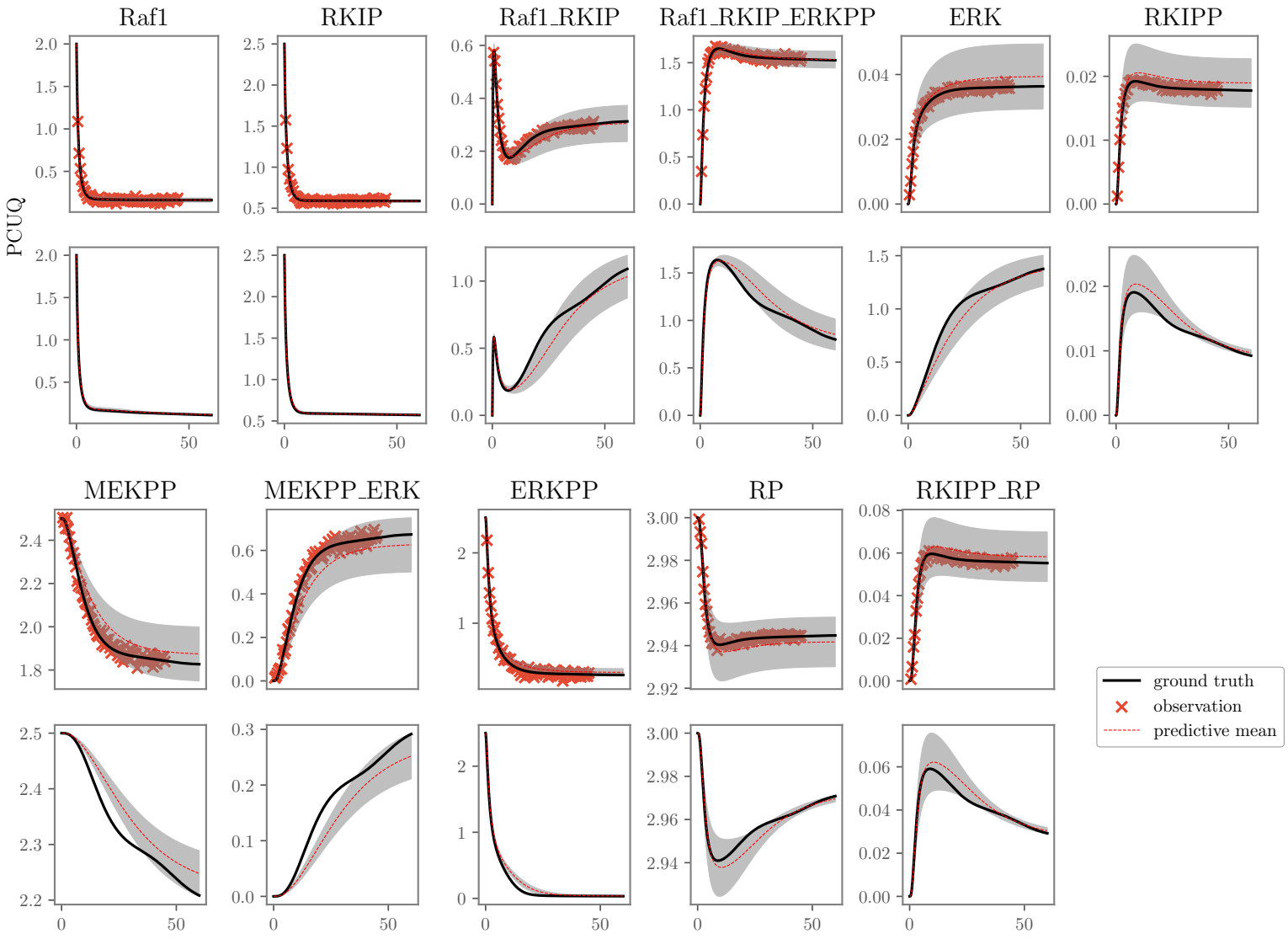

Figure: PCUQ predictive for the ERK signalling model.

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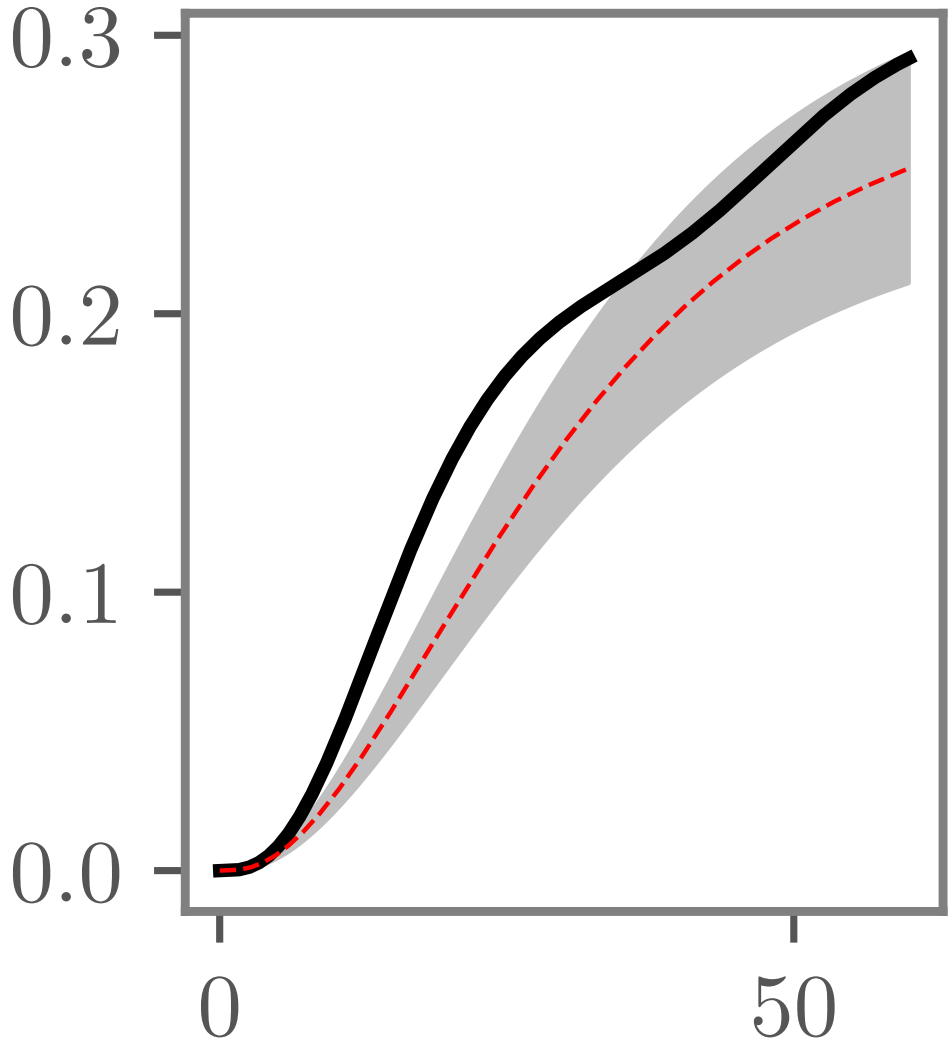

Figure: PCUQ predictive for the ERK signalling model.

A Bit More Detail

Predictive Fit via MMD

To define the *predictive fit* for PCUQ, we need:

- kernel $k : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, e.g. $k(y, y') = (yy') + (yy')^2$
- *reproducing kernel Hilbert space* (RKHS) $\mathcal{H}(k)$ [see Berlinet and Thomas-Agnan, 2011, for background]
- *kernel mean embedding*

$$\mu_k(P) := \int k(\cdot, y) \, \mathrm{d}P(y) \in \mathcal{H}(k).$$

The divergence of a candidate $P \in \mathcal{P}(\mathcal{Y})$ from the data-generating distribution $P_\star$ can be quantified using *maximum mean discrepancy* (MMD):

$$\begin{aligned} \mathrm{MMD}(P_\star, P) &= \|\mu_k(P_\star) - \mu_k(P)\|_{\mathcal{H}(k)} \\ &\overset{\text{e.g.}}{=} \left\| \begin{bmatrix} \mathbb{E}_{Y \sim P_\star}[Y] \\ \mathbb{E}_{Y \sim P_\star}[Y^2] \end{bmatrix} - \begin{bmatrix} \mathbb{E}_{Y \sim P}[Y] \\ \mathbb{E}_{Y \sim P}[Y^2] \end{bmatrix} \right\| \end{aligned}$$

The MMD is a proper metric if k is a *characteristic* kernel [Sriperumbudur et al., 2011]; our use of MMD is justified by its interpretation as a statistical divergence induced by a *proper scoring rule* [Dawid, 1986].

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This reveals one possible interpretation of (1) as a *kernel Stein discrepancy* [Chwialkowski et al., 2016, Liu et al., 2016, Gorham and Mackey, 2017] corresponding to the *Stein kernel* $\kappa_{P_\star}$ [Oates et al., 2017].

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Sensible in the Well-Specified Context
If $P_\star = P_{\theta_\star}$ for some unique $\theta_\star \in \Theta$, then (1) is uniquely minimised by $Q = \delta_{\theta_\star}$ provided k is a characteristic kernel.

Predictive Fit via MMD

The mixture model P_Q has kernel mean embedding

$$\mu_k(P_Q) = \iint k(\cdot, y)\, \mathrm{d}P_\theta(y)\mathrm{d}Q(\theta) = \int \mu_k(P_\theta)\, \mathrm{d}Q(\theta),$$

so the MMD between $P_\star$ and P_Q can be written as

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Estimation
Of course, the true data-generating distribution $P_\star$ in (1) is unknown and must be approximated. In PCUQ we use the empirical distribution P_n in lieu of $P_\star$.

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Regularisation
A plug-in approximation necessitates additional regularisation, since otherwise minimisation of $Q \mapsto \mathrm{MMD}(P_n, P_Q)$ would result in a discrete distribution where each atom corresponds to a value of θ that explains one of the data points well.

Approximating Q_n via Gradient Flow

The output Q_n of PCUQ is a minimiser of the entropy-regularised objective

$$\mathcal{F}_n(Q) = \mathcal{E}_n(Q) + \lambda_n \int \log q(\theta)\, \mathrm{d}Q(\theta), \tag{2}$$

where the *free energy* $\mathcal{E}_n(Q)$ is identical, after algebraic manipulation, to

$$\mathcal{E}_n(Q) \overset{+C}{=} \int v(\theta)\, \mathrm{d}Q(\theta) + \frac{1}{2} \iint \kappa_{P_n}(\theta, \vartheta)\, \mathrm{d}Q(\theta)\mathrm{d}Q(\vartheta),$$

and where q and q_0 are respectively densities for Q and Q_0.

Wasserstein Gradient Flow

For the entropy-regularised functional $\mathcal{F}_n$ (2), we can simulate a Wasserstein gradient flow via a McKean–Vlasov process [Ambrosio et al., 2008]

$$\mathrm{d}\theta_t = -\nabla_{\mathrm{W}} \mathcal{E}_n(Q^t)(\theta_t) + \sqrt{2\lambda_n}\mathrm{d}W_t, \tag{3}$$

$$\nabla_{\mathrm{W}} \mathcal{E}_n(Q^t)(\theta_t) = \nabla v(\theta_t) + \int \nabla_1 \kappa_{P_n}(\theta_t, \vartheta)\, \mathrm{d}Q^t(\vartheta)$$

where $Q^t = \mathrm{law}(\theta_t)$, ∇_{W} denotes the Wasserstein gradient, $(W_t)_{t \geq 0}$ is a Wiener process on $\mathbb{R}^p$ and, for the bivariate function κ_{P_n}, the notation $\nabla_1 \kappa_{P_n}$ denotes differentiation with respect to the first argument.

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Simulation as an Interacting Particle System
Discretise Q^t into a system of N evolving particles $\theta_t^1, \theta_t^2, \ldots, \theta_t^N$, whose evolution is governed by the following system of *stochastic differential equations* (SDEs):

$$\mathrm{d}\theta_t^i = -\left(\nabla v(\theta_t^i) + \frac{1}{N-1} \sum_{j \neq i} \nabla_1 \kappa_{P_n}(\theta_t^i, \theta_t^j)\right)\mathrm{d}t + \sqrt{2\lambda_n}\mathrm{d}W_t^i,$$

where $(W_t^i)_{t \geq 0}$ are N independent Wiener processes on $\mathbb{R}^p$. An Euler–Maruyama discretisation incurs per-iteration computational complexity $O(nN^2)$ and storage complexity (with caching) of $O(n + N)$.

Approximating Q_n via Gradient Flow

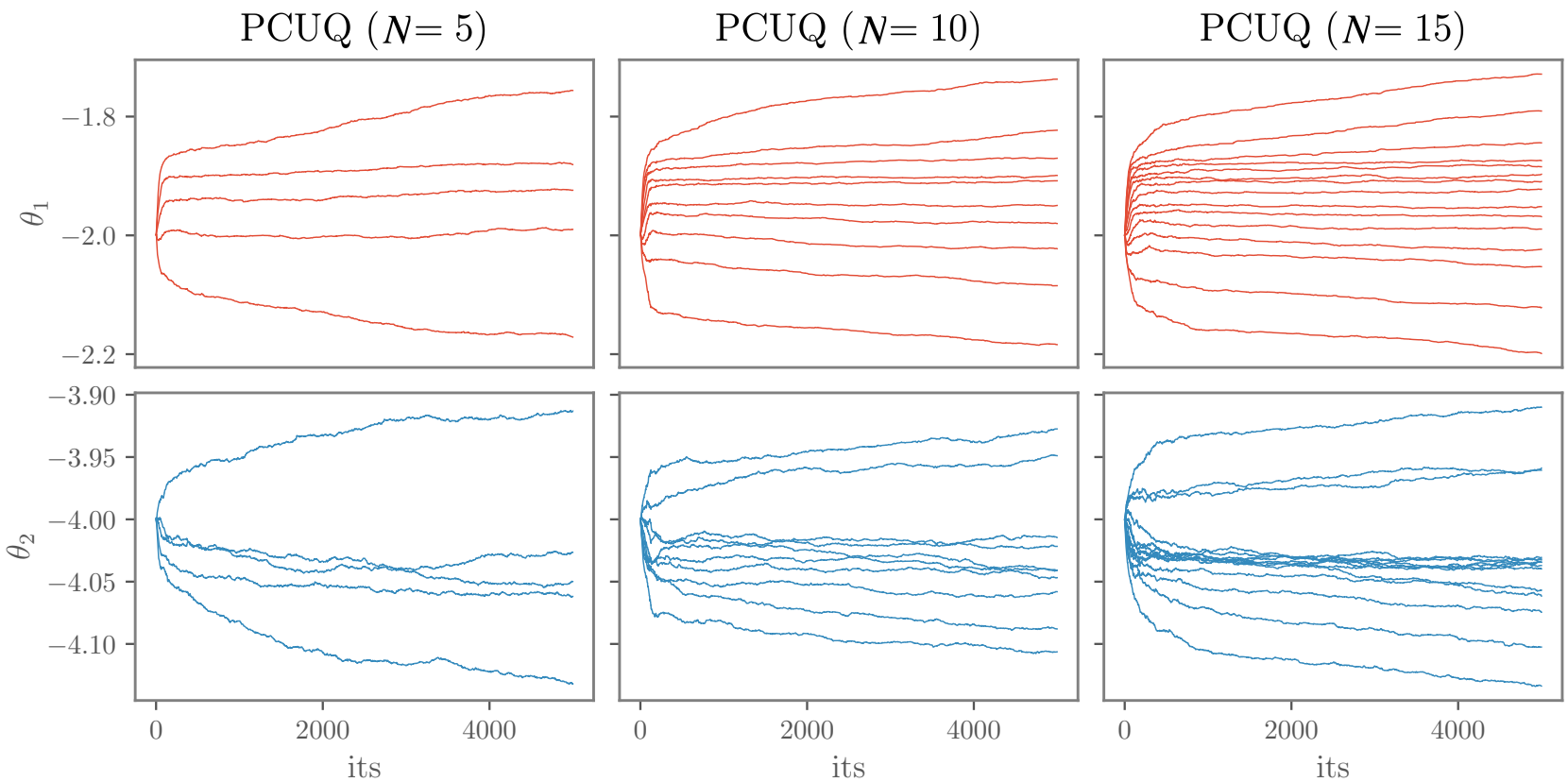
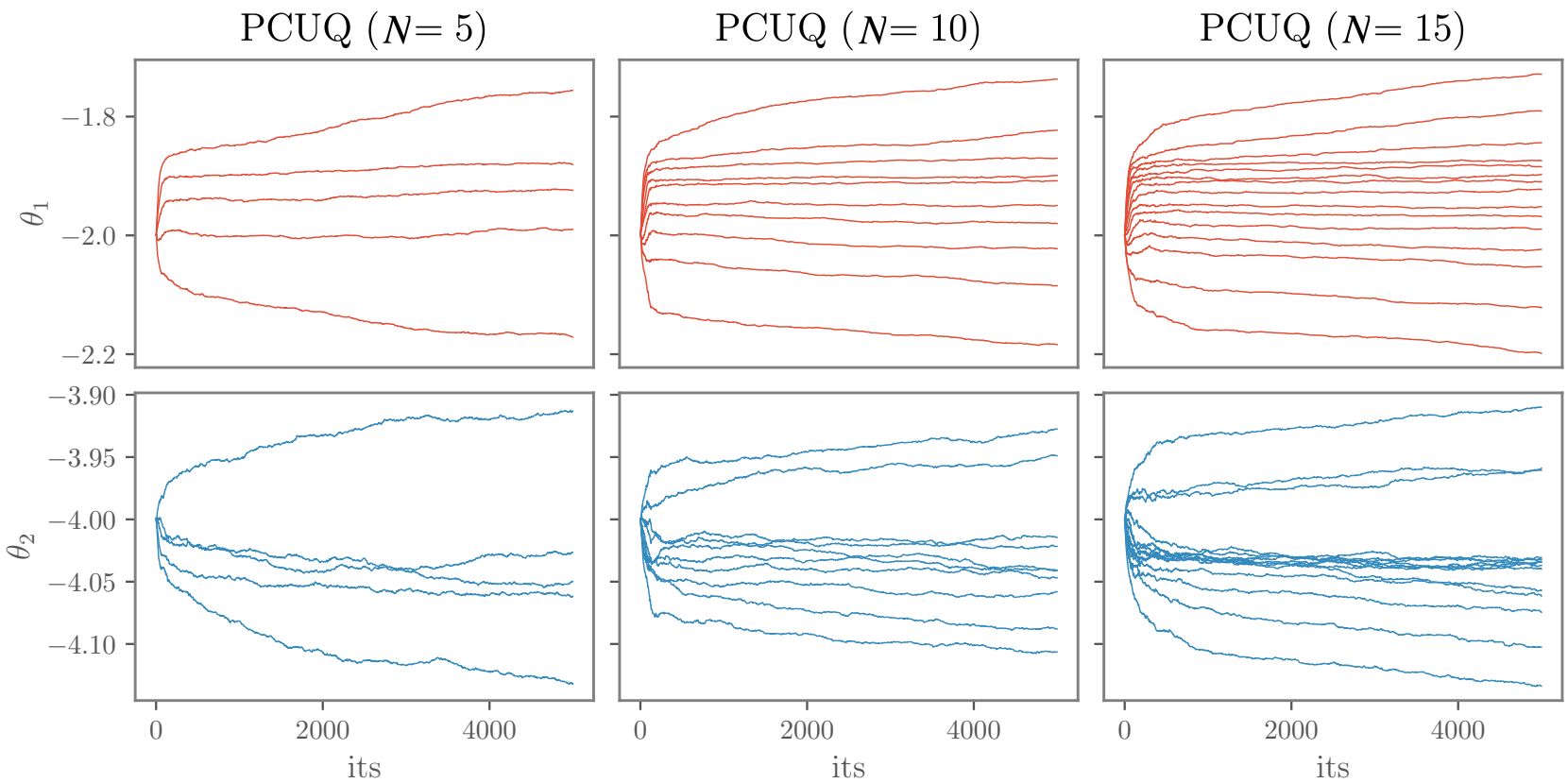


Figure: Interacting particle system for approximation of Q_n. (N = number of particles used)

Convergence of the Gradient Flow

Though theoretically convex, in practice gradients are small in low probability region; we mitigated this by initialising close to the Bayesian MAP $\theta^\dagger$.

Approximating Q_n via Gradient Flow



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Extension to Dependent Data

- each y_i is associated with a covariate $x_i \in \mathcal{X}$ and generated according to an (unknown) conditional distribution $P_\star(\cdot|x_i)$
- have a conditional model $\{P_\theta(\cdot|x)\}_{\theta\in\Theta}$ for each $x \in \mathcal{X}$

Idea: Suppose that [Alquier and Gerber, 2024]

$$\{(x_i, y_i)\}_{i=1}^n \overset{\text{iid}}{\sim} \bar{P}_\star(\mathrm{d}x, \mathrm{d}y) := \frac{1}{n}\sum_{i=1}^n \delta_{x_i}(\mathrm{d}x)\, P_0(\mathrm{d}y|x_i)$$

and consider the extended model

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Choice of Kernel
For example, if $\mathcal{X} \subset \mathbb{R}^{d_\mathcal{X}}$ and $\mathcal{Y} \subset \mathbb{R}^{d_\mathcal{Y}}$, we may consider the Gaussian kernel

$$k((x, y), (x', y')) = \exp\left(-\frac{\|x - x'\|^2}{\ell_\mathcal{X}^2} - \frac{\|y - y'\|^2}{\ell_\mathcal{Y}^2}\right)$$

with bandwidths $\ell_\mathcal{X}$ and $\ell_\mathcal{Y}$ to be specified. (We take $\ell_\mathcal{X} \to 0$, as recommended in Alquier and Gerber [2024].)

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Summary

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The main claims:

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- Methodology should probably be tailored to specific communities.
- Prediction-centric approaches are not new, but they are an interesting alternative to generalised Bayes!

Notable omissions:

- Bayesian exponentially tilted empirical likelihood, conformal prediction, martingale posteriors (next chapter!), ...

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