Standard IVP model:

$$Y_i = \mathcal{G}(x(t_i)) + \varepsilon_i \,, \qquad \varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, \theta) \,, \qquad x(0) = X_0$$

(assume $\mathcal{G}$ is linear, X_0 is known, f is autonomous)

$$\pi(\theta|Y) \propto \pi(Y|\theta)\pi(\theta)$$

$$\pi(Y|\theta) \longrightarrow \mathbb{E}_{\omega}\pi(Y|Z)\pi(Z|\theta,\omega)$$

- We introduce randomness ω to the integrator as a surrogate for the numerical error.
- Under the assumption that the scale etc. of this randomness can be calibrated to some justifiable notion of uncertainty in the method, we can treat this 'distribution over numerical solutions' the same way as the 'posterior' in 'Bayesian' PN.
- Marginalising it out then gives a parameter posterior which takes account of the numerical error.

[Lie et al. (2017b)]

- Generate a numerical sequence $z_1, z_2, \ldots, z_N$ (using an iterative procedure) which has provable proximity to the true values $x(t_1), x(t_2) \ldots, x(t_N)$.
- Iteration: $z_{i+1} \leftarrow\!\shortmid \{z_i, z_{i-1}, \ldots\}$

$$\sup_i \|z_i - x(t_i)\| < Ch^r$$

[Conrad et al. (2016)]

- Generate a numerical sequence $Z_1, Z_2, \ldots, Z_N$ (using a probabilistic iterative procedure) which has provable proximity to the true values $x(t_1), x(t_2) \ldots, x(t_N)$.
- Iteration: $z_{i+1} \leftarrow\!\shortmid \{z_i, z_{i-1}, \ldots, \omega\}$

$$\sup_i \mathbb{E}_\omega \left\| Z_i - x(t_i) \right\| < Ch^r$$

[Conrad et al. (2016)]

PROBABILISTIC EULER METHOD

$$
\begin{aligned}
Z_0 &\mapsfrom X_0 \\
F_i &\mapsfrom f(Z_i, \theta) \\
Z_{i+1} &\mapsfrom Z_i + hF_i + \xi_i(h)
\end{aligned}
\Bigg| \circlearrowleft
$$

THEOREM [Conrad et al. (2016)] If $\mathbb{E}[\xi_i(h)\xi_i(h)^T] < kh^3$, the order of convergence of the probabilistic method is equal to that of the Euler method.

[Conrad et al. (2016), Lie et al. (2017a)]

PROBABILISTIC ONE-STEP METHOD

$$
\left.
\begin{aligned}
Z_0 &\leftarrow\!\shortmid X_0 \\
F_i &\leftarrow\!\shortmid f(Z_i, \theta) \\
Z_{i+1} &\leftarrow\!\shortmid \Psi(Z_i) + \xi_i(h)
\end{aligned}
\right| \circlearrowleft
$$

$\Psi(Z_i)$ — numerical map of a one-step method of order p

THEOREM [Conrad et al. (2016)] If $\mathbb{E}[\xi_i(h)\xi_i(h)^T] < kh^{2p+1}$, the order of convergence of the probabilistic method is equal to that of the underlying deterministic method defined by Ψ.

[Conrad et al. (2016), Lie et al. (2017a)]

EXTENSION TO MULTISTEP METHOD

$$
\begin{aligned}
Z_0, \ldots, Z_s &\leftarrow X_0, \ldots, \tilde{X}_s \\
F_i &\leftarrow f(Z_i, \theta) \\
Z_{i+1} &\leftarrow Z_i + h \sum_{j=0}^{s-1} \beta_j F_{i-j} + \xi_i(h)
\end{aligned}
\Bigg| \circlearrowleft
$$

- The s-step Adams-Bashforth method is of order s.

THEOREM [Teymur et al. (2016)] If $\mathbb{E}[\xi_i(h)\xi_i(h)^T] < kh^{2s+1}$, the order of convergence of the probabilistic method is equal to that of the underlying deterministic method.

[Teymur et al. (2016)]

- Recall Adams-Bashforth relation $Z_{i+1} \leftarrow\!\shortmid Z_i + h \sum_{j=0}^{s-1} \beta_j F_{i-j}$.
- Implicit multistep method (Adams-Moulton) defined by

$$Z_{i+1} = Z_i + h \left[\beta_{-1} f(Z_{i+1}) + \sum_{j=0}^{s-1} \beta_j F_{i-j} \right].$$

- Requires a loop to calculate Z_{i+1}.
- Not clear how to randomise this (add a zero-mean Gaussian without knowing what we are adding it to...?).

- Rearrange as *function* of F_{i+1}:

$$F_{i+1}(z) = \frac{z - Z_i}{h} - \sum_{j=0}^{s-1} \beta_j F_{i-j}$$

- Form a distribution which directly penalises the discrepancy d between these two:

$$d(z) := \left(\frac{z - Z_i}{h} - \sum_{j=0}^{s-1} \beta_j F_{i-j} \right) - f(z)$$

[Teymur, Lie, Sullivan & Calderhead *(forthcoming)*]

$$
\begin{aligned}
Z_0, \ldots, Z_s &\leftarrowtail X_0, \ldots, \tilde{X}_s \\
F_i &\leftarrowtail f(Z_i, \theta) \\
p(Z_{i+1} = z | Z_i, Z_{i-1}, \ldots, Z_{i-(s-1)}) &\propto \exp\left(-\frac{d(z)^2}{2\eta^2}\right) \Bigg| \circlearrowleft
\end{aligned}
$$

THEOREM [Teymur, Lie, Sullivan & Calderhead] If $\eta = kh^s$, the method proposed above converges at the same rate as the underlying Adams-Moulton method.

CURRENT RESEARCH AND QUESTIONS

- Some approaches to calibration discussed in referenced papers (and in longer version of this talk!)
- Multidimensional generalisation accounts for non-trivial cross-correlations in errors.
- Can be tricky to implement (but some proposals in related papers about eg. how to set up the MCMC).
- Relatively expensive to calibrate but once this is done, can treat the inverse problem in the standard fashion.
- Effect on parameter posteriors being explored elsewhere.
- Maybe possible to make 'a priori' calibration statements exploiting known features of underlying method?
- Theoretical results presented in given papers — experiments ongoing.

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