REPORT – ANALYTICAL POSTERIORS IN A SIMPLE CASE

Let us consider as a toy problem the one dimensional ODE

$$y' = -y, \quad y(0) = y_0.$$

We consider the inferential problem of determining the true initial condition y_0^* from the observations. Given $h > 0$, we consider a single observation $d = y^{y_0^*}(h) + \eta$, where $y^{y_0^*}(h) = y_0^* e^{-h}$ is the true solution at time $t = h$ and $\eta \sim \mathcal{N}(0, \sigma^2)$ is a source of noise. If a Gaussian prior $\pi_0 = \mathcal{N}(0, 1)$ is given for y_0, the posterior distribution is computable analytically and is given by

$$\pi(y_0 \mid d) = \mathcal{N}\Big(y_0; \frac{de^{-h}}{\sigma^2 + e^{-2h}}, \frac{\sigma^2}{\sigma^2 + e^{-2h}}\Big),$$

where $\mathcal{N}(x; \mu, \alpha^2)$ is the density of a Gaussian random variable of mean μ and variance α^2 evaluated in x. Consistently, if $\sigma^2 \to 0$, we have that $d \to y_0^* e^{-h}$ and therefore $\pi(y_0 \mid d) \to \delta_1 = \delta_{y_0^*}$.

If we approximate $y^{y_0}(h)$ for a given initial condition y_0 with a single step of the explicit Euler method (i.e., with step size h), we get $y^{y_0}(h) \approx (1-h)y_0$. Computing the posterior distribution obtained with this approximation leads to

$$\pi_{\mathrm{EE}}(y_0 \mid d) = \mathcal{N}\Big(y_0; \frac{(1-h)d}{\sigma^2 + (1-h)^2}, \frac{\sigma^2}{\sigma^2 + (1-h)^2}\Big).$$

In the limit of $\sigma^2 \to 0$, we get in this case that the posterior distribution tends to $\pi_{\mathrm{EE}}(y_0 \mid d) \to \delta_{\bar{y}}$, where $\bar{y} = e^{-h} y_0^* / (1-h)$. If, for example, $y_0^* = 1$ and $h = 1/2$, we would have $\bar{y} \approx 1.213$. The posterior distribution is hence tending to a biased Dirac delta with respect to the true value.

Let us consider the additive noise explicit Euler (AN-EE), i.e., the approximation $y^{y_0}(h) \approx Y_1$, where $Y_1 = (1-h)y_0 + \xi$ and ξ is a random variable $\mathcal{N}(0, h^3)$, so that the method converges consistently with the deterministic method. In this case, the posterior distribution is given by

$$\pi_{\mathrm{EE}}(y_0 \mid d) = \mathcal{N}\Big(y_0; \frac{(1-h)d}{\tilde{\sigma}^2 + (1-h)^2}, \frac{\tilde{\sigma}^2}{\tilde{\sigma}^2 + (1-h)^2}\Big).$$

where $\tilde{\sigma}^2 = \sigma^2 + h^3$. In this case, taking the limit $\sigma^2 \to 0$ leads to

$$\pi_{\mathrm{AN-EE}}(y_0 \mid d) \to \mathcal{N}\Big(y_0; \frac{(1-h)e^{-h} y_0^*}{h^3 + (1-h)^2}, \frac{h^3}{h^3 + (1-h)^2}\Big),$$

which shows that while the asymptotic mean is still biased with respect to the true value, the uncertainty in the forward model is reflected by a positive variance. In case $h = 1/2$ and $y_0^* = 1$, we get that the mean under the posterior is approximately 0.809 and the variance is 1/3.

Let us now consider the random time step explicit Euler (RTS-EE) with step size distribution $H \sim \mathcal{U}(h - h^p, h + h^p)$. In this case, the forward model acts as

$$Y_1 = y_0 - Hy_0 = (1-h)y_0 + (h - H)y_0, \quad U \sim \mathcal{U}(-h^p, h^p).$$

The posterior distribution over y_0 can be computed as

$$\begin{aligned} \pi_{\mathrm{RTS-EE}}(y_0 \mid d) &\propto \pi_0(y_0)\, \mathbb{E}^U\, \pi(d \mid y_0) \\ &\propto \exp\Big(-\frac{y_0^2}{2}\Big)\, \mathbb{E}^U \exp\Big(-\frac{(d - (1-h)y_0 - Uy_0)^2}{2\sigma^2}\Big). \end{aligned}$$

Let us compute the likelihood term. With a change of variable $z = Uy_0$ we obtain

$$\mathbb{E}^U\, \pi(d \mid y_0) = \frac{1}{2h^p y_0} \int_{y_0 h^p}^{y_0 h^p} \exp\Big(-\frac{(d - (1-h)y_0 - z)^2}{2\sigma^2}\Big) \mathrm{d}z.$$

Now a change of variable $w = (z - (d - (1-h)y_0))/\sigma$ gives

$$\mathbb{E}^U\, \pi(d \mid y_0) = \frac{\sigma}{2h^p y_0} \int_{(-y_0 h^p - (d-(1-h)y_0))/\sigma}^{(y_0 h^p - (d-(1-h)y_0))/\sigma} \exp\Big(-\frac{w^2}{2}\Big) \mathrm{d}z,$$

Hence the likelihood can be expressed in terms of the cumulative distribution function Φ of a standard Gaussian random variable, i.e.,

$$\mathbb{E}^U\, \pi(d \mid y_0) = \frac{\sigma\sqrt{2\pi}}{2h^p y_0} \Big(\Phi\Big(\frac{((1-h)+h^p)y_0 - d}{\sigma}\Big) - \Phi\Big(\frac{((1-h)-h^p)y_0 - d}{\sigma}\Big)\Big).$$

Disregarding all multiplicative constant that are independent of y_0, we get the posterior

$$\pi_{\mathrm{RTS-EE}}(y_0 \mid d) \propto \exp\Big(-\frac{y_0^2}{2}\Big)\frac{1}{y_0}\Big(\Phi\Big(\frac{((1-h)+h^p)y_0 - d}{\sigma}\Big) - \Phi\Big(\frac{((1-h)-h^p)y_0 - d}{\sigma}\Big)\Big).$$

The natural choice of p is $p = q + 1/2 = 3/2$, hence

$$\pi_{\mathrm{RTS-EE}}(y_0 \mid d) \propto \exp\Big(-\frac{y_0^2}{2}\Big)\frac{1}{y_0}\Big(\Phi\Big(\frac{((1-h)+h^{3/2})y_0 - d}{\sigma}\Big) - \Phi\Big(\frac{((1-h)-h^{3/2})y_0 - d}{\sigma}\Big)\Big).$$

In the limit for $\sigma \to 0$, the difference between the cumulative distribution functions of tends to 1 or to 0 depending on the sign of the argument. Hence, the limiting distribution is

$$\pi_{\mathrm{RTS-EE}}(y_0 \mid d) \propto \exp\Big(-\frac{y_0^2}{2}\Big)\frac{1}{y_0}\chi_{\{y_{\min} \le y_0 \le y_{\max}\}},$$

where the interval $[y_{\min}, y_{\max}]$ is given by

$$y_{\min} = \frac{e^{-h} y_0^*}{((1-h)+h^{3/2})}, \quad y_{\max} = \frac{e^{-h} y_0^*}{((1-h)-h^{3/2})},$$

as in the limit of $\sigma \to 0$, we have $d \to e^{-h} y_0^*$. In order to compute moments of y_0 under the limiting posterior distribution with respect to σ, we need first to compute the normalising constant of the posterior, i.e.

$$C = \int_{-\infty}^{\infty} \exp\Big(-\frac{y_0^2}{2}\Big)\frac{1}{y_0}\chi_{\{y_{\min} \le y_0 \le y_{\max}\}} \mathrm{d}y_0 = \frac{1}{2}\Big(\mathrm{Ei}\big(\frac{y_{\min}^2}{2}\big) - \mathrm{Ei}\big(\frac{y_{\max}^2}{2}\big)\Big),$$

where Ei is the exponential integral function, which is defined as

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty} \frac{e^{-t}}{t} \mathrm{d}t.$$

The mean of y_0 under the posterior is then given by

$$\mathbb{E}_{\pi_{\mathrm{RTS-EE}}(y_0|d)}(y_0) = \frac{1}{C}\int_{-\infty}^{\infty} \exp\Big(-\frac{y_0^2}{2}\Big)\chi_{\{y_{\min} \le y_0 \le y_{\max}\}} \mathrm{d}y_0 = \sqrt{2\pi}\frac{\Phi(y_{\max}) - \Phi(y_{\min})}{C}.$$

The second moment of y_0 is instead given by

$$\mathbb{E}_{\pi_{\mathrm{RTS-EE}}(y_0|d)}(y_0^2) = \frac{1}{C}\int_{-\infty}^{\infty} y_0 \exp\Big(-\frac{y_0^2}{2}\Big)\chi_{\{y_{\min} \le y_0 \le y_{\max}\}} \mathrm{d}y_0 = \frac{e^{-y_{\min}^2/2} - e^{-y_{\max}^2/2}}{C},$$

which gives the variance

$$\mathrm{Var}_{\pi_{\mathrm{RTS-EE}}(y_0|d)}(y_0) = \frac{e^{-y_{\min}^2/2} - e^{-y_{\max}^2/2}}{C} - \Big(\sqrt{2\pi}\frac{\Phi(y_{\max}) - \Phi(y_{\min})}{C}\Big)^2.$$

In case $h = 1/2$ and $y_0^* = 1$, we get $\mathbb{E}_{\pi_{\mathrm{RTS-EE}}(y_0|d)}(y_0) \approx 1.154$ and $\mathrm{Var}_{\pi_{\mathrm{RTS-EE}}(y_0|d)}(y_0) \approx 0.166$.

We represent graphically the posterior distributions obtained with the exact and approximated forward models in Figure 1 and 2. We vary $\sigma = \{0.1, 0.05, 0.025, 0.0125\}$ and consider $y_0^* = 1$ and $h = 1/2$.

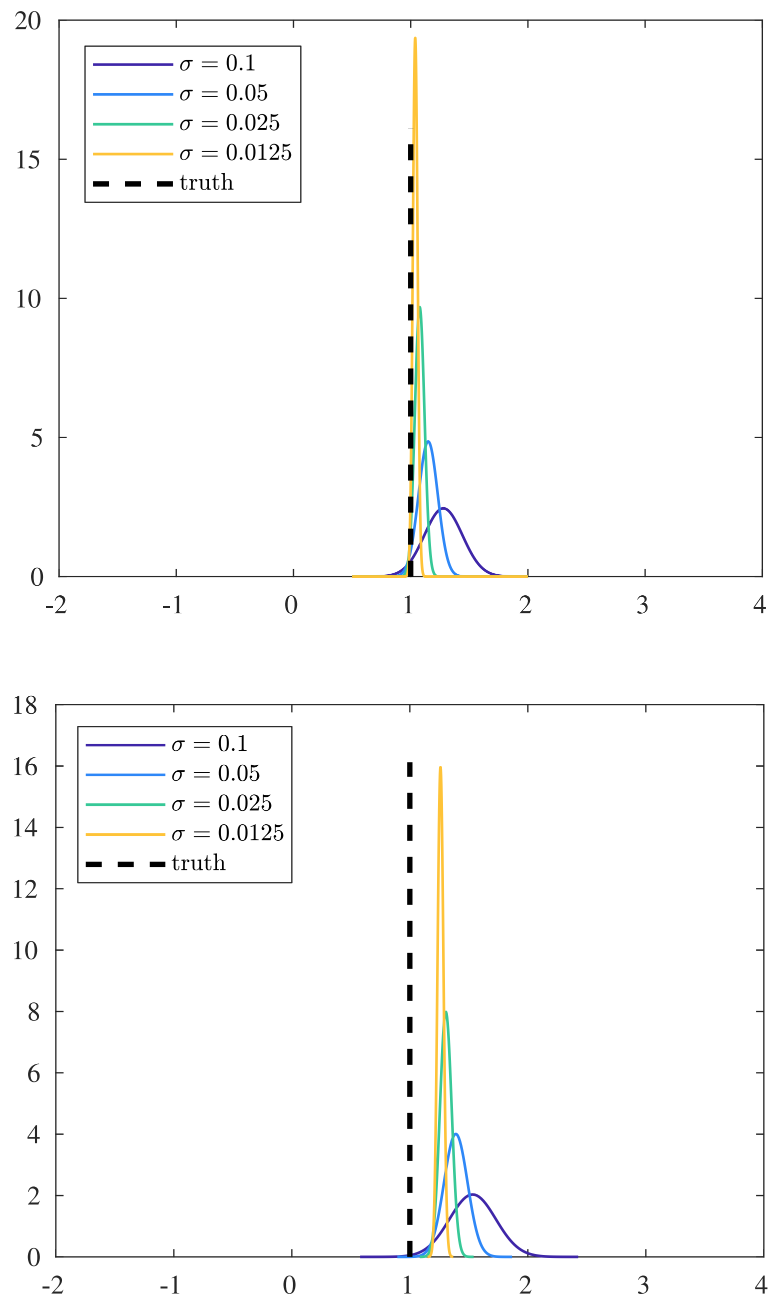

Fig. 1: Exact posterior distribution and explicit Euler posterior.

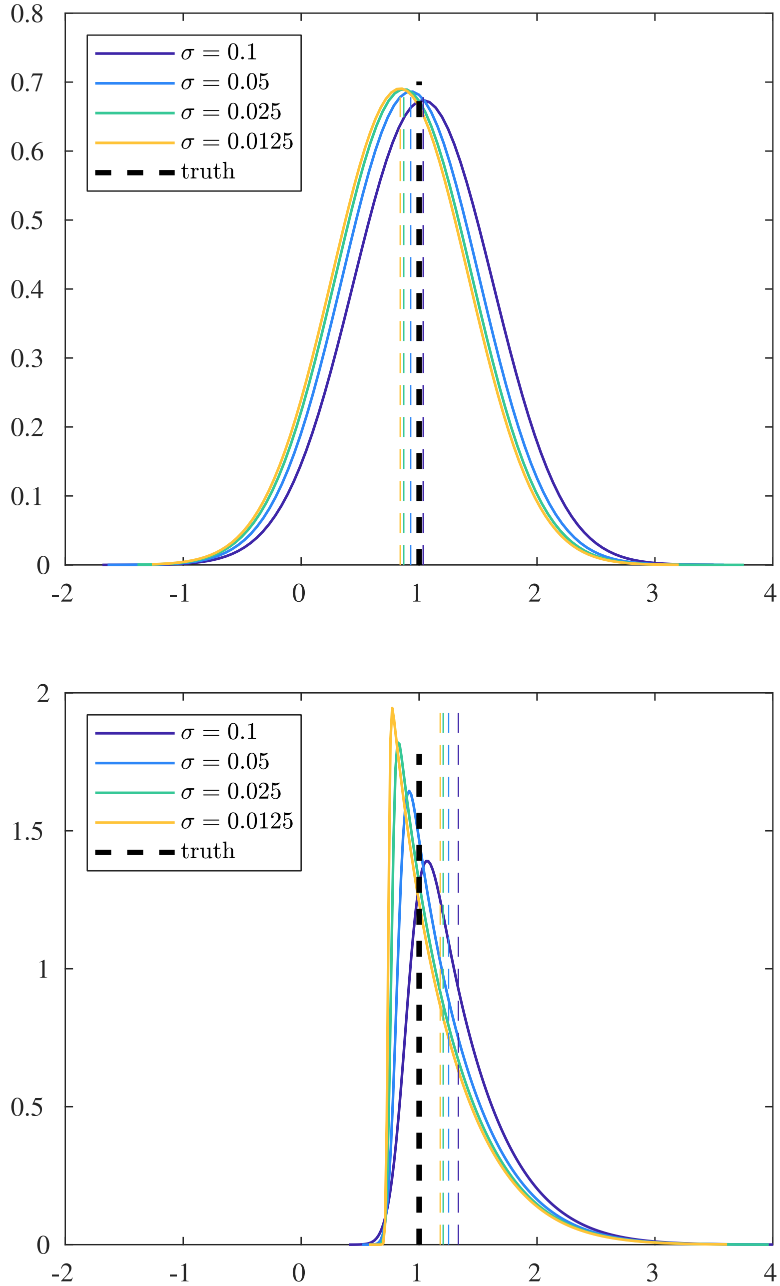

Fig. 2: Posterior distributions for the AN-EE (top) and the RTS-EE (bottom) methods. The mean of the posterior distribution is represented by vertical dashed lines for the different values of σ.