A Probabilistic Model for the Numerical Solution of Initial Value Problems

by Schober, Särkkä and Hennig

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- In this paper it is shown that for those priors, the predictive posterior corresponds to a linear multistep method for solving the ODE in Nordsieck form\(^1\).

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• In this paper it is shown that for those priors, the predictive posterior corresponds to a linear multistep method for solving the ODE in Nordsieck form\(^1\).
• This allows us to establish global error results in a consistent fashion.

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Standard Solvers and Nordsieck Form
Problem Setup

We have an IVP:

\[ y'(x) = f(t, y(t)) \]

where

- \( t \in T := [t_0, T] \subset \mathbb{R} \)
- \( y : T \to \mathbb{R} \)
- \( f : T \times \mathbb{R} \to \mathbb{R} \)
- \( y(t_0) = y_0 \).
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Produce a solution on a grid \( \{t_n\} \), \( n = 0, 1, 2, \ldots, N \). Let \( y_n \) be the approximation to \( y \) at time \( t_n \), and \( h_n = t_n - t_{n-1} \). Let \( z_n = f(t_n, y_n) \).
Only consider explicit methods.
Only consider **explicit** methods.

The most basic: **Explicit Euler**

\[ y_n = y_{n-1} + h z_{n-1} \]

Problems: global error \( O(h) \), unstable.

We would like methods of order \( q \) - that is, with global error \( O(h^q) \)
(Explicit) Linear Multistep Methods approximate the solution as a linear combination of previous evaluations of $f$ and estimates of $y$

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h \sum_{i=1}^{k} \beta_i z_{n-i}$$

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(1)

Two predominant methods:

- Adams-Bashforth
- Adams-Moulton

[See also: Teymur et al. [2016]]
Runge Kutta Methods evaluate $f$ at multiple locations between time-steps:

$$k_i = f(t_n + c_i h, y + h \sum_{j<i} a_{ij} k_j)$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$$
Runge Kutta Methods

Butcher Tableau for $q = s = 2$:

\[
\begin{align*}
    k_1 &= f(t_n, y_n) \\
    k_2 &= f(t_n + \alpha h, y_n + \alpha h k_1) \\
    y_{n+1} &= y_n + h \left(1 - \frac{1}{2\alpha}\right) k_1 + \frac{h}{2\alpha} k_2
\end{align*}
\]

Midpoint method: $\alpha = \frac{1}{2}$

Heun’s method: $\alpha = 1$

\[
\begin{array}{c|cc}
0 & \alpha & \alpha \\
\alpha & (1 - \frac{1}{2\alpha}) & \frac{1}{2\alpha}
\end{array}
\]
All Linear Multistep Methods\(^2\) can be written in **Nordsieck form**:

\[
x_n = \left( y_n, h y'_n, \ldots, \frac{h^q y^{(q)}(n)}{q!} \right)
\]

\[
x_{n+1} = \left( I - L e_1^T \right) P x_n + h L z_n
\]

where \( z_n \) solves

\[
[P x_n]_1 + [L]_1 z_n = h f(t_n + h, [P x_n]_0 + h[L]_0 z_n)
\]

\( P \) the Pascal Triangle matrix.

\(^2\)and some Runge-Kutta Methods?
For suitable choices of $L$, Nordsieck methods can achieve local truncation error (at least) $q$. 
A Probabilistic Model
For a probability space \((\Omega, \mathcal{F}, P)\)...

- \(X_t\) the prior distribution for the solution \(y(t)^3\), taking values in \(\mathbb{R}^{q+1}\).
- \(Y\) the *true* solution
- \(Y'\) its first derivative.

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- \(X_t\) the prior distribution for the solution \(y(t)^3\), taking values in \(\mathbb{R}^{q+1}\).
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We also let \(\mathcal{F}_t\) denote the *filtration* generated by \(X_t\).

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Obervation: certain GPs can be written as a Linear Time Invariant (LTI) SDE:

\[ dX_t = FX_t dt + LdW_t \]

\( F \) the “state feedback matrix” and \( L \) the “diffusion vector”. \( W_t \) a Wiener process, \( dW(t) \sim \mathcal{N}(0, \sigma^2 dt) \).
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\[ dW(t) \sim \mathcal{N}(0, \sigma^2 dt). \]

We assume \( Y_t \) and \( Y'_t \) are related to \( X_t \) by

\[ Y_t = H_0 X_t \]
\[ Y'_t = H_1 X_t \]
Given a $X_{t_*} \sim \mathcal{N}(m_*, C_*)$, for $t > t_*$ we have that $X_t$ is also Gaussian.
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Let $A(h) = \exp(Fh)$. Then

$$m_t = A(t - t^*) m_*$$
$$\text{cov}(X_t, X_{t'}) = A(t' - t^*) C_* A(t - t^*)^T$$
$$+ \int_{t^*}^{\min(t, t')} A(t - \tau) L \sigma^2 L^T A(t' - \tau)^T d\tau$$
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Let $A(h) = \exp(Fh)$. Then

$$m_t = A(t - t_*)m_*$$

$$\text{cov}(X_t, X_{t'}) = A(t' - t_*)C_*A(t - t_*)^T$$

$$+ \int_{t_*}^{\min(t, t')} A(t - \tau)L\sigma^2L^TA(t' - \tau)^T d\tau$$

For the practical algorithm we only ever need $\text{cov}(X_{t+h}, X_{t+h})$, so let

$$Q(h) = \int_{t}^{t+h} A(h)L\sigma^2L^TA(h)^T d\tau$$
The advantage of this formulation is that if we view solution as a filtering problem, it allows us to express predictive means in Nordsieck form.
The Kalman Filter

Assuming:

1. Observations $z_t$ are linked to a hidden state $x_t$ by a **Linear** operator:

   $$z_t = H x_t + \xi_t$$

   where $\xi_t \sim \mathcal{N}(0, R)$
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2. We have some Prediction equation

$$x_{t+1}^- = A x_t + \eta_t$$

where $\eta_t \sim \mathcal{N}(0, Q)$
The Kalman Filter

Assuming:

1. Observations $z_t$ are linked to a hidden state $x_t$ by a Linear operator:

   $$z_t = H x_t + \xi_t$$

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   $$x_{t+1}^- = Ax_t + \eta_t$$

   where $\eta_t \sim \mathcal{N}(0, Q)$

3. We endow $x_0$ with a Gaussian prior.
The Kalman Filter

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the Kalman filter describes how to exactly update the posterior distribution as new observations are obtained.
The Kalman Filter

More or less...

1. **Predict**: $\mathbf{x}_{t+1}^- | \mathbf{z}_t$
2. **Update**: $\mathbf{x}_{t+1} | \mathbf{z}_{t+1}$

Under the assumptions, distributions on $\mathbf{x}_t$ and $\mathbf{x}_t^-$ are **Gaussian** for all $t$. 
The Kalman Filter

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Under the assumptions, distributions on $x_t$ and $x_t^-$ are **Gaussian** for all $t$.

Kalman’s equations tell us how to efficiently update the mean and covariance matrices for each new piece of information.
Start with a Gaussian distribution $X_0$. For $n = 0, \ldots, N$ do...

1. Compute the predictive distribution $X_{t_n}^- | Z_{[n-1]}$
2. Compute $z_n = f(t_n, X_{t_n}^-)$ (noiseless)
3. Find $X_{t_n} | Z[n]$

Problem: Step 2 is not tractable.
Solution: replace step 2 with something explicitly computable:

1. Compute the **predictive distribution** $\mathbf{X}_{t_n} | z_{n-1}$
2. Compute $z_n = f(t_n, \mathbb{E}(\mathbf{X}_{t_n}))$ (noiseless)
3. Find $\mathbf{X}_{t_n} | z_n$
The Algorithm
Runge Kutta Means
This formulation makes simpler the earlier result\textsuperscript{4} regarding Runge Kutta Means.

\textsuperscript{4}Schober et al. [2014]
This formulation makes simpler the earlier result\(^4\) regarding Runge Kutta Means. In what follows we will use an **Integrated Wiener Process** of order \(q\) (IWP\((q)\)) form for \(X_t\):

\[
dX_t = U_{q+1}X dt + e_q dW
\]

Where \(U_q\) is the **upper shift matrix** of size \(q\). This gives a convenient closed-form for \(A(h), Q(h)\).

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Where \(U_q\) is the upper shift matrix of size \(q\). This gives a convenient closed-form for \(A(h), Q(h)\).

Choose the prior mean to be \(m_{t-1}^- \equiv 0\) and the prior covariance to be \(C_{t-1}^-\).

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The **predictive mean** at $t = 1$ is equivalent to **Explicit Euler**.
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\[ m_{t-1} = \begin{pmatrix} y_0 \\ m_{t_0,1}^- \end{pmatrix} \]

\[ c_{t-1} = \begin{pmatrix} 0 & 0 \\ 0 & c_{t_0,11}^- \end{pmatrix} \]

for some $m_{t_0,1}^-$ and $c_{t_0,11}^-$
The predictive mean at $t = 1$ is equivalent to Explicit Euler.

\[
\begin{align*}
&\bullet
t_{-1} &\quad &\bullet
t_0 &\quad &\circ
t_1 \\
m_{t_0} = \begin{pmatrix} y_0 \\ z_0 \end{pmatrix} \\
C_{t_0} = 0
\end{align*}
\]
The predictive mean at $t = 1$ is equivalent to Explicit Euler.

\[ m_{t_1}^- = \begin{pmatrix} y_0 + hz_0 \\ z_0 \end{pmatrix} \]

\[ c_{t_1}^- = Q(h) \]
The **predictive mean** at $t = 1$ is equivalent to **Explicit Euler**.

\[
m_{t_1} = \begin{pmatrix} y_0 + \frac{h}{2}(z_0 + z_1) \\ z_1 \end{pmatrix}
\]

\[
C_{t_1} = \sigma^2 \begin{pmatrix} \frac{h^3}{12} & 0 \\ 0 & 0 \end{pmatrix}
\]

This corresponds to an RK2 scheme. (Heun’s Method, $\alpha = 1$).
Continuing this past $t_1$ we see that the scheme no longer matches any known numerical method (not even Heun’s method).
For an IWP(2) model we fix the prior covariance to be $C_{t-1}^\tau = Q(\tau)$ for some $\tau > 0$. 
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\[
\begin{bmatrix}
& t_{-1} & t_0 & t_0 + h \alpha & t_1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
 m_{t_0 + h \alpha}^- \end{bmatrix}_0 = y_0 + h \alpha z_0 + \frac{h^2 \alpha^2}{2} \left( \frac{4z_0}{\tau} - \frac{20y_0}{3\tau} \right)
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\begin{array}{cccc}
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\bullet & \bullet & \bullet & \bigcirc \\
\end{array}
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\]

For equivalence with RK2 we require

\[
\begin{bmatrix} m_{t_0+h\alpha}^- \end{bmatrix}_0 = y_0 + h\alpha z_0
\]

Solution (?): Send \( \tau \to \infty \)}
$\tau \rightarrow \infty$

- Equivalent to using an improper prior.
- More severe ramifications for continuation.
- Challenging computationally.
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- More severe ramifications for continuation.
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Difficult to justify given that the domain is restricted to \([t_0, T]\\)
Convergence Analysis and Nordiseck Methods
The posterior mean **does not** correspond to an RK method past $t_1$...

$\implies$ no global error results from this route!
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It does correspond to a general linear method in Nordsieck form.
We re-scale the state vector:

\[ \tilde{X} = \begin{pmatrix} Y_t \\ hY'_t \\ \frac{h^2}{2!} Y''_t \\ \vdots \\ \frac{h^q}{q!} Y^{(q)}_t \end{pmatrix} = BX_t \]

yielding the new SDE

\[ d\tilde{X}_t = BU_{q+1}B^{-1}\tilde{X}_t dt + Be_q dW \]

which makes \( \tilde{A}(h) \) independent of \( h \).
Proposition 1

The probabilistic Nordsieck method arising from the once-integrated Wiener process is equivalent in predictive posterior mean with the trapezoidal rule.
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The probabilistic Nordsieck method arising from the once-integrated Wiener process is equivalent in predictive posterior mean with the trapezoidal rule.

This means that the IWP(1) probabilistic Nordsieck method is actually of order 2 rather than order 1!
Theorem 1

The predictive posterior mean of the IWP(2) with fixed step size $h$ is a third order Nordsieck method.
Calibration and Experiments
Three parameters to tune: $q, \sigma^2, h$. $q$ is fixed to 2.
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As with standard solvers we adapt $h_n$ at each step to not exceed a tolerance.
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As with standard solvers we adapt $h_n$ at each step to not exceed a tolerance. $\sigma$ is chosen by maximising the marginal likelihood of the residual:

$$
\hat{\sigma} := \arg \min_{\sigma} p \left( z_n - \left[ m_{t_n} \right]_1 \mid \sigma \right)
$$
Experiments

[To the paper!]
Conclusions
• The choice of $z_n = f(t_n, \mathbb{E}(X_{t_n}^-))$. 

Criticisms

- The choice of $z_n = f(t_n, \mathbb{E}(X_{t_n}))$.
- The filtration assumption.
Further Work

- How does this relate to the fully Bayesian posterior distribution?
Further Work

• How does this relate to the fully Bayesian posterior distribution?
• What about implicit schemes?
Thanks!
References


