

On tree-based methods for (partial) differential equations

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(joint work with Guillaume Penent and Jiang Yu Nguwi)

Stochastic branching mechanisms have been used to represent the solutions of partial differential equations in [15], [7], [10], [8], and recently extended in [6] to the treatment of polynomial nonlinearities in first order gradient terms. This talk reviews an extension of such tree-based methods to functional nonlinearities with gradients of arbitrary orders.

Consider the ODE

$$(1) \quad u'(t) = f(u(t)), \quad u(0) = u_0 \in \mathbb{R}^d, \quad t \in \mathbb{R}_+,$$

whose solution can be expanded as

$$u(t) = u_0 + tf(u_0) + \frac{t^2}{2}f'f(u_0) + \frac{t^3}{6}f'f'f(u_0) + \frac{t^3}{6}f''[f, f](u_0) + \dots$$

which rewrites as the sum

$$u(t) = u_0 + \sum_{\mathcal{T}} \frac{t^{r(\mathcal{T})}}{\sigma(r(\mathcal{T}))\gamma(r(\mathcal{T}))} F(\mathcal{T})$$

over the family of Butcher trees \mathcal{T} , see [1], [2], Chapters 4-6 of [4], and [9], based on early work of [3]. In order to solve (1), we may also write

$$u(s) = u_0 + \int_0^s u'(r)dr = u_0 + \int_0^s f(u(r))dr,$$

and more generally we can expand the derivative $f^{(l)}(u(r))$ as

$$f^{(l)}(u(r)) = f^{(l)}(u_0) + \int_0^r f(u(r))f^{(l+1)}(u(v))dv, \quad l \geq 1.$$

We note that the above family of equations can be rewritten as

$$(2) \quad c(u)(t) = c(u)(0) + \sum_{Z \in \mathcal{M}(c)} \int_0^t \prod_{z \in Z} z(u)(s)ds$$

where c runs through a set $\mathcal{C} := \{\text{Id}, f^{(l)}, l \geq 0\}$, of functions called *codes* and $\mathcal{M}(c)$ is defined by letting $\mathcal{M}(\text{Id}) := \{f\}$ and $\mathcal{M}(g) := \{(f, g')\}$ for g a smooth function on $\mathbb{R}_+ \times \mathbb{R}$, see [12].

Next, consider a nonlinear PDE of the form

$$(3) \quad \begin{cases} \partial_t u(t, x) + \frac{1}{2} \Delta u(t, x) + f(u(t, x)) = 0 \\ u(T, x) = \phi(x), \quad (t, x) \in [0, T] \times \mathbb{R}. \end{cases}$$

Letting $v(t, x) := g(u(t, x))$, we now have

$$\begin{aligned} \partial_t v(t, x) + \frac{1}{2} \Delta v(t, x) &= g'(u(t, x)) \left(\partial_t u(t, x) + \frac{1}{2} \Delta u(t, x) \right) + \frac{1}{2} (\partial_x u(t, x))^2 g''(u(t, x)) \\ &= -f(u(t, x)) g'(u(t, x)) + \frac{1}{2} (\partial_x u(t, x))^2 g''(u(t, x)), \end{aligned}$$

which shows that the functions u , $\partial_x u$, $af^{(k)} \circ u$ satisfy the integral equations

$$\left\{ \begin{array}{l} u(t, x) = \int_{-\infty}^{\infty} \varphi(T-t, y-x) \phi(y) dy + \int_t^T \int_{-\infty}^{\infty} \varphi(s-t, y-x) f(u(s, y)) dy ds \\ af^{(k)}(u(t, x)) = \int_{-\infty}^{\infty} \varphi(T-t, y-x) af^{(k)}(\phi(y)) dy \\ + \int_t^T \int_{-\infty}^{\infty} \varphi(s-t, y-x) \\ \quad \times \left(af(u(s, y)) f^{(k+1)}(u(s, y)) - \frac{a}{2} (\partial_x u(s, y))^2 f^{(k+2)}(u(s, y)) \right) dy ds \\ \partial_x u(t, x) = \int_{-\infty}^{\infty} \varphi(T-t, y-x) \partial_x \phi(y) dy \\ + \int_t^T \int_{-\infty}^{\infty} \varphi(s-t, y-x) f'(u(s, y)) \partial_x u(s, y) dy ds, \end{array} \right.$$

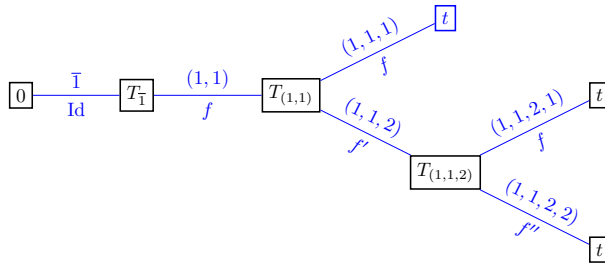
$a \neq 0$, $k \in \mathbb{N}$. We note that the above set of equations admits a formulation identical to (2) provided that we use the codes

$$\mathcal{C} := \{\text{Id}, \partial_x, af^{(k)}, a \neq 0, k \in \mathbb{N}\}$$

and the mechanism defined as

$$\mathcal{M}(\text{Id}) := \{f^*\}, \quad \mathcal{M}(g^*) := \left\{ (f^*, (g')^*), \left(\partial_x, \partial_x, -\frac{1}{2} (g'')^* \right) \right\},$$

and $\mathcal{M}(\partial_x) := \{((f')^*, \partial_x)\}$.



We consider a random coding tree $\mathcal{T}_{t,x,c}$ illustrated by the above sample, started at (t, x) with a code $c \in \mathcal{C}$ and partitioned as $\mathcal{K}^\partial \cup \mathcal{K}^\circ$, where \mathcal{K}° denotes the set of leaves. In the next result, we use the random functional

$$\mathcal{H}(\mathcal{T}_{t,x,c}) := \prod_{\bar{k} \in \mathcal{K}^\circ} \frac{1}{q_{c_{\bar{k}}} \rho(\tau_{\bar{k}})} \prod_{\bar{k} \in \mathcal{K}^\partial} \frac{c_{\bar{k}}(u)(T, X_{T_{\bar{k}}})}{\bar{F}(T - T_{\bar{k}})}.$$

of the random coding tree $\mathcal{T}_{t,x,c}$, in which branching at a node \bar{k} occurs at the random time $T_{\bar{k}}$, the interjump time $\tau_{\bar{k}} = T_{\bar{k}} - T_{\bar{k}-}$ has tail CDF \bar{F} and PDF ρ , and $(X_t^{\bar{k}})_{t \geq T_{\bar{k}-}}$ is an independent Brownian motion started at time $T_{\bar{k}-}$.

Theorem 1. ([13]) *Assume that the integral solution of the system (2) is unique and that there exists a constant $K > 0$ such that:*

$$|f^{(k)} \circ \phi|_{\infty} \leq K, \quad k \geq 0, \quad |\phi|_{\infty} \leq K, \quad |\phi'|_{\infty} \leq K.$$

Then, there exists $T > 0$ such that the solution of (3) admits the probabilistic representation

$$u(t, x) = \mathbb{E} [\mathcal{H}(\mathcal{T}_{t,x,\text{Id}})], \quad (t, x) \in [0, T] \times \mathbb{R}.$$

The above method also extends to fully nonlinear PDEs of the form

$$\begin{cases} \partial_t u(t, x) + \frac{1}{2} \Delta u(t, x) + f(u(t, x), \nabla u(t, x), \dots, \nabla^n u(t, x)) = 0, \\ u(T, x) = \phi(x), \quad (t, x) = (t, x_1, \dots, x_d) \in [0, T] \times \mathbb{R}^d, \end{cases}$$

$d \geq 1$, see [13], [11]. As an example, we consider a cosine nonlinearity with a gradient of order four, for which our method appears more accurate than the deep Galerkin method [14]. Related comparisons can be found in [11] with respect to the deep BSDE method [5].

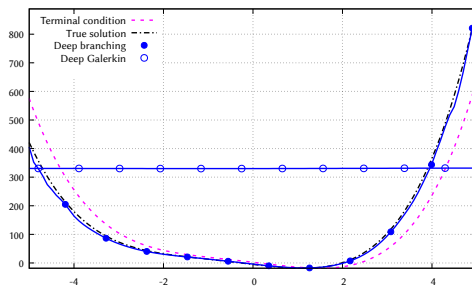


FIGURE 1. Comparison graphs in dimension $d = 5$.

REFERENCES

- [1] J.C. Butcher. Coefficients for the study of Runge-Kutta integration processes. *J. Austral. Math. Soc.*, 3:185–201, 1963.
- [2] J.C. Butcher. *Numerical methods for ordinary differential equations*. John Wiley & Sons, Ltd., Chichester, third edition, 2016.
- [3] A. Cayley. On the theory of the analytical forms called trees. *Philosophical Magazine*, 13(85):172–176, 1857.
- [4] P. Deuffhard and F. Bornemann. *Scientific Computing with Ordinary Differential Equations*, volume 42 of *Texts in Applied Mathematics*. Springer-Verlag, New York, 2002.
- [5] J. Han, A. Jentzen, and W. E. Solving high-dimensional partial differential equations using deep learning. *Proceedings of the National Academy of Sciences*, 115(34):8505–8510, 2018.

- [6] P. Henry-Labordère, N. Oudjane, X. Tan, N. Touzi, and X. Warin. Branching diffusion representation of semilinear PDEs and Monte Carlo approximation. *Ann. Inst. H. Poincaré Probab. Statist.*, 55(1):184–210, 2019.
- [7] N. Ikeda, M. Nagasawa, and S. Watanabe. Branching Markov processes I, II, III. *J. Math. Kyoto Univ.*, 8-9:233–278, 365–410, 95–160, 1968-1969.
- [8] H.P. McKean. Application of Brownian motion to the equation of Kolmogorov-Petrovskii-Piskunov. *Comm. Pure Appl. Math.*, 28(3):323–331, 1975.
- [9] R.I. McLachlan, K. Modin, H. Munthe-Kaas, and O. Verdier. Butcher series: a story of rooted trees and numerical methods for evolution equations. *Asia Pac. Math. Newsl.*, 7(1):1–11, 2017.
- [10] M. Nagasawa and T. Sirao. Probabilistic treatment of the blowing up of solutions for a nonlinear integral equation. *Trans. Amer. Math. Soc.*, 139:301–310, 1969.
- [11] J.Y. Nguwi, G. Penent, and N. Privault. A deep branching solver for fully nonlinear partial differential equations. Preprint arXiv:2203.03234, 17 pages, 2022.
- [12] G. Penent and N. Privault. Numerical evaluation of ODE solutions by Monte Carlo enumeration of Butcher series. Preprint arXiv:2201.05998, 22 pages, 2021.
- [13] G. Penent and N. Privault. A fully nonlinear Feynman-Kac formula with derivatives of arbitrary orders. Preprint arXiv:2201.03882, 25 pages, 2022.
- [14] J. Sirignano and K. Spiliopoulos. DGM: A deep learning algorithm for solving partial differential equations. *Journal of Computational Physics*, 375:1339–1364, 2018.
- [15] A.V. Skorokhod. Branching diffusion processes. *Teor. Veroyatnost. i Primenen.*, 9:492–497, 1964.