# On the Use of Hybrid Coarse-Level Models in Multilevel Minimization Methods

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# **1** Introduction

We consider the following minimization problem:

$$\min_{\mathbf{x}\in\mathbb{D}^n} f(\mathbf{x}),\tag{1}$$

where  $f : \mathbb{R}^n \to \mathbb{R}$  is a bounded, twice continuously differentiable objective function and  $n \in \mathbb{N}$  is typically very large. Our goal is to minimize (1) using a nonlinear multilevel minimization (NMM) method, e.g., MG-OPT [11] or RMTR [7]. The main idea behind NMM methods is to employ a hierarchy of so-called coarselevel objective functions, denoted by  $\{f^\ell\}_{\ell=1}^L$ , where L > 1. These functions are typically obtained by exploring the structure of the underlying minimization problem, e.g., by discretizing the underlying infinite-dimensional problem with a varying discretization parameter. During the solution process, the functions  $\{f^\ell\}_{\ell=1}^L$  are utilized in order to construct the search-directions for the minimization problem at hand in a computationally efficient manner.

The overall efficiency of NMM methods relies on the ability of the coarse-level objective functions  $\{f^{\ell}\}_{\ell=1}^{L}$  to approximate the function f well. Indeed, the convergence theory of the majority of NMM methods requires that the local behavior of the coarse-level objective functions is at least first-order coherent with the local behavior of f. The coherence is commonly ensured by employing the so-called  $\tau$ -correction [1], which corrects the coarse-level objective function  $f^{\ell}$  in an additive manner. Although this approach is almost universally employed in the multilevel literature, other approaches were also considered, e.g., a second-order additive correction approach [7, 12], or Galerkin-based coarse-level models [7, 9]. In this work, we explore techniques from the surrogate-based/multi-fidelity optimization [4] in order to construct the first-order coherent coarse-level models in the context of NMM methods. In particular, we discuss how to correct functions  $\{f^{\ell}\}_{\ell=1}^{L}$  using additive, multiplicative, and hybrid approaches.

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#### 2 Nonlinear multilevel minimization framework

In this work, we minimize (1) using the NMM method. To this aim, we consider a hierarchy of *L* levels. Each level  $\ell = 1, ..., L$  is associated with some model  $h^{\ell} : \mathbb{R}^{n^{\ell}} \to \mathbb{R}$ , where we assume that  $h^{\ell-1}$  is computationally cheaper to minimize than  $h^{\ell}$  and that  $n^{\ell-1} < n^{\ell}$ . As we will discuss in Section 3, the models  $\{h^{\ell}\}_{\ell=1}^{L}$  are constructed during the minimization process by correcting the objective functions  $\{f^{\ell}\}_{\ell=1}^{L}$  by taking into account the knowledge of the current iterate. Through this work, we assume that  $h^{L} := f^{L} := f$ . Transfer of the data between different levels of the multilevel hierarchy is performed using the prolongation operator  $\mathbf{I}_{\ell+1}^{\ell+1} : \mathbb{R}^{n^{\ell}} \to \mathbb{R}^{n^{\ell+1}}$ , and the restriction operator  $\mathbf{R}_{\ell+1}^{\ell} : \mathbb{R}^{n^{\ell+1}} \to \mathbb{R}^{n^{\ell}}$  to transfer iterates from the level  $\ell + 1$  to  $\ell$ . The operator  $\mathbf{P}_{\ell+1}^{\ell}$  is constructed such that  $\mathbf{x}^{\ell} = \mathbf{P}_{\ell+1}^{\ell}(\mathbf{I}_{\ell}^{\ell+1}\mathbf{x}^{\ell})$ , for any  $\mathbf{x}^{\ell} \in \mathbb{R}^{n^{\ell}}$ .

Using the aforementioned definitions, we now describe a generic NMM method in the form of a V-cycle, summarized in Algorithm 1. During the description, we use a superscript to denote the level and a subscript to denote the iteration index. Starting from the finest level,  $\ell = L$ , and initial guess  $\mathbf{x}_0^{\ell}$ , the NMM method performs  $\mu_s$ nonlinear smoothing steps to approximately minimize model  $h^{\ell}$ . The choice of the nonlinear smoother depends on the particular choice of the NMM method. For instance, one can employ a first-order method equipped with a line-search or trustregion globalization strategy if a variant of multilevel line-search or trustregion method is considered. The outcome of this minimization process, iterate  $\mathbf{x}_{\mu_s}^{\ell}$ , is then used to construct a coarse-level model  $h^{\ell-1}$  and initial guess  $\mathbf{x}_0^{\ell-1} = \mathbf{P}_{\ell}^{\ell-1} \mathbf{x}_{\mu_s}^{\ell}$ . This process is repeated recursively until the coarsest level is reached.

On the coarsest level,  $\ell = 1$ , an NMM method approximately minimizes  $h^{\ell}$ using  $\mu_c$  steps of a nonlinear solution strategy, giving rise to  $\mathbf{x}_{*}^{\ell}$ . Afterwards, the prolongated coarse-level correction  $\mathbf{s}_{\mu_s+1}^{\ell+1} := \mathbf{I}_{\ell}^{\ell+1}(\mathbf{x}_{*}^{\ell} - \mathbf{x}_{0}^{\ell})$  is used to update the current iterate  $\mathbf{x}_{\mu_s}^{\ell+1}$  on level  $\ell + 1$ . However, before this update is performed, the correction  $\mathbf{s}_{\mu_s+1}^{\ell}$  has to undergo some convergence control. The type of convergence control again depends on the particular type of the NMM method. For example, if the multilevel trust-region method is used, then  $\mathbf{s}_{\mu_s+1}^{\ell+1}$  is required to provide a decrease in  $h^{\ell+1}$  to be accepted by the algorithm. If a variant of a line-search method is used, then an appropriate step size has to be determined. In the end, the algorithm performs  $\mu_s$ post-smoothing steps, starting from  $\mathbf{x}_{\mu_s+1}^{\ell+1}$  and giving rise to  $\mathbf{x}_{*}^{\ell+1}$ . This process is again repeated on all levels until the finest level is reached.

# 3 Construction of coarse-level models

On each level  $\ell$ , the NMM methods minimize the model  $h^{\ell} : \mathbb{R}^{n^{\ell}} \to \mathbb{R}$  approximately. The result of this minimization, the iterate  $\mathbf{x}_{*}^{\ell}$ , is then used to construct the search On the Use of Hybrid Coarse-Level Models in Multilevel Minimization Methods

Algorithm 1 NMM( $\ell$ ,  $h^{\ell}$ ,  $\mathbf{x}_0^{\ell}$ )

**Require:**  $\ell \in \mathbb{N}, h^{\ell} : \mathbb{R}^{n^{\ell}} \to \mathbb{R}, \mathbf{x}_{0}^{\ell} \in \mathbb{R}^{n^{\ell}} \text{ and } \mu_{s}, \mu_{c} \in \mathbb{N}$ 1:  $\mathbf{x}_{\mu_{s}}^{\ell} = \text{Nonlinear\_smoothing}(h^{\ell}, \mathbf{x}_{0}^{\ell}, \mu_{s})$ 2: Construct  $h^{\ell-1}$  using  $\mathbf{x}_{\mu_{s}}^{\ell}$ , and  $\nabla h^{\ell}(\mathbf{x}_{\mu_{s}}^{\ell})$ 3: **if**  $\ell = 2$  **then** 4:  $\mathbf{x}_{*}^{\ell-1} = \text{Nonlinear\_solve}(h^{\ell-1}, \mathbf{P}_{\ell}^{\ell-1}\mathbf{x}_{\mu_{s}}^{\ell}, \mu_{c})$ 5: **else** 6:  $\mathbf{x}_{*}^{\ell-1} = \text{NMM}(\ell - 1, h^{\ell-1}, \mathbf{P}_{\ell}^{\ell-1}\mathbf{x}_{\mu_{s}}^{\ell})$ 7: **end if** 8:  $\mathbf{x}_{\mu_{s}+1}^{\ell} = \text{Convergence\_control}(h^{\ell}, \mathbf{x}_{\mu_{s}}^{\ell}, \mathbf{I}_{\ell-1}^{\ell}(\mathbf{x}_{*}^{\ell-1} - \mathbf{P}_{\ell}^{\ell-1}\mathbf{x}_{\mu_{s}}^{\ell}))$ 9:  $\mathbf{x}_{*}^{\ell} = \text{Nonlinear\_smoothing}(h^{\ell}, \mathbf{x}_{\mu_{s}+1}^{\ell}, \mu_{s})$ 

direction for the minimization on the next finer level. As a consequence, the overall efficiency of NMM methods depends on the capabilities of the models  $\{h^{\ell}\}_{\ell=1}^{L}$  to approximate f as accurately as possible.

Given an initial guess  $\mathbf{x}_0^{\ell} = \mathbf{P}_{\ell+1}^{\ell} \mathbf{x}_{\mu_s}^{\ell+1}$ , the model  $h^{\ell}$  is constructed during each V-cycle by correcting the function  $f^{\ell}$ , such that the following condition holds:

$$\nabla h^{\ell}(\mathbf{x}_{0}^{\ell}) = \mathbf{R}_{\ell+1}^{\ell} \nabla h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}).$$
<sup>(2)</sup>

This ensures that  $h^{\ell}$  and  $h^{\ell+1}$  are locally first-order coherent and that the following relation holds:  $\langle \nabla h^{\ell}(\mathbf{x}_0^{\ell}), \mathbf{s}^{\ell} \rangle = \langle \nabla h^{\ell+1}(\mathbf{x}_{\mu_s}^{\ell+1}), \mathbf{I}_{\ell}^{\ell+1}\mathbf{s}^{\ell} \rangle$ . In this work, we discuss three different approaches for constructing models  $\{h^{\ell}\}_{\ell=1}^{L}$ , namely additive, multiplicative and hybrid. Our discussion considers only the first-order coherent models, constructed using the Taylor approximation of the associated correction function. However, models enforcing higher-order coherency as well as different approximations of the correction function could also be considered.

# 3.1 An additive approach

Using the additive approach, the coarse-level model  $h_{add}^{\ell} \colon \mathbb{R}^{n^{\ell}} \to \mathbb{R}$  is obtained by correcting the low-cost function  $f^{\ell}$  as follows

$$h_{\text{add}}^{\ell}(\mathbf{x}^{\ell}) = f^{\ell}(\mathbf{x}^{\ell}) + \gamma_{\text{add}}^{\ell}(\mathbf{x}^{\ell}), \qquad (3)$$

where the additive correction function  $\gamma_{\text{add}}^{\ell} \colon \mathbb{R}^{n^{\ell}} \to \mathbb{R}$  accounts for the difference between the value of  $f^{\ell}$  and the fine-level model  $h^{\ell+1}$ , i.e.,

$$\gamma_{\text{add}}^{\ell}(\mathbf{x}^{\ell}) \coloneqq h^{\ell+1}(\mathbf{I}_{\ell}^{\ell+1}\mathbf{x}^{\ell}) - f^{\ell}(\mathbf{x}^{\ell}).$$

$$\tag{4}$$

Unfortunately, the evaluation of  $\gamma_{add}^{\ell}$  at any given  $\mathbf{x}^{\ell}$  requires an evaluation of the fine-level model  $h^{\ell+1}$  at  $\mathbf{I}_{\ell}^{\ell+1}\mathbf{x}^{\ell}$ . As a consequence, numerical computations involving  $h_{add}^{\ell}$  are computationally more demanding than computations performed using  $h^{\ell+1}$  directly. To ease the computational burden, we evaluate  $\gamma_{add}^{\ell}$  exactly only at the initial coarse-level iterate  $\mathbf{x}_{0}^{\ell} = \mathbf{P}_{\ell}^{\ell+1}\mathbf{x}_{\mu_{s}}^{\ell+1}$ . Thus, we impose

$$\gamma_{\mathrm{add}}^{\ell}(\mathbf{x}_0^{\ell}) \coloneqq h^{\ell+1}(\mathbf{x}_{\mu_s}^{\ell+1}) - f^{\ell}(\mathbf{x}_0^{\ell}),$$

only at  $\mathbf{x}_0^{\ell}$ . For any other  $\mathbf{x}^{\ell}$ , we approximate the correction function  $\gamma_{add}^{\ell}$  by means of the first-order Taylor approximation, defined around  $\mathbf{x}_0^{\ell}$  as follows

$$\tilde{\gamma}_{\text{add}}^{\ell}(\mathbf{x}^{\ell}) = \gamma_{\text{add}}^{\ell}(\mathbf{x}_{0}^{\ell}) + \langle \nabla \gamma_{\text{add}}^{\ell}(\mathbf{x}_{0}^{\ell}), \ \mathbf{x}^{\ell} - \mathbf{x}_{0}^{\ell} \rangle.$$

Replacing  $\gamma_{add}^{\ell}$  with  $\tilde{\gamma}_{add}^{\ell}$  in (3) gives rise to

$$h_{\text{add}}^{\ell}(\mathbf{x}^{\ell}) \coloneqq f^{\ell}(\mathbf{x}^{\ell}) + h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}) - f^{\ell}(\mathbf{x}_{0}^{\ell}) + \langle \nabla \gamma_{\text{add}}^{\ell}(\mathbf{x}_{0}^{\ell}), \mathbf{x}^{\ell} - \mathbf{x}_{0}^{\ell} \rangle, \tag{5}$$

where

$$\nabla \gamma_{\text{add}}^{\ell}(\mathbf{x}_{0}^{\ell}) := \mathbf{R}_{\ell+1}^{\ell} \nabla h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}) - \nabla f^{\ell}(\mathbf{x}_{0}^{\ell}).$$
(6)

Note, the quantity  $h^{\ell+1}(\mathbf{x}_{\mu_s}^{\ell+1}) - f^{\ell}(\mathbf{x}_0^{\ell})$  enforces zeroth-order coherence between  $h^{\ell+1}$ and  $h_{add}^{\ell}$  at  $\mathbf{x}_{\mu_s}^{\ell+1}$  and  $\mathbf{x}_0^{\ell}$ , respectively, i.e.,  $h_{add}^{\ell}(\mathbf{x}_0^{\ell}) = h^{\ell+1}(\mathbf{x}_{\mu_s}^{\ell+1})$ . However, this term does not affect the evaluation of the derivatives of  $h_{add}^{\ell}$ , and therefore it is often neglected in practice. We also point out that the term  $\nabla \gamma_{add}^{\ell}(\mathbf{x}_0^{\ell})$ , known in the multilevel literature as  $\tau$ -correction, ensures that condition (2) holds.

#### 3.2 A multiplicative approach

Optimization methods that exploit multiple fidelities often employ multiplicative correction functions [4]. In this case, the low-cost approximation  $f^{\ell}$  associated with level  $\ell$  is made coherent with the model  $h^{\ell+1}$  as follows:

$$h_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) = \gamma_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) f^{\ell}(\mathbf{x}^{\ell}).$$
(7)

Here, the multiplicative correction function  $\gamma_{\text{mult}}^{\ell} \colon \mathbb{R}^{n^{\ell}} \to \mathbb{R}$  is given as

$$\gamma_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) \coloneqq \frac{h^{\ell+1}(\mathbf{I}_{\ell}^{\ell+1}\mathbf{x}^{\ell}) + \kappa}{f^{\ell}(\mathbf{x}^{\ell}) + \kappa},\tag{8}$$

where  $\kappa \approx \epsilon$  ensures numerical stability as the value of  $f^{\ell}(\mathbf{x}^{\ell})$  approaches zero.

Similar to the additive approach, evaluating  $\gamma_{\text{mult}}^{\ell}$  precisely at all coarse-level iterates is computationally expensive. Therefore, we impose (8) only at  $\mathbf{x}_{0}^{\ell}$ , i.e.,

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$$\gamma_{\text{mult}}^{\ell}(\mathbf{x}_0^{\ell}) := \frac{h^{\ell+1}(\mathbf{x}_{\mu_s}^{\ell+1}) + \kappa}{f^{\ell}(\mathbf{x}_0^{\ell}) + \kappa},$$

where we explored that  $\mathbf{x}_{\mu_s}^{\ell+1} = \mathbf{I}_{\ell}^{\ell+1} \mathbf{x}_0^{\ell}$ . At any other iterate  $\mathbf{x}^{\ell}$ , we approximate  $\gamma_{\text{mult}}^{\ell}$  by means of the first-order Taylor approximation, defined around  $\mathbf{x}_0^{\ell}$  as

$$\tilde{\gamma}_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) = \gamma_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell}) + \langle \nabla \gamma_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell}), \ \mathbf{x}^{\ell} - \mathbf{x}_{0}^{\ell} \rangle.$$
(9)

Replacing  $\gamma_{\text{mult}}^{\ell}$  with  $\tilde{\gamma}_{\text{mult}}^{\ell}$  in (7) then gives rise to the first-order coherent model

$$h_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) \coloneqq \tilde{\gamma}_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) \ f^{\ell}(\mathbf{x}^{\ell}).$$
(10)

The numerical evaluation of  $\tilde{\gamma}_{\text{mult}}^{\ell}$  amounts to

$$\tilde{\gamma}_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}) := \frac{h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}) + \kappa}{f^{\ell}(\mathbf{x}_{0}^{\ell}) + \kappa} + \langle \nabla \gamma_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell}), \ \mathbf{x}^{\ell} - \mathbf{x}_{0}^{\ell} \rangle,$$

where  $\nabla \gamma_{\text{mult}}^{\ell}(\mathbf{x}_0^{\ell})$  is given by

$$\nabla \gamma_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell}) := \frac{1}{f^{\ell}(\mathbf{x}_{0}^{\ell}) + \kappa} \big( \mathbf{R}_{\ell+1}^{\ell} \nabla h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}) \big) - \frac{h^{\ell+1}(\mathbf{x}_{\mu_{s}}^{\ell+1}) + \kappa}{(f^{\ell}(\mathbf{x}_{0}^{\ell}) + \kappa)^{2}} \nabla f^{\ell}(\mathbf{x}_{0}^{\ell}).$$

Straightforward calculations show that model  $h_{\text{mult}}^{\ell}$ , defined by (10), is zeroth-order and first-order coherent with  $h^{\ell+1}$  at  $\mathbf{x}_{0}^{\ell}$  and  $\mathbf{x}_{\mu_{s}}^{\ell+1}$ , respectively.

# 3.3 A hybrid approach

From a computational point of view, additive and multiplicative approaches are comparable. However, their behavior is very different. The additive approach adds new terms to  $f^{\ell}$ , which can be interpreted as uniform translation (zeroth-order), and rotation (first-order) of the function graph; see also Fig. 1. In contrast, the multiplicative approach introduces skewing, which might not be desirable if f and  $f^{\ell}$  are in good agreement, at least locally. However, if functions  $f^{\ell}$  and f are not in good agreement, then additional skewing can be beneficial [3], e.g., if the polynomial order of f is higher than the polynomial order of  $f^{\ell}$ . Moreover, multiplication of  $f^{\ell}$  with  $\tilde{\gamma}^{\ell}_{mult}$  can introduce new minima on level  $\ell$ , where  $\ell < L$ . For instance, let us suppose that  $f^{\ell}$  is a second-order polynomial. Its multiplication with  $\tilde{\gamma}^{\ell}_{mult}$  increases the order of the polynomial, i.e., we obtain a model  $h^{\ell}_{mult}$  which is quartic and has, in general, more minima than quadratic function.

In general, it is not known a priori whether the additive or the multiplicative model is more suitable for a given optimization problem. To overcome this difficulty, a hybrid approach [6] can be employed. A coarse-level model  $h_{mix}^{\ell}$  is then obtained

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Fig. 1 Coarse-level models constructed around  $x_0^{L-1} = 2.5$  and  $x_0^{L-1} = 6.0$ .

as a convex combination of the additive  $h_{add}^{\ell}$  and the multiplicative  $h_{mult}^{\ell}$  models, i.e.,

$$h_{\text{mix}}^{\ell}(\mathbf{x}^{\ell}) := w_{\text{add}}^{\ell} h_{\text{add}}^{\ell}(\mathbf{x}^{\ell}) + w_{\text{mult}}^{\ell} h_{\text{mult}}^{\ell}(\mathbf{x}^{\ell}), \qquad (11)$$

where  $w_{\text{add/mult}}^{\ell} \in \mathbb{R}$  and  $w_{\text{add}}^{\ell} + w_{\text{mult}}^{\ell} = 1$ . In order to maximize the approximation properties of  $h_{\text{mix}}^{\ell}$ , the weights  $w_{\text{add}}^{\ell}, w_{\text{mult}}^{\ell}$  have to be chosen carefully. Below, we describe two different strategies for selecting the values  $w_{\text{add}}^{\ell}$  and  $w_{\text{mult}}^{\ell}$ .

# **3.3.1** Matching function values (MFV) at the previously evaluated fine-level iterate

Following [2], the weights  $w_{add}^{\ell}$ ,  $w_{mult}^{\ell}$  can be selected by matching the function value at the previously evaluated fine-level iterate, denoted by  $\mathbf{x}_p^{\ell+1}$ , as in

$$w_{\text{add}}^{\ell} = \frac{h^{\ell+1}(\mathbf{x}_{p}^{\ell+1}) - h_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell})}{h_{\text{add}}^{\ell}(\mathbf{x}_{0}^{\ell}) - h_{\text{mult}}^{\ell}(\mathbf{x}_{0}^{\ell})} \qquad \text{and} \qquad w_{\text{mult}}^{\ell} = 1 - w_{\text{add}}^{\ell}.$$
(12)

From a computational point of view, evaluating (12) is cheap as  $h^{\ell+1}(\mathbf{x}_p^{\ell+1})$  is readily available, for instance from the  $\mu_s - 1$  pre-smoothing step performed on level  $\ell + 1$ .

#### 3.3.2 Bayesian updating approach

To maximize the approximation properties of  $h_{\text{mix}}^{\ell}$ , it might be beneficial to take into account the history of the  $d^{\ell}$  previously evaluated fine-level iterates [3]. Therefore, we consider the dataset  $\mathcal{D}^{\ell} = \{(h^{\ell+1}(\mathbf{x}_p^{\ell+1}), h_{\text{add}}^{\ell}(\mathbf{P}_{\ell+1}^{\ell}\mathbf{x}_p^{\ell+1}), h_{\text{mult}}^{\ell}(\mathbf{P}_{\ell+1}^{\ell}\mathbf{x}_p^{\ell+1})\}_{p=1}^{d^{\ell}}$ , where each sample contains the function value of  $h^{\ell+1}$  at  $\mathbf{x}_p^{\ell+1}$ , as well as the function values of the coarse-level models  $h_{\text{add/mult}}^{\ell}$  obtained at  $\mathbf{P}_{\ell+1}^{\ell}\mathbf{x}_p^{\ell+1}$ . In this work, we construct  $\mathcal{D}^{\ell}$  by taking into account the last  $d^{\ell}$  iterates which were transferred from level  $\ell + 1$  to level  $\ell$ . For example, if  $d^{\ell} = 3$ , then  $\mathcal{D}^{\ell}$  is constructed by taking into account the iterate  $\mathbf{x}_p^{\ell+1} = \mathbf{x}_{\mu_s}^{\ell+1}$ , obtained as a result of the pre-smoothing step during the previous three V-cycles. For simplicity, we use the notation  $d^{\ell} = \infty$  to denote all previous V-cycles.

Having constructed the dataset  $\mathcal{D}^{\ell}$ , we can now employ the Bayesian posterior updating approach [3] to determine the values of  $w_{\text{add/mult}}^{\ell}$ . Starting from  $w_{\text{add/mult}}^{\ell} = 0.5$ , the weights are updated every time the model  $h^{\ell}$  is constructed as follows:

$$w_{\text{add/mult}}^{\ell} = \frac{w_{\text{add/mult}}^{\ell}\psi_{\text{add/mult}}^{\ell}}{w_{\text{mult/add}}^{\ell}\psi_{\text{mult/add}}^{\ell} + w_{\text{add/mult}}^{\ell}\psi_{\text{add/mult}}^{\ell}}.$$
(13)

The model likelihoods  $\psi_{\text{add/mult}}^{\ell}$  in (13) are evaluated as

$$\psi_{\rm add/mult}^{\ell} = \left(2\pi\sigma_{\rm add/mult}^2\right)^{-d^{\ell}/2} \exp(-d^{\ell}/2),\tag{14}$$

and the maximum likelihood estimator of the model variance is given by

$$\sigma_{\text{add/mult}}^2 = \frac{1}{d^{\ell}} \sum_{p=1}^{d^{\ell}} (h^{\ell+1}(\mathbf{x}_p^{\ell+1}) - h_{\text{add/mult}}^{\ell}(\mathbf{P}_{\ell+1}^{\ell}\mathbf{x}_p^{\ell+1})).$$
(15)

#### 4 Numerical results and discussion

In this section, we investigate the influence of different coarse-level models on the performance of the NMM method using numerical examples from the field of supervised learning, namely classification using ResNets [8]. Given a dataset  $S = \{(\mathbf{z}_s, \mathbf{c}_s)\}_{s=1}^{n_s}$ , where  $\mathbf{z}_s \in \mathbb{R}^{n_{in}}$  and  $\mathbf{c}_s \in \mathbb{R}^{n_{out}}$ , our goal is to find parameters  $\mathbf{x} \in \mathbb{R}^n$  of a ResNet, defined as RN:  $\mathbb{R}^{n_{in}} \times \mathbb{R}^n \to \mathbb{R}^{n_{out}}$ , by solving the following minimization problem:

$$\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}) \coloneqq \frac{1}{n_s} \sum_{s=1}^{n_s} g(\mathrm{RN}(\mathbf{z}_s, \mathbf{x}), \mathbf{c}_s),$$
(16)

where g denotes the cross-entropy loss function.

Since (16) is a non-convex function, we choose the NMM method to be a variant of the RMTR method [7]. The multilevel hierarchy and transfer operators are constructed by leveraging the fact that the ResNet can be interpreted as a forward Euler discretization of an ordinary differential equation; see [10, 5] for details. Here, we construct a hierarchy of ResNets by uniformly refining a ResNet with three layers three times. Fig. 4 demonstrates the number of effective gradient evaluations<sup>1</sup> of the RMTR method with respect to different coarse-level models for three different datasets.

As we can observe, the choice of the coarse-level model has a significant impact on the overall efficiency of the multilevel method. For all three examples, hybrid approaches outperform purely additive and multiplicative ones. In terms of hybrid

<sup>&</sup>lt;sup>1</sup> The number of effective gradient evaluations is obtained as  $\sum_{\ell=1}^{L} 2^{\ell-L} W_{\ell} C_L$ , where  $C_L$  represents a cost associated with an evaluation of the gradient on the level L,  $W_{\ell}$  describes a number of gradient evaluations performed on a level  $\ell$ , and  $2^{\ell-L}$  is a coarsening factor in 1D.

	Model/Example	Blobs	Smiley	Spiral
	$h_{\rm add}$	29 ± 5.3%	$676 \pm 11.2\%$	$203 \pm 12.3\%$
	$h_{ m mult}$	$32 \pm 6.1\%$	$485 \pm 15.1\%$	$153 \pm 15.9\%$
-		$38 \pm 4.8\%$	$404 \pm 10.3\%$	$297 \pm 11.3\%$
	$h_{\rm mix}({ m MFV})$	$25 \pm 4.2\%$	$352 \pm 6.5\%$	<b>123 ± 7.1</b> %
	$h_{\rm mix}(d^\ell=5)$	$25 \pm 3.4\%$	$514\pm6.3\%$	$197\pm6.8\%$
			$471 \pm 7.7\%$	$156 \pm 7.4\%$
	$h_{\min}(d^{\ell} = \infty)$	$25 \pm 3.8\%$	<b>301 ± 6.9</b> %	$126 \pm 9.9\%$

**Fig. 2** *Left:* Blobs, Smiley, and Spiral datasets (*Top* to *Down*). Each class is illustrated by different color. *Right:* The average number of effective gradient evaluations of the RMTR method (4 levels). Averages are obtained from 5 independent runs.

models, we observe that the Bayesian approach performs similar, or superior to MFV, especially if all prior fine-level iterates are considered ( $d^{\ell} = \infty$ ).

Given our (limited) numerical experience, we believe that employing hybrid, and possibly other types of novel coarse-level models, provides a promising future direction for improving the efficiency and the reliability of NMM methods.

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