High-order multilevel optimization strategies and their application to the training of artificial neural networks

E. Riccietti (IRIT-INP, Toulouse)

Joint work with: H. Calandra (Total)
S. Gratton (IRIT-INP, Toulouse)
X. Vasseur (ISAE-SUPAERO, Toulouse)

Toulouse- 11 March 2018

Context

We consider large-scale nonlinear unconstrained optimization problems:

$$\min_x f(x)$$

Context

We consider large-scale nonlinear unconstrained optimization problems:

$$\min_x f(x)$$

Classical iterative optimization methods:

$$f(x_k + s) \simeq T_2(x_k, s)$$

with $T_2(x_k, s)$ Taylor model of order 2. At each iteration we compute a step s_k to update the iterate:

$$\min_s m_{q,k}(x_k, s) = T_2(x_k, s) + r(\lambda_k), \qquad \lambda_k > 0$$

$r(\lambda_k)$ regularization term.

A classical example

- Adaptive Cubic Regularization method (ARC):

$$m(x_k, s) = f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T \nabla^2 f(x_k) s + \frac{\lambda_k}{3} \|s\|^3$$

C. Cartis, N. Gould, Ph. Toint, 'Adaptive cubic regularisation methods for unconstrained optimization', 2009

Extension to higher-order methods ($q > 2$)

E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 'Worst-case evaluation complexity for unconstrained nonlinear optimization using high-order regularized models', 2017

Model of order q:

$$\min_s m_{q,k}(x_k, s) = T_q(x_k, s) + \frac{\lambda_k}{q+1}\|s\|^{q+1}, \qquad \lambda_k > 0.$$

$$T_q(x_k, s) = \sum_{i=1}^{q} \frac{1}{i!} \nabla^i f(x_k)(\overbrace{s, \ldots, s}^{i \text{ times}})$$

Tensor of order 3

Definition

Let $T \in \mathbb{R}^{n^3}$, and $u, v, w \in \mathbb{R}^n$. Then $T(u, v, w) \in \mathbb{R}$, $T(v, w) \in \mathbb{R}^n$

$$T(u, v, w) = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} T(i, j, k) u(i) v(j) w(k),$$

$$T(v, w)(i) = \sum_{j=1}^{n} \sum_{k=1}^{n} T(i, j, k) v(j) w(k), \quad i = 1, \ldots, n.$$

Tensor of order i

Definition

Let $i \in \mathbb{N}$ and $T \in \mathbb{R}^{n^i}$, and $u \in \mathbb{R}^n$. Then $T(\underbrace{u, \ldots, u}_{i \text{ times}}) \in \mathbb{R}$,

$T(\underbrace{u, \ldots, u}_{i-1 \text{ times}}) \in \mathbb{R}^n$ and

$$T(\underbrace{u, \ldots, u}_{i \text{ times}}) = \sum_{j_1=1}^{n} \cdots \sum_{j_i=1}^{n} T(j_1, \ldots, j_i) u(j_1) \ldots u(j_i),$$

$$T(\underbrace{u, \ldots, u}_{i-1 \text{ times}})(j_1) = \sum_{j_2=1}^{n} \cdots \sum_{j_i=1}^{n} T(j_1, \ldots, j_i) u(j_2), \ldots u(j_i), \quad j_1 = 1, \ldots, n.$$

High order methods

E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 'Worst-case evaluation complexity for unconstrained nonlinear optimization using high-order regularized models', 2017

Unifying framework for global convergence and worst-case complexity is presented.

☺ better complexity
☹ needs higher-order derivatives, model is expensive to minimize

Bottelneck: Subproblem solution

Solving

$$\min_s T_q(x_k, s) + \frac{\lambda_k}{q+1}\|s\|^{q+1}$$

represents greatest cost per iteration, which depends on the size of the problem.

$$\Downarrow$$

S. Gratton, A. Sartenaer, PH. Toint, 'Multilevel trust region method' 2008

Hierarchy of problems

- $\{f_l(x_l)\}$, $x_l \in \mathcal{D}_l$
- $|\mathcal{D}_l| < |\mathcal{D}_{l+1}|$
- f_l is cheaper to optimize compared to f_{l+1}

Our contributions

E. G. Birgin, J. L. Gardenghi, J. M. Martinez, S. A. Santos and Ph. L. Toint, 2017

- one level methods: non-scalable

S. Gratton, A. Sartenaer, PH. Toint, 2008

- method for second order models

$$\Downarrow$$

We propose a family of scalable multilevel methods using high-order models.

Outline

- Part I: multilevel extension of iterative high-order optimization methods
  - global convergence
  - worst-case complexity
  - local convergence rate

Outline

- Part I: multilevel extension of iterative high-order optimization methods
  - global convergence
  - worst-case complexity
  - local convergence rate
- Part II: use of the multilevel methods for the training of artificial neural network
  - multilevel methods in the literature used just for problems with a geometrical structure

Part I

1. Multilevel extension of iterative high-order optimization methods

Multilevel setting

- At each level l, $x \in \mathbb{R}^{n_l}$. $l_{\max}$ finest level, 0 coarsest level.

level $l_{\max}$	$\mathbb{R}^n$	$x^{l_{\max}}$	$f^{l_{\max}} = f$	$\mu^{l_{\max}} = f$
$\vdots$		$\vdots$	$\vdots$	$\vdots$
level $l+1$	$\mathbb{R}^{n_{l+1}}$	x^{l+1}	f^{l+1}	μ^{l+1}
	$R^{l+1} \Downarrow \quad \Uparrow P^{l+1}$			
level l	$\mathbb{R}^{n_l}$	x^l	f^l	μ^l
$\vdots$		$\vdots$	$\vdots$	$\vdots$
level 0	$\mathbb{R}^{n_0}$	x^0	f^0	μ^0

- f^l represents f on the coarse spaces (it is e.g. the discretization of f on a coarse space)
- The functions μ^l are modifications of the f^l to ensure inter-level coherence.
- $R^l = \alpha (P^l)^T$, for some $\alpha > 0$.

One level strategy

At level $l = l_{\max}$, let x_k^l be the current approximation. We look for a correction s_k^l to define the new approximation $x_{k+1}^l = x_k^l + s_k^l$.

x_k^l

One level strategy

At level $l = l_{\max}$, let x_k^l be the current approximation. We look for a correction s_k^l to define the new approximation $x_{k+1}^l = x_k^l + s_k^l$.

$$x_k^l \xrightarrow{T_q^l} x_{k+1}^l = x_k^l + s_k^l$$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:

$$x_k^l$$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:

$$x_k^l \xrightarrow{T_q^l} x_{k+1}^l = x_k^l + s_k^l$$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:
   - if $\|\nabla \mu_{q,k}^{l-1}(x_{0,k}^{l-1})\| = \|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$, $\kappa > 0$,
   - if $\|R\nabla f^l(x_k^l)\| > \epsilon^l$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:
   - if $\|\nabla \mu_{q,k}^{l-1}(x_{0,k}^{l-1})\| = \|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$, $\kappa > 0$,
   - if $\|R\nabla f^l(x_k^l)\| > \epsilon^l$

x_k^l

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:
   - if $\|\nabla \mu_{q,k}^{l-1}(x_{0,k}^{l-1})\| = \|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$, $\kappa > 0$,
   - if $\|R\nabla f^l(x_k^l)\| > \epsilon^l$

$$x_k^l$$
$$\downarrow R^l$$
$$R^l x_k^l := x_{0,k}^{l-1}$$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:
   - if $\|\nabla \mu_{q,k}^{l-1}(x_{0,k}^{l-1})\| = \|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$, $\kappa > 0$,
   - if $\|R\nabla f^l(x_k^l)\| > \epsilon^l$

$$
\begin{array}{ccc}
x_k^l & & \\
\Big\downarrow R^l & & \\
R^l x_k^l := x_{0,k}^{l-1} & \xrightarrow{\quad\mu^{l-1}\quad} & x_{*,k}^{l-1}
\end{array}
$$

Multilevel strategy

Two choices:

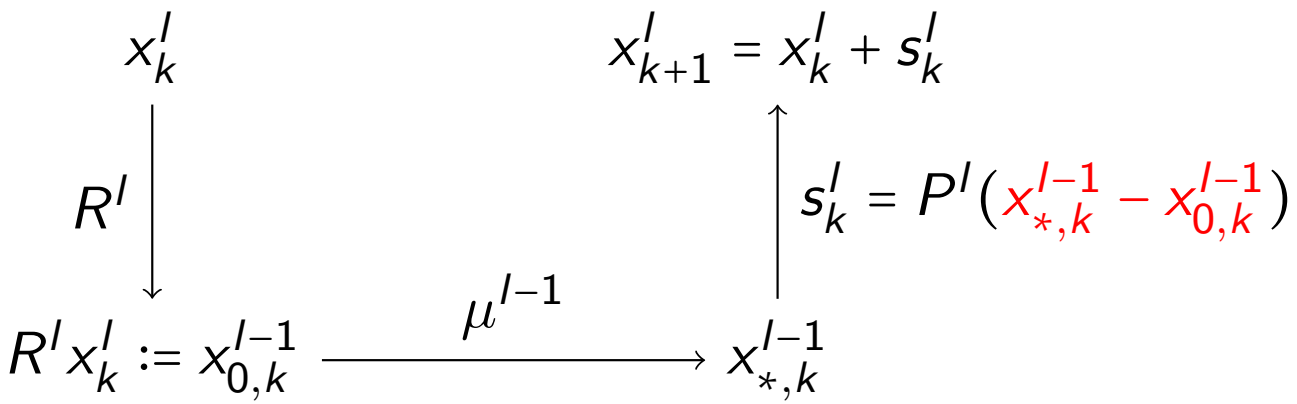
1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}:
   - if $\|\nabla \mu_{q,k}^{l-1}(x_{0,k}^{l-1})\| = \|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$, $\kappa > 0$,
   - if $\|R\nabla f^l(x_k^l)\| > \epsilon^l$

$$
\begin{array}{ccc}
x_k^l & & x_{k+1}^l = x_k^l + s_k^l \\
\Big\downarrow R^l & & \Big\uparrow s_k^l = P^l(x_{*,k}^{l-1} - x_{0,k}^{l-1}) \\
R^l x_k^l := x_{0,k}^{l-1} & \xrightarrow{\quad\mu^{l-1}\quad} & x_{*,k}^{l-1}
\end{array}
$$

Multilevel strategy

Two choices:

1. minimize regularized Taylor model, get s_k^l,
2. choose lower level model μ^{l-1}: if $\|R\nabla f^l(x_k^l)\| \geq \kappa \|\nabla f^l(x_k^l)\|$



- The lower level model is cheaper to optimize.
- The procedure is recursive: more levels can be used.

Coherence between levels, $q = 1$

Lower level model:

- Let $x_{0,k}^{l-1} = Rx_k^l$. Model with first order correction:

$$\mu_{1,k}^{l-1} = f^{l-1}(x_{0,k}^{l-1}, s^{l-1}) + (R^l \nabla f^l(x_k^l) - \nabla f^{l-1}(x_k^{l-1}))^T s^{l-1}$$

This ensures that

$$\nabla \mu_{1,k}^{l-1}(x_{0,k}^{l-1}) = R^l \nabla f^l(x_k^l)$$

$\rightarrow$ first-order behaviours of f^l and μ^{l-1} are coherent in a neighbourhood of the current approximation. If $s^l = P^l s^{l-1}$

$$\nabla f^l(x_k^l)^T s^l = \nabla f^l(x_k^l)^T P^l s^{l-1} = \nabla \mu_{1,k}^{l-1}(x_{0,k}^{l-1})^T s^{l-1}.$$

Coherence between levels, $q = 2$

Lower level model: Let $x_{0,k}^{l-1} = Rx_k^l$. We define $\mu_{q,k}^{l-1}$ as

$$\mu_{2,k}^{l-1}(x_{0,k}^{l-1} + s^{l-1}) = f^{l-1}(x_{0,k}^{l-1} + s^{l-1}) + (R^l \nabla f^l(x_k^l) - \nabla f^{l-1}(x_k^{l-1}))^T s^{l-1}$$
$$+ \frac{1}{2}(s^{l-1})^T ((R^l)^T \nabla f^l(x_k^l) P^l - \nabla^2 f^{l-1}(x_k^{l-1}))s^{l-1}$$

$\rightarrow$ We can generalize this up to order q to have the behaviours of f^l and $\mu_{q,k}^{l-1}$ to be coherent up to order q in a neighbourhood of the current approximation.

Coherence up to order q

We define

$$\mu_{q,k}^{l-1}(x_{0,k}^{l-1}, s^{l-1}) = f^{l-1}(x_{0,k}^{l-1} + s^{l-1}) + \sum_{i=1}^{q} \frac{1}{i!}[\mathcal{R}(\nabla^i f^l(x_k)) - \nabla^i f^{l-1}(x_{0,k}^{l-1})] \underbrace{(s^{l-1}, \ldots, s^{l-1})}_{i \text{ times}},$$

where $\mathcal{R}(\nabla^i f^l(x_k^l))$ is such that for all $i = 1, \ldots, q$ and $s_1^{l-1}, \ldots, s_i^{l-1} \in \mathbb{R}^{n_{l-1}}$

$$[\mathcal{R}(\nabla^i f^l(x_k^l))](s_1^{l-1}, \ldots, s_i^{l-1}) := \nabla^i f^l(x_k^l, Ps_1^{l-1}, \ldots, Ps_i^{l-1}),$$

where $\nabla^i f^l$ denotes the i-th order tensor of f^l.

Basic iterative optimization algorithm

Until convergence

- Define the local model m_k of f around x_k, depending on λ_k
- Compute a trial point $x_k + s_k$ that decreases this model
- Compute the predicted reduction $m_k(x_k) - m_k(x_k + s_k)$
- Evaluate change in the objective function $f(x_k) - f(x_k + s_k)$
- If achieved change $\sim$ predicted reduction then
  - Accept trial point as new iterate $x_{k+1} = x_k + s_k$

  else
  - Reject the trial point $x_{k+1} = x_k$
  - Increase λ_k

Recursive multilevel q-order methods

Until convergence

- Choose either a q-order Taylor model or the lower level model.
  - Taylor model: compute a Taylor step satisfying a sufficient decrease property
  - Lower level: apply the algorithm recursively
- Evaluate change in the objective function and in the model
- If achieved change $\sim$ predicted reduction then
  - Accept trial point as new iterate

  else
  - Reject the trial point
  - Increase λ_k

Theoretical results: Assumptions

Assumption 1

Let us assume that for all l the q-th derivative tensors of f^l are Lipschitz continuous.

Assumption 2

There exist strictly positive scalars $\kappa_{EB}, \rho > 0$ such that

$$\operatorname{dist}(x, \mathcal{X}) \leq \kappa_{EB} \|\nabla_x f(x)\|, \quad \forall x \in \mathcal{N}(\mathcal{X}, \rho),$$

where $\mathcal{X}$ is the set of second-order critical points of f, $\operatorname{dist}(x, \mathcal{X})$ denotes the distance of x to $\mathcal{X}$ and $\mathcal{N}(\mathcal{X}, \rho) = \{x \mid \operatorname{dist}(x, \mathcal{X}) \leq \rho\}$.

Yue, M.C. and Zhou, Z. and So, A.M.C. 'On the Quadratic Convergence of the Cubic Regularization Method under a Local Error Bound Condition', 2018: generalized to higher-order methods

Theoretical results: 1) global convergence

Theorem

Let Assumption 1 hold. Then, the sequence of iterates generated by the algorithm converges globally to a first-order stationary point.

Theoretical results: 1) global convergence

Theorem

Let Assumption 1 hold. Then, the sequence of iterates generated by the algorithm converges globally to a first-order stationary point.

- E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 2017: generalized to multilevel framework
- Gratton, Sartenaer, Toint, 2008: extended to higher-order models and simplified

Theoretical results: 2) complexity

Theorem

Let Assumption 1 hold. Let f_{low} be a lower bound on f. Then, the method requires at most

$$\frac{K_3}{\epsilon^{\frac{q+1}{q}}}(f(x_{k_1}) - f_{low})\left(1 + \frac{|\log \gamma_1|}{\log \gamma_3}\right) + \frac{1}{\log \gamma_3}\log\left(\frac{\lambda_{\max}}{\lambda_0}\right)$$

iterations to achieve an iterate x_k such that $\|\nabla f(x_k)\| \leq \epsilon$, where

$$K_3 := \frac{q+1}{\eta_1 \lambda_{\min}} \max\{K_1^{1/q}, K_2^{1/q}\}.$$

E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 2017: $k = O(\epsilon^{\frac{q+1}{q}})$ Complexity of standard method is maintained

Theoretical results: 2) complexity

Theorem

Let Assumption 1 hold. Let f_{low} be a lower bound on f. Then, the method requires at most

$$\frac{K_3}{\epsilon^{\frac{q+1}{q}}}(f(x_{k_1}) - f_{low})\left(1 + \frac{|\log \gamma_1|}{\log \gamma_3}\right) + \frac{1}{\log \gamma_3}\log\left(\frac{\lambda_{\max}}{\lambda_0}\right)$$

iterations to achieve an iterate x_k such that $\|\nabla f(x_k)\| \leq \epsilon$, where

$$K_3 := \frac{q+1}{\eta_1 \lambda_{\min}} \max\{K_1^{1/q}, K_2^{1/q}\}.$$

E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 2017: $k = O(\epsilon^{\frac{q+1}{q}})$ Complexity of standard method is maintained

Theoretical result: 3) local convergence

Theorem

Let Assumptions 1 and 2 hold. Assume that $\mathcal{L}(f(x_k^h))$ is bounded for some $k \geq 0$ and that it exists an accumulation point x^* such that $x^* \in \mathcal{X}$. Then, the whole sequence $\{x_k^h\}$ converges to x^* and it exist strictly positive constants $c \in \mathbb{R}$ and $\bar{k} \in \mathbb{N}$ such that:

$$\frac{\|x_{k+1}^h - x^*\|}{\|x_k^h - x^*\|^q} \leq c, \quad \forall k \geq \bar{k}.$$

Theoretical result: 3) local convergence

Theorem

Let Assumptions 1 and 2 hold. Assume that $\mathcal{L}(f(x_k^h))$ is bounded for some $k \geq 0$ and that it exists an accumulation point x^* such that $x^* \in \mathcal{X}$. Then, the whole sequence $\{x_k^h\}$ converges to x^* and it exist strictly positive constants $c \in \mathbb{R}$ and $\bar{k} \in \mathbb{N}$ such that:

$$\frac{\|x_{k+1}^h - x^*\|}{\|x_k^h - x^*\|^q} \leq c, \quad \forall k \geq \bar{k}.$$

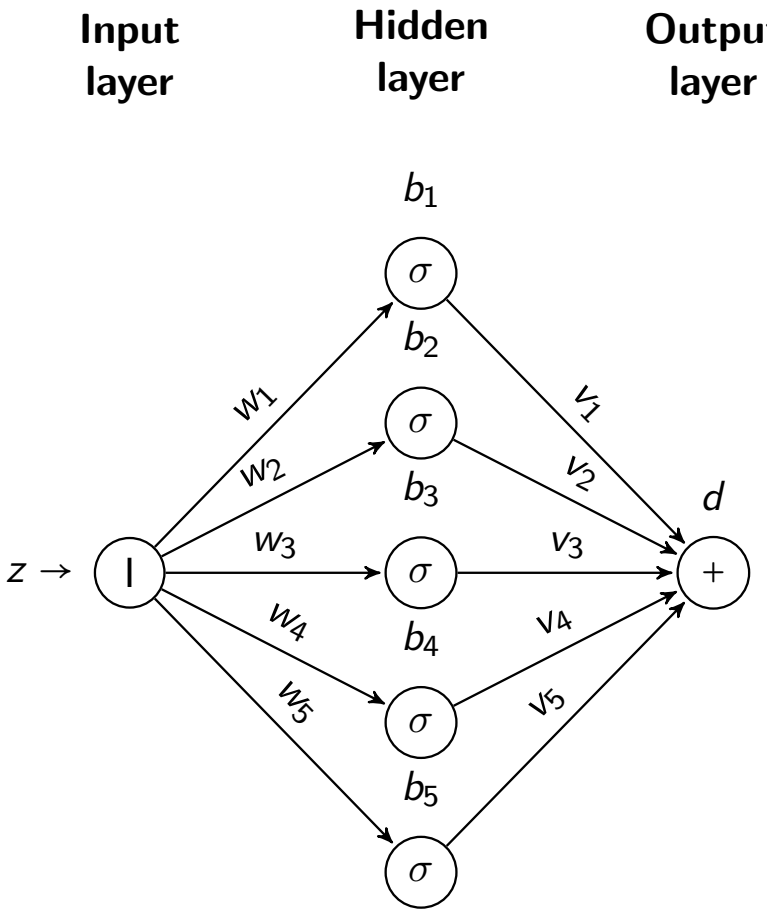

E. G. Birgin, J. L. Gardenghi, J. M. Martnez, S. A. Santos and Ph. L. Toint, 2017: local convergence not proved


Gratton, Sartenaer, Toint, 2008: local convergence not proved

Part II

1. Use of the multilevel methods for the training of artificial neural networks

Artificial neural networks



$z \in \mathbb{R}$,
$p = [v, w, b, d]^T$
$\hat{g}(p, z) \sim g(z)$

Activation funct. σ,
sigmoid: $\sigma(z) = \frac{e^z - 1}{e^z + 1}$,
tanh: $\sigma(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$,
logit: $\sigma(z) = \frac{e^z}{e^z + 1}$, soft-
plus: $\sigma(z) = \log(e^z + 1)$.

Exploit multilevel method for training of ANNs

Training problem:

$$\min_p \mathcal{L}(p, z) = \mathcal{F}(\hat{g}(p, z) - g(z)), \qquad z \in \mathcal{T}$$

$$\hat{g}(p, z) = \sum_{i=1}^{r} v_i \sigma(w_i z + b_i) + d$$

where $\mathcal{L}$ is the loss function, $\mathcal{T}$ training set.

Exploit multilevel method for training of ANNs

Training problem:

$$\min_{p} \mathcal{L}(p, z) = \mathcal{F}(\hat{g}(p, z) - g(z)), \qquad z \in \mathcal{T}$$

$$\hat{g}(p, z) = \sum_{i=1}^{r} v_i \sigma(w_i z + b_i) + d$$

where $\mathcal{L}$ is the loss function, $\mathcal{T}$ training set.

Large-scale problem: can we exploit multilevel methods for the training?

Exploit multilevel method for training of ANNs

Training problem:

$$\min_{p} \mathcal{L}(p, z) = \mathcal{F}(\hat{g}(p, z) - g(z)), \qquad z \in \mathcal{T}$$

$$\hat{g}(p, z) = \sum_{i=1}^{r} v_i \sigma(w_i z + b_i) + d$$

where $\mathcal{L}$ is the loss function, $\mathcal{T}$ training set.

Large-scale problem: can we exploit multilevel methods for the training?

- How to build the coarse problem? The variables to be optimized are the network's weights:
  NO evident geometrical structure to exploit!

Exploit multilevel method for training of ANNs

Training problem:

$$\min_{p} \mathcal{L}(p, z) = \mathcal{F}(\hat{g}(p, z) - g(z)), \qquad z \in \mathcal{T}$$

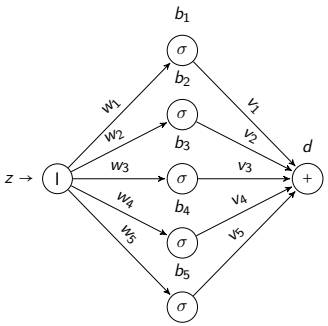
$$\hat{g}(p, z) = \sum_{i=1}^{r} v_i \sigma(w_i z + b_i) + d$$

where $\mathcal{L}$ is the loss function, $\mathcal{T}$ training set.

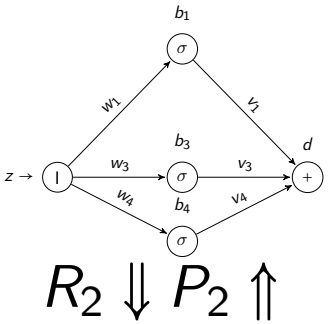
Large-scale problem: can we exploit multilevel methods for the training?

- How to build the coarse problem? The variables to be optimized are the network's weights:
  NO evident geometrical structure to exploit!
- The network possesses a purely algebraic structure: can we exploit it?

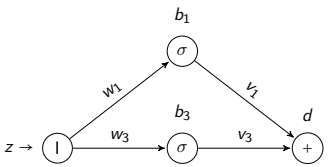
Exploit multilevel method for training of ANNs



$$\mathcal{F}_1 : \mathbb{R}^{3r_1} \to \mathbb{R}$$
$$\hat{g}(p, z) = \sum_{i \in I_1} v_i \sigma(w_i z + b_i) + d$$
$$|I_1| = r_1$$



$$\mathcal{F}_2 : \mathbb{R}^{3r_2} \to \mathbb{R}$$
$$\hat{g}(p, z) = \sum_{i \in I_2} v_i \sigma(w_i z + b_i) + d$$
$$I_2 \subset I_1, \ |I_2| = r_2 < r_1$$



$$\mathcal{F}_3 : \mathbb{R}^{3r_3} \to \mathbb{R}$$
$$\hat{g}(p, z) = \sum_{i \in I_3} v_i \sigma(w_i z + b_i) + d$$
$$I_3 \subset I_2, \ |I_3| = r_3 < r_2$$

How do we select the hierarchy of variables?

Algebraic multigrid: C/F splitting

Ruge and Stueben C/F splitting for $Ax = b$

- Two variables i, j are said to be *coupled* if $a_{i,j} \neq 0$.
- We say that a variable i is strongly coupled to another variable j, if $-a_{i,j} \geq \epsilon \max_{a_{i,k}<0} |a_{i,k}|$ for a fixed $0 < \epsilon < 1$, usually $\epsilon = 0.25$.

Prolongation-Restriction operators

$P = [I; \Delta]$, $R = P^T$.

Which matrix should we use?

Assume to use a second-order model:

$$m(x_k, s) = f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T \nabla^2 f(x_k) s + \frac{\lambda_k}{3} \|s\|^3$$

$$m(x_k, s) = f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T B_k s + \frac{\lambda_k}{2} \|s\|^2$$

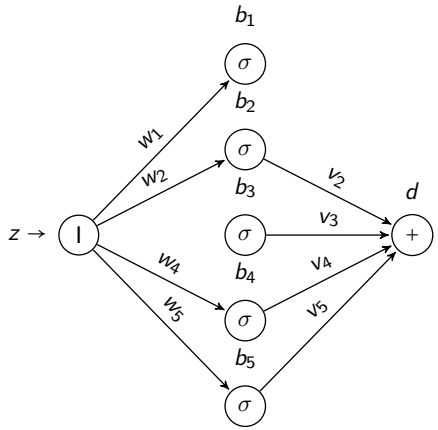
At each iteration we have to solve a linear system of the form:

$$(B_k + \tilde{\lambda}_k I)s = -\nabla f(x_k), \quad \tilde{\lambda}_k > 0.$$

As in AMG for linear systems, we use information contained in matrix B_k.

Which matrix should we use?

Remark
Variables are coupled!
$\{w_i, b_i, v_i\}$



We do not use the full matrix B_k and we define A as:

$$B_k = \begin{bmatrix} f_{v,v} & .. & .. \\ .. & f_{w,w} & .. \\ .. & .. & f_{b,b} \end{bmatrix} \to A = \frac{f_{v,v}}{\|f_{v,v}\|_\infty} + \frac{f_{w,w}}{\|f_{w,w}\|_\infty} + \frac{f_{b,b}}{\|f_{b,b}\|_\infty}$$

We define the coarse/fine splitting based on the auxiliary matrix A.

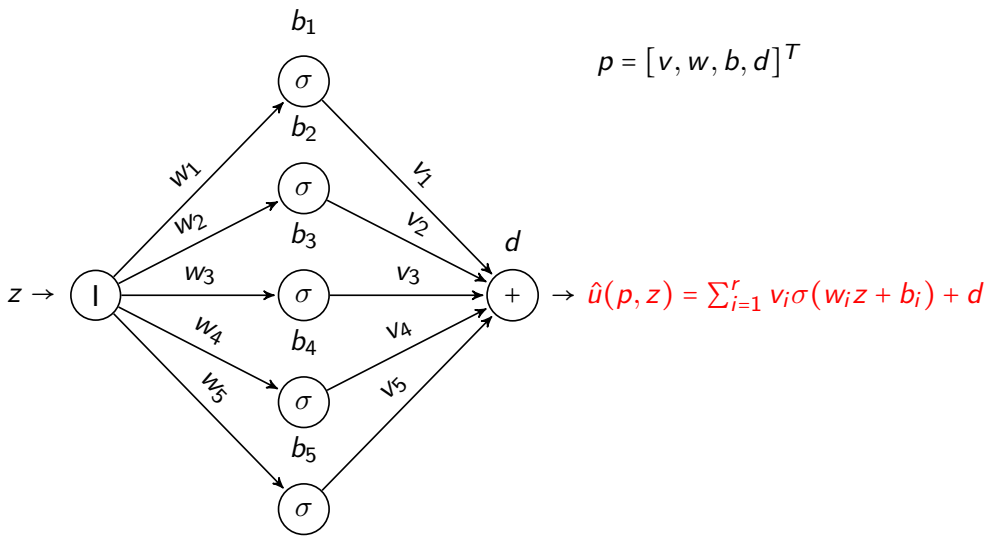
Application: solution of PDEs

Approximate the solution $u(z)$ of a PDE:

$$D(z, u(z)) = g(z), \ z \in (a, b);$$
$$u(a) = A, \ u(b) = B.$$

We approximate the solution of the PDE with a neural network:

$$u(z) \sim \hat{u}(p, z), \quad p \in \mathbb{R}^n$$



Application: solution of PDEs

We select a training set $\mathcal{T}$ s.t. $|\mathcal{T}| = t$:

$$z = [z_1, \dots, z_t]^T, \quad a \le z_1 < \cdots < z_t \le b$$

We define

$$\mathcal{L}(p, z) = \frac{1}{2t}(\|D(z, \hat{u}(z)) - g(z)\|^2 + \lambda_p(\|\hat{u}(a) - A\|^2 + \|\hat{u}(b) - B\|^2))$$

for $\hat{u}(z) \in \mathbb{R}^t$.

Advantages

- No need of discretization: we get an analytical expression of the solution, with good generalization properties (also for points outside the interval)
- We can solve also nonlinear equations, or equations with highly-nonlinear solution
- Overcome the curse of dimensionality

Choice of the true solution

$$D(z, u(z)) = g(z), \ z \in (a, b);$$

- We choose g to have true solution $u_T(z, \nu)$ depending on ν

Remark

- As ν increases the function becomes more oscillatory and it is harder to approximate.
- The size of the problem increases with the number of nodes.
- $\mathcal{T}$: equispaced points in $(0, 1)$ with $h = \frac{1}{3\nu}$ (Shannon's criterion).

Least-squares problem → multi-level Levenberg-Marquardt method

Preliminary results: Poisson's equation 10 runs

1D		$\nu = 20$	$r = 2^9$		$\nu = 25$	$r = 2^{10}$
Solver	iter	RMSE	save	iter	RMSE	save
LM	869	1.e-4		1439	1.e-3	
MLM	507	1.e-4	1.1-2.6-4.3	1325	1.e-3	1.2-1.7-2.8

Table: 1D Poisson's equation, $u_T(z, \nu) = cos(\nu z)$, 10 runs

2D		$\nu = 5$	$r = 2^{10}$		$\nu = 6$	$r = 2^{11}$
Solver	iter	RMSE	save	iter	RMSE	save
LM	633	1.e-3		1213	1.e-3	
MLM	643	1.e-3	1.1-1.5-2.1	1016	1.e-3	1.2-1.9-2.4

Table: 2D Poisson's equation, $u_T(z, \nu) = cos(\nu z)$, 10 runs

save(min,average,max)=ratio between total number of flops required for matrix-vector products

Helmholtz's and nonlinear equations, 10 runs

		$\nu = 5$	$r = 2^{10}$
Solver	iter	RMSE	save
LM	1159	1.e-3	
MLM	1250	1.e-3	1.2-1.9-3.1

Table: Helmholtz's equations. $\Delta u(z) + \nu^2 u(z) = 0$, $u_T(z, \nu) = sin(\nu z) + cos(\nu z)$

		$\nu = 20$	$r = 2^9$		$\nu = 1$	$r = 2^9$
Method	iter	RMSE	save	iter	RMSE	save
LM	950	10^{-5}		270	10^{-3}	
MLM	1444	10^{-5}	0.8-2.9-5.3	320	10^{-3}	1.2-1.7-1.8

Table: Left: $\Delta u + \sin u = g_1$ (1D) $u_T(z, \nu) = 0.1 \cos(\nu z)$. Right: $\Delta u + e^u = g_1$ (2D), $u_T(z, \nu) = \log\left(\frac{\nu}{z_1 + z_2 + 10}\right)$

Conclusions

- Theoretical contribution: We have presented a class of multilevel high-order methods for optimization and proved their global and local convergence and complexity.
- Practical contribution: We have got further insight on the methods proposing a AMG strategy to build coarse representations of the problem to use some methods in the family for the training of artificial neural networks.

Thank you for your attention!

If $q = 1$, the regularized model is defined as

$$f(x_k) + \nabla f(x_k) + \frac{\lambda_k}{2}\|s\|^2, \tag{1}$$

where in case of a least-squares problem $\nabla f(x_k) = J(x_k)^T F(x_k)$. For a positive definite matrix $M \in \mathbb{R}^{n\times n}$ and $x \in \mathbb{R}^n$, we can define the following norm:

$$\|x\|_M = x^T M x.$$

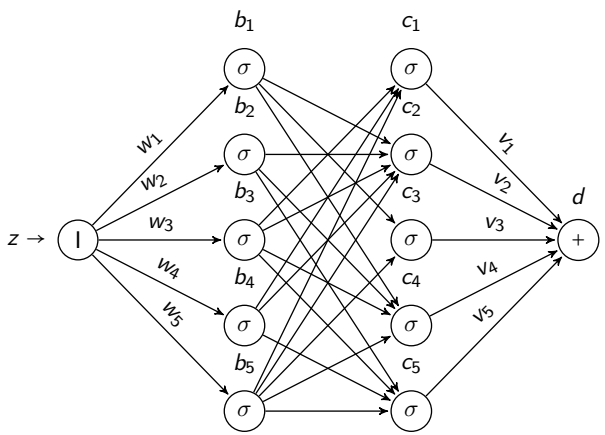
If we define $M = \frac{B_k}{\lambda_k} + I$, then we have $\frac{\lambda_k}{2}\|s\|_M^2 = \frac{1}{2}s^T B_k s + \frac{\lambda_k}{2}\|s\|^2$, so that the model

$$m_k(x_k, s) = f(x_k) + \nabla f(x_k) + \frac{\lambda_k}{2}\|s\|_M^2,$$

corresponds to $q = 1$, just with a different norm for the regularization term.

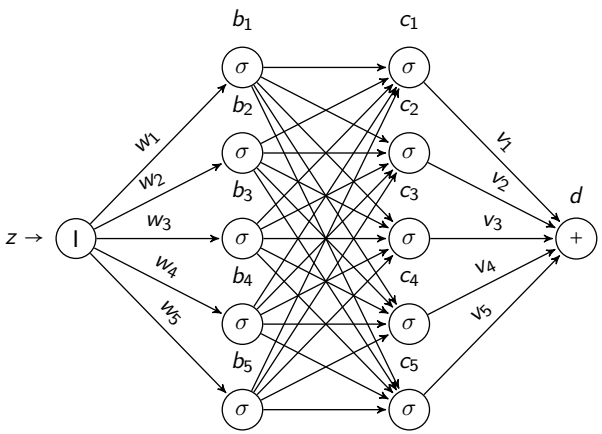
Future work 1: Extend the method to multilayer networks.

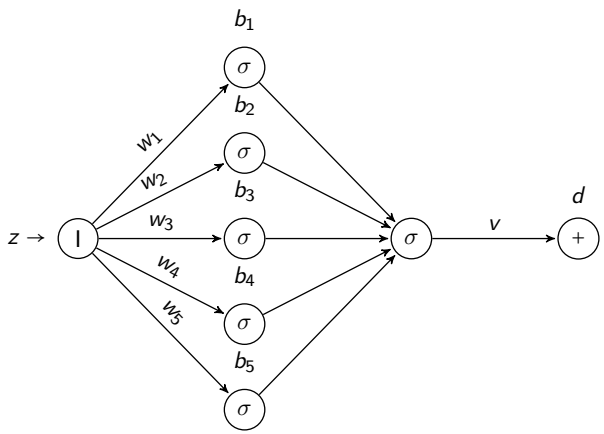
- Extend the method as it is: use a sparse network.



Future work 1: Extend the method to multilayer networks.

- Extend the method as it is: use a sparse network.
- Change strategy to build coarse problems: compress variables in a layer to exploit the structure of the multilayer network.





Future work 2: Hessian-free method

- Make it a competitive training method: method needs to compute and store the Hessian matrix (for step computation and to build transfer operators): too expensive for large-scale problems.
- Hessian complete calculation needed just once (first iteration) to compute R and P.

Thank you for your attention!

For more details:

On high-order multilevel optimization strategies and their application to the training of artificial neural networks

Prolongation operator

$$x_i^h = (Px^H)_i = \begin{cases} x_i^H & \text{if } i \in C, \\ \sum_{k \in P_i} \delta_{i,k} x_k^H & \text{if } i \in F, \end{cases}$$

with

$$\delta_{i,k} = \begin{cases} -\alpha_i a_{i,k}/a_{i,i} & \text{if } k \in P_i^-, \\ -\beta_i a_{i,k}/a_{i,i} & \text{if } k \in P_i^+, \end{cases} \qquad \alpha_i = \frac{\sum_{j \in N_i} a_{i,j}^-}{\sum_{k \in P_i} a_{i,k}^-}, \qquad \beta_i = \frac{\sum_{j \in N_i} a_{i,j}^+}{\sum_{k \in P_i} a_{i,k}^+},$$

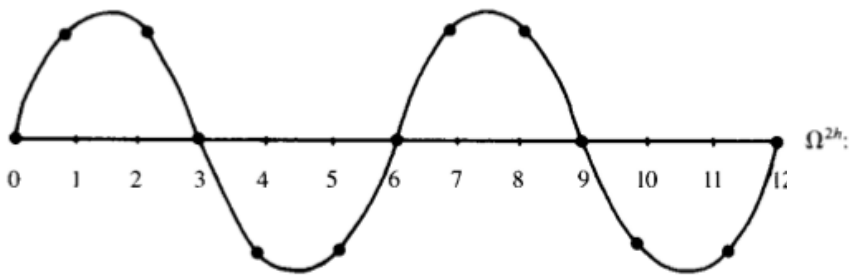
where $a_{i,j}^+ = \max\{a_{i,j}, 0\}$, $a_{i,j}^- = \min\{a_{i,j}, 0\}$, N_i is the set of variables connected to i (i.e. all j such that $a_{i,j} \neq 0$), P_i the set of coarse variables strongly connected to i, which is partitioned in P_i^- (negative couplings) and P_i^+ (positive couplings). The interpolation operator, assuming to have regrouped and ordered the variables to have all those corresponding to indexes in C at the beginning, is then defined as $P = [I; \Delta]$ where I is the identity matrix of size $|C|$ and Δ is the matrix such that $\Delta_{i,j} = \delta_{i,j}$.

Classical multigrid methods

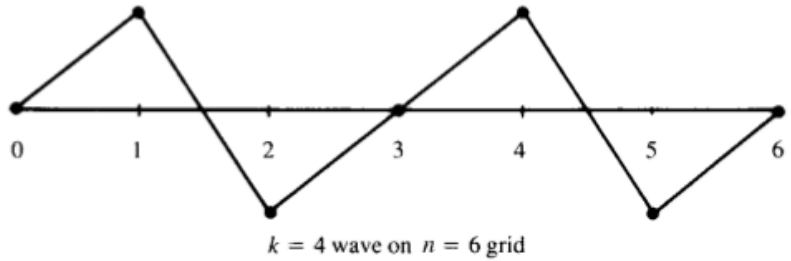
- Consider a linear elliptic PDE: $D(z, u(z)) = f(z)\ z \in \Omega$ + b.c.
- Discretize on grid h. Get a large-scale linear system $A_h x_h = b_h$.

Consider the discretization of the same PDE problem on a coarser grid: $A_H x_H = b_H$, $H > h$.

- Relaxation methods fails to eliminate smooth components of the error efficiently.
- Smooth components projected on a coarser grid appear more oscillatory.



$k = 4$ wave on $n = 12$ grid



$k = 4$ wave on $n = 6$ grid

Coarse problem construction

Define transfer grid operators: P prolongation and R restriction to project vectors from a grid to another: $x_H = Rx_h$, $x_h = Px_H$, such that $R = \alpha P^T$.

Geometry exploitation

The geometrical structure of the problem is exploited to build R and P.

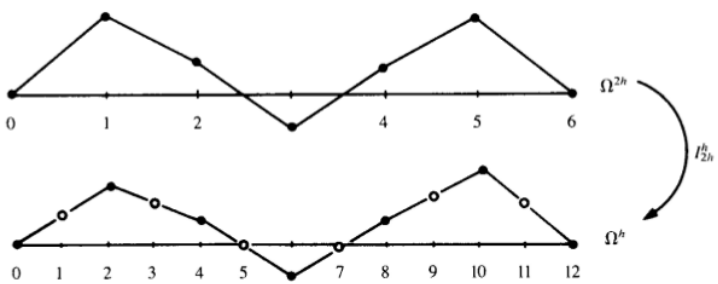


Figure 3.2: *Interpolation of a vector on coarse grid Ω^{2h} to fine grid Ω^{h}.*

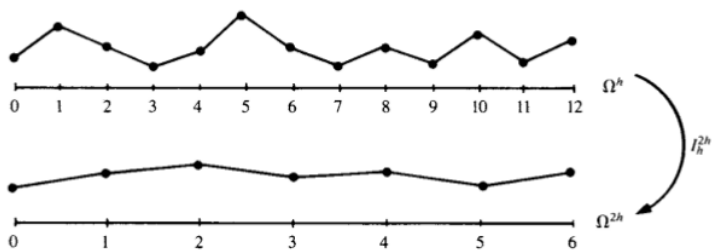


Figure 3.4: *Restriction by full weighting of a fine-grid vector to the coarse grid.*