Convolutional Neural Networks and PDEs

Numerical Methods for Deep Learning

Recall - Deep Network

$$\mathbf{Y}_{j+1} = \mathbf{P}_j \mathbf{Y}_j + \sigma(\mathbf{K}_j \mathbf{Y}_j + b_j)$$

Problems/Challenges

- The state can grow (explosion) $\Rightarrow$ $\mathbf{Y}_N$ very sensitive to $\mathbf{Y}_0$ and $\mathbf{K}_j$ (exploding gradients)
- The state can go to 0 $\Rightarrow$ $\mathbf{Y}_N$ independent to $\mathbf{Y}_0$ and to the $\mathbf{K}_j$'s (vanishing gradients)
- In both cases the optimization can fail

Today: Deep Convolutional Neural Networks

Deep network with convolution operators parameterized by stencils. Common

$$\mathbf{Y}_{j+1} = \mathbf{P}_j \mathbf{Y}_j + h\mathbf{K}_{j,2}\sigma(\mathbf{K}_{j,1}\mathbf{Y}_j + b_j)$$

Motivation for second convolution?

- approximation properties of double layer
- if $\sigma(x) = \max(x, 0)$ entries in $\mathbf{Y}$ can only grow.

Learning tasks:

- image classification
- semantic segmentation

Convolutions and PDEs

Let $\mathbf{y}$ be 1D grid function, $\mathbf{y} \leftrightarrow y$ (n cells of width $h_x = 1/n$)

$$
\begin{aligned}
K(\theta)\mathbf{y} &= [\theta_1 \ \theta_2 \ \theta_3] * \mathbf{y} \\
&= \left(\frac{\beta_1}{4}[1 \ \ 2 \ \ 1] + \frac{\beta_2}{2h_x}[-1 \ \ 0 \ \ 1] + \frac{\beta_3}{h_x^2}[-1 \ \ 2 - 1] \right) * \mathbf{y}
\end{aligned}
$$

Relation between β and θ given by

$$
\underbrace{\begin{pmatrix} 1/4 & -1/(2h_x) & -1/h_x^2 \\ 1/2 & 0 & 2/h_x^2 \\ 1/4 & 1/(2h_x) & -1/h_x^2 \end{pmatrix}}_{=\mathbf{A}(h_x)} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix}.
$$

In the limit $h_x \to 0$ this gives

$$
K(\theta(t)) = \beta_1(t) + \beta_2(t)\partial_x + \beta_3(t)\partial_x^2.
$$

Scaling Convolution Operators: Rediscretization

Let $\mathbf{y}_c$ and $\mathbf{y}_f$ be 1D grid functions $\mathbf{y} \leftrightarrow y$ (grid: $n_c = n$ and $n_f = 2n$ cells of width $h_c = 1/n_c$ and $h_f = 1/n_f$, respectively)

Ex: Let $y(x) = (cos(2\pi x^4)) + x - 0.8(x-0.5)^2$, $n = 8$, and

$$\theta_{\rm coarse} = (-67, 129, -59)^\top.$$

Find corresponding kernel, $\theta_{\rm fine}$ on fine mesh.

Strategy:

1. setup $\mathbf{A}(h_c)$ and compute β
2. setup $\mathbf{A}(h_f)$ and compute $\theta_{\rm fine}$

`E15CoarseToFineConv1D.m`

Convolution and PDEs - 2D Case

Similar arguments apply in two and more dimensions. Let $\theta \in \mathbb{R}^{3\times 3}$ be a given stencil then

$$
\begin{aligned}
K(\theta) =& \beta_1 + \beta_2 \partial_x + \beta_3 \partial_y + \beta_4 \partial_{xy} + \beta_5 \partial_{xx} \\
&+ \beta_6 \partial_{yy} + \beta_7 \partial_{x^2 y} + \beta_8 \partial_{xy^2} + \beta_9 \partial_{x^2 y^2}
\end{aligned}
$$

How to get the coefficients? Let $h_x > 0$ pixel size, use

$$
\left(\begin{array}{rrr|rrr|rrr}
1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\
2 & -2 & 0 & 2 & -2 & 0 & 2 & 0 & 2 \\
1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\
2 & 0 & -2 & -2 & 2 & 0 & 0 & 2 & 2 \\
4 & 0 & 0 & -4 & -4 & 0 & 0 & 0 & -4 \\
2 & 0 & 2 & -2 & -2 & 0 & 0 & -2 & 2 \\
1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\
2 & 2 & 0 & 2 & -2 & 0 & -2 & 0 & 2 \\
1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1
\end{array}\right) \cdot \mathrm{diag} \begin{pmatrix} 1/16. \\ 1/6h_x \\ 1/6h_x \\ 1/4h^2 \\ 1/4h^2 \\ 1/h^2 \\ 1/2h^3 \\ 1/2h^3 \\ 1/2h^3 \end{pmatrix}
$$

Algebraic Prolongation of Convolution Kernels

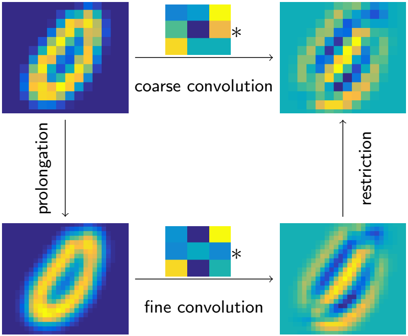
$$\mathbf{K}_H = \mathbf{R}\mathbf{K}_h\mathbf{P},$$

where

- $\mathbf{K}_h$ fine mesh operator (given)
- $\mathbf{R}$ restriction (e.g., averaging)
- $\mathbf{P}$ prolongation (e.g., interpolation)

Remarks:

- Galerkin: $\mathbf{R} = \gamma\mathbf{P}^\top$
- Coarse $\rightarrow$ Fine: unique if kernel size constant.
- only small linear solve required



Scaling Convolution Operators: Algebraic

Let $n_c = 3$, $n_f = 6$ (see `E15CoarseToFineConv1D.m`)

Prolongation and restriction

$$\mathbf{P} = \begin{pmatrix} 1 & & \\ 3/4 & 1/4 & \\ 1/4 & 3/4 & \\ & 3/4 & 1/4 \\ & 1/4 & 3/4 \\ & & 1 \end{pmatrix},$$

$$\mathbf{R} = \begin{pmatrix} 1/2 & 1/2 & & & & \\ & & 1/2 & 1/2 & & \\ & & & & 1/2 & 1/2 \end{pmatrix}$$

1. build $\mathbf{K}_H = \mathbf{R}\mathbf{K}_h\mathbf{D}$ for jth unit vector as stencil
2. extract a column associated with interior node
3. reshape and get patch around node
4. vectorize and use as one column

Stability of Convolutional ResNets

Residual Neural Network is discretization of

$$\partial_t \mathbf{y}(t) = \mathbf{K}_2(t)\sigma\left(\mathbf{K}_1(t)\mathbf{y} + b(t)\right), \quad \mathbf{y}(0) = \mathbf{y}_0.$$

To analyze stability need to look at eigenvalues of

$$\mathbf{J}(t) = \mathbf{K}_2(t)\mathrm{diag}\left(\sigma'(\mathbf{K}_1(t)\mathbf{y} + b)\right)\mathbf{K}_1(t)$$

Difficult to analyze eigenvalues for general $\mathbf{K}_2$ and $\mathbf{K}_1$.
Easy option: Set $\mathbf{K}_2 = -\mathbf{K}_1^\top$ (and drop subscript index).
Doing so gives:

$$\mathbf{J}_{sym}(t) - \mathbf{K}(t)^\top\mathrm{diag}\left(\sigma'(\mathbf{K}_1(t)\mathbf{y} + b)\right)\mathbf{K}(t)$$

symmetric negative definite $\leadsto$ stability if $\partial_t \mathbf{K}$ small

`E15ParabolicCNN.m`

Parabolic CNN

In original Residual Net choose $\mathbf{K}_2 = -\mathbf{K}_1^\top = \mathbf{K}^\top$. This gives parabolic CNN

$$\partial_t \mathbf{Y}_t = -\mathbf{K}(t)^\top \sigma(\mathbf{K}(t)\mathbf{Y} + \mathbf{b}(t)), \quad \mathbf{Y}(0) = \mathbf{Y}_0$$

Theorem

If σ is monotonically non-decreasing, then the forward propagation is stable, i.e., there is a $M > 0$ such that

$$\|\mathbf{Y}(T) - \mathbf{Y}_\epsilon(T)\|_F \le M \|\mathbf{Y}(0) - \mathbf{Y}_\epsilon(0)\|_F,$$

where $\mathbf{Y}$ and $\mathbf{Y}_\epsilon$ are solutions for different initial values.

Use forward Euler discretization with h small enough

$$\mathbf{Y}_{j+1} = \mathbf{Y}_j - h\mathbf{K}_j^\top \sigma(\mathbf{K}_j \mathbf{Y} + \mathbf{b}_j), \quad j = 0, 1, \dots, N-1$$

Similar to anisotropic diffusion (popular in image processing) [1]

Proof: Stability of Parabolic Networks

For ease of notation, assume no bias. We show that

$$\partial_t \|\mathbf{Y}(t) - \mathbf{Y}_\epsilon(t)\|_F^2 \le 0.$$

Integrating this over $[0, T]$ yields the stability result.
Why? Note that for all $t \in [0, T]$ taking derivative gives

$$\begin{aligned}\big(-\mathbf{K}(t)^\top \sigma(\mathbf{K}(t)\mathbf{Y}) + \mathbf{K}(t)^\top \sigma(\mathbf{K}(t)\mathbf{Y}_\epsilon), \mathbf{Y} - \mathbf{Y}_\epsilon\big) \\ -\left(\sigma(\mathbf{K}(t)\mathbf{Y}) - \sigma(\mathbf{K}(t)\mathbf{Y}_\epsilon), \mathbf{K}(t)(\mathbf{Y} - \mathbf{Y}_\epsilon)\right) \quad \le 0.\end{aligned}$$

Where $(\cdot, \cdot)$ is inner product and the inequality follows from the monotonicity of the activation function.

Relation to Total Variation

Note that the parabolic network can be seen as a gradient flow for

$$\phi(\mathbf{Y}) = s(\mathbf{K}(t)\mathbf{Y}(t) + b(t)),$$

where $\sigma(x) = s'(x)$. What is s?

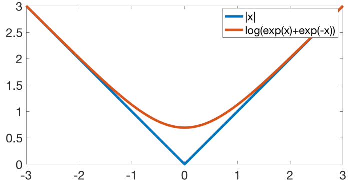
- $\sigma = \max(x, 0)$:

$$s(x) = \max(x, 0)^2$$

- $\sigma = \tanh(x)$:

$$s(x) = \log(\exp(x) - \exp(-x))$$

For $\mathbf{K}(t) = \nabla$, this shows a relation to total variation [3].



thanks to Stanley Osher for providing this example

Normalization

Goal: Make sure $\|\mathbf{Y}_j\|$ does not change too much.

1. Compute

$$\mathbf{Z}_j = \mathbf{K}_j \mathbf{Y}_j$$

2. "Normalize"

$$\widehat{\mathbf{Z}}_j = N(\mathbf{Z}_j)$$

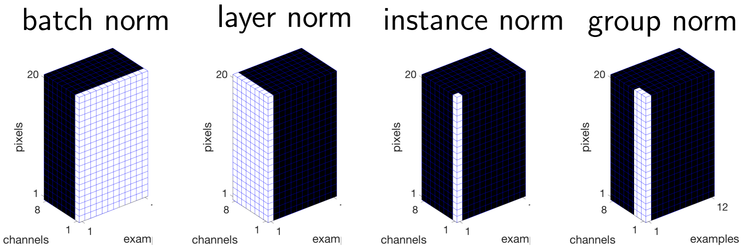
3. Update

$$\mathbf{Y}_{j+1} = \mathbf{P}_j \mathbf{Y}_j - h \mathbf{K}_j^\top \sigma(\alpha_j \widehat{\mathbf{Z}}_j + \beta_j),$$

where α_j, β_j are trainable weights.

How to normalize?

Normalization



Represent image data as a multidimensional array

$$\underbrace{\textit{Height} \times \textit{Width}}_{\textit{pixels}} \times \textit{Channels} \times \textit{Examples}$$

We can normalize over each one of those.

Normalization

Normalization along `dir` is done by

- Reducing the mean

  `Y = Y - mean(Y,dir)`

- Dividing by the standard deviation

  `Y = Y ./ sqrt(Y.^2+eps)`

  where `eps`>0 is a conditioning parameter.

Questions:

- How to compute derivatives?
- The effect of batch size?
- How well does this work?

Batch Normalization

- the first normalization suggested [2]
- coupling across examples. Intuitive?
- sensitive to batch size
- works very well (i.e., better performance of SGD)

`E15BatchNorm.m`

Instance Normalization

Suggested recently [4] but has much older roots
Equivalent to total variation in image denoising [3]

$$TV(\mathbf{Y}) = \frac{\nabla \mathbf{Y}}{\sqrt{|\nabla \mathbf{Y}|^2 + \epsilon}}$$

Can we utilize this to do better?

`E15InstanceNorm.m`

References

[1] Y. Chen and T. Pock. Trainable Nonlinear Reaction Diffusion: A Flexible Framework for Fast and Effective Image Restoration. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 39(6):1256–1272, June 2017.

[2] S. Ioffe and C. Szegedy. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. *arXiv preprint [cs.LG] 1502.03167v3*, 2015.

[3] L. I. Rudin, S. Osher, and E. Fatemi. Nonlinear total variation based noise removal algorithms. *Physica D: Nonlinear Phenomena*, 60(1-4):259–268, 1992.

[4] D. Ulyanov, A. Vedaldi, and V. Lempitsky. Instance Normalization: The Missing Ingredient for Fast Stylization. *arxiv preprint [cs.CV] 1607.08022v3*, 2016.