Parametric Models

Numerical Methods for Deep Learning

Motivation

Recall single layer

$$\mathbf{Z} = \sigma(\mathbf{YK} + b),$$

where $\mathbf{Y} \in \mathbb{R}^{n \times n_f}$, $\mathbf{K} \in \mathbb{R}^{n_f \times m}$, $b \in \mathbb{R}$, and σ element-wise activation.

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Possible remedies:

- **Regularization:** penalize $\mathbf{K}$
- **Parametric model:** $\mathbf{K}(\theta)$ where $\theta \in \mathbb{R}^p$ with $p \ll m \cdot n_f$.

Some Simple Parametric Models

- Diagonal scaling:

$$\mathbf{K}(\theta) = \mathrm{diag}(\theta) \in \mathbb{R}^{n_f \times n_f}$$

Advantage: preserves size and structure of data.

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- Antisymmetric kernel

$$\mathbf{K}(\theta) = \begin{pmatrix} 0 & \theta_1 & \theta_2 \\ -\theta_1 & 0 & \theta_3 \\ -\theta_2 & -\theta_3 & 0 \end{pmatrix}$$

  Advantage?: $\mathrm{real}(\lambda_i(\mathbf{K}(\theta))) = 0$.

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- M-matrix

$$\mathbf{K}(\theta) = \begin{pmatrix} \theta_1 + \theta_2 & -\theta_1 & -\theta_2 \\ -\theta_3 & \theta_3 + \theta_4 & -\theta_4 \\ -\theta_5 & -\theta_6 & \theta_5 + \theta_6 \end{pmatrix} \quad \theta \geq 0$$

  Advantage: like differential operator

Differentiating Parametric Models

Need derivatives of model to optimize θ in

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$$\mathbf{K}(\theta) = \mathrm{mat}(\mathbf{Q}\,\theta)$$

Therefore, matrix-vector products with the Jacobian simply are

$$\mathbf{J}_\theta(\mathbf{K}(\theta))\mathbf{v} = \mathrm{mat}(\mathbf{Q}\ \mathbf{v}) \quad \text{and} \quad \mathbf{J}_\theta(\mathbf{K}(\theta))^\top \mathbf{w} = \mathbf{Q}^\top \mathbf{w}$$

where $\mathbf{v} \in \mathbb{R}^p$ and $\mathbf{w} \in \mathbb{R}^m$.

Example: Derivative of M-matrix

$$\mathbf{K}(\theta) = \begin{pmatrix} \theta_1 + \theta_2 & -\theta_1 & -\theta_2 \\ -\theta_3 & \theta_3 + \theta_4 & -\theta_4 \\ -\theta_5 & -\theta_6 & \theta_5 + \theta_6 \end{pmatrix} \quad \theta \geq 0$$

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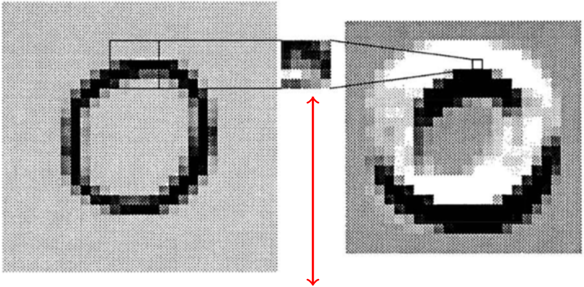
verify that this can be written as $K(\theta) = \mathrm{mat}(\mathbf{Q}\,\theta)$ where

$$\mathbf{Q} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \in \mathbb{R}^{9\times 6}$$

Note: not efficient to construct $\mathbf{Q}$ when p large but helpful when computing derivatives

Convolutional Neural Networks

$\mathbf{y} \in \mathbb{R}^{28\times 28}$ input features $\quad$ $\mathbf{z} \in \mathbb{R}^{24\times 24}$ output features



$\theta \in \mathbb{R}^{5\times 5}$ convolution kernel

- useful for speech, images, videos, ...
- efficient parameterization, efficient codes (GPUs, ...)
- now: CNNs as parametric model and PDEs, simple code

Y LeCun, BE Boser, JS Denker
Handwritten digit recognition with a back-propagation network.
Advances in neural information processing systems,396404, 1990.

Convolutions in 1D

Let $y, z, \theta : \mathbb{R} \to \mathbb{R}$, $z : \mathbb{R} \to \mathbb{R}$ be continuous functions then

$$z(x) = (\theta * y)(x) = \int_{-\infty}^{\infty} \theta(x - t)y(t)dt.$$

Assume $\theta(x) \neq 0$ only in interval $[-a, a]$ (compact support).

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A few properties

- $\theta * y = \mathcal{F}^{-1}((\mathcal{F}\theta)(\mathcal{F}y))$, $\mathcal{F}$ is Fourier transform
- $\theta * y = y * \theta$

Discrete Convolutions in 1D

Let $\theta \in \mathbb{R}^{2k+1}$ be stencil, $\mathbf{y} \in \mathbb{R}^{n_f}$ grid function

$$\mathbf{z}_i = (\theta * \mathbf{y})_i = \sum_{j=-k}^{k} \theta_j \mathbf{y}_{i-1}.$$

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Example: Discretize $\theta \in \mathbb{R}^3$ (non-zeros only), $\mathbf{y}, \mathbf{z} \in \mathbb{R}^4$ on regular grid

$$\begin{aligned}
\mathbf{z}_1 &= \theta_3 \mathbf{w}_1 + \theta_2 \mathbf{x}_1 + \boldsymbol{\theta}_1 \mathbf{x}_2 \\
\mathbf{z}_2 &= \theta_3 \mathbf{x}_1 + \theta_2 \mathbf{x}_2 + \boldsymbol{\theta}_1 \mathbf{x}_3 \\
\mathbf{z}_3 &= \theta_3 \mathbf{x}_2 + \theta_2 \mathbf{x}_3 + \boldsymbol{\theta}_1 \mathbf{x}_4 \\
\mathbf{z}_4 &= \theta_3 \mathbf{x}_3 + \theta_2 \mathbf{x}_4 + \boldsymbol{\theta}_1 \mathbf{w}_2
\end{aligned}$$

where $\mathbf{w}_1, \mathbf{w}_2$ are used to implement different boundary conditions (right choice? depends ...).

Structured Matrices - 1

$$\begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{z}_3 \\ \mathbf{z}_4 \end{pmatrix} = \begin{pmatrix} \theta_3 & \theta_2 & \theta_1 & & & \\ & \theta_3 & \theta_2 & \theta_1 & & \\ & & \theta_3 & \theta_2 & \theta_1 & \\ & & & \theta_3 & \theta_2 & \theta_1 \end{pmatrix} \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \\ \mathbf{w}_2 \end{pmatrix}$$

Different boundary conditions lead to different structures

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Different boundary conditions lead to different structures

- Zero boundary conditions: $\mathbf{w}_1 = \mathbf{w}_2 = 0$

$$\begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{z}_3 \\ \mathbf{z}_4 \end{pmatrix} = \begin{pmatrix} \theta_2 & \theta_1 & & \\ \theta_3 & \theta_2 & \theta_1 & \\ & \theta_3 & \theta_2 & \theta_1 \\ & & \theta_3 & \theta_2 \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix}$$

This is a *Toeplitz matrix* (constant along diagonals).

Structured Matrices - 2

- Periodic boundary conditions: $\mathbf{w}_1 = \mathbf{x}_4$ and $\mathbf{w}_2 = \mathbf{x}_1$

$$\begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{z}_3 \\ \mathbf{z}_4 \end{pmatrix} = \begin{pmatrix} \theta_2 & \theta_1 & & \theta_3 \\ \theta_3 & \theta_2 & \theta_1 & \\ & \theta_3 & \theta_2 & \theta_1 \\ \theta_1 & & \theta_3 & \theta_2 \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix}$$

this is a *circulant matrix* (each row/column is periodic shift of previous row/column)

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An attractive property of a cirulant matrix is that we can efficiently compute its eigendecomposition

$$\mathbf{K}(\theta) = \mathbf{F}^* \mathrm{diag}(\lambda) \mathbf{F}$$

where $\mathbf{F}$ is the discrete Fourier transform and the eigenvalues, $\lambda \in \mathbb{C}^4$, can be computed using first column

$$\lambda = \mathbf{F}(\mathbf{K}(\theta)\mathbf{u}_1) \quad \text{where} \quad \mathbf{u}_1 = (1, 0, 0, 0)^\top.$$

Coding: 1D Convolution using FFTs

Let $\theta \in \mathbb{R}^3$ be some stencil and $n_f = m = 16$

1. build a sparse matrix $\mathbf{K}$ for computing the convolution with periodic boundary conditions. Hint: `spdiags`
2. compute the eigenvalues of $\mathbf{K}$ using `eig(full(K))` and using `fft` and first column of $\mathbf{K}$. Compare!
3. verify that `norm(K*y - real(ifft(lam.*fft(y))))` is small.
4. repeat previous item for transpose.
5. write code that computes eigenvalues for arbitrary stencil size without building $\mathbf{K}$. Hint: `circshift`

Derivatives of 1D Convolution - 1

Recall that we need a way to compute

$$\mathbf{J}_\theta(\mathbf{YK}(\theta))\mathbf{v} \quad \text{and} \quad \mathbf{J}_\theta(\mathbf{YK}(\theta))^\top\mathbf{w}, \quad (\mathbf{J}_\theta \in \mathbb{R}^{n_f \times p})$$

(note that we have put $\mathbf{Y}$ inside the bracket to avoid tensors)

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Assume single example, $\mathbf{y}$. Since we have periodic boundary conditions

$$\begin{aligned}(\mathbf{y}^\top \mathbf{K}(\theta))^\top &= \mathbf{K}(\theta)^\top \mathbf{y} = \mathrm{real}(\mathbf{F}(\lambda(\theta) \odot \mathbf{F}^* \mathbf{y})) \\ &= \mathrm{real}(\mathbf{F}\ \mathrm{diag}(\mathbf{F}^* \mathbf{y})\ \lambda(\theta)), \quad \lambda(\theta) = \mathbf{F}(\mathbf{K}(\theta)\mathbf{u}_1).\end{aligned}$$

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Need to differentiate eigenvalues w.r.t. θ. Note linearity

$$\mathbf{K}(\theta)\mathbf{u}_1 = \mathbf{Q}\theta, \quad \mathbf{Q} = ?$$

Derivatives of 1D Convolution - 2

Assume we have

$$\mathbf{K}(\theta)^\top \mathbf{y} = \mathrm{real}(\mathbf{F}\ \mathrm{diag}(\mathbf{F}^* \mathbf{y})\ \mathbf{F}\mathbf{Q}\theta))$$

Then mat-vecs with Jacobian are easy to compute

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Code this and check Jacobian and its transpose using `conv1D.m`!

Extension 1: Many Examples

Let now $n > 1$. in MATLAB beneficial to avoid for-loop over examples.

$$(\mathbf{YK}(\theta))^\top = \mathbf{K}(\theta)^\top \mathbf{Y}^\top = \mathrm{real}(\mathbf{F}\mathrm{diag}(\lambda(\theta))\mathbf{F}^*\mathbf{Y}^\top)$$

$$(\mathbf{ZK}(\theta)^\top)^\top = \mathbf{K}(\theta)\mathbf{Z}^\top = \mathrm{real}(\mathbf{F}^*\mathrm{diag}(\lambda(\theta))\mathbf{F}\mathbf{Z}^\top)$$

These require almost no change to the code. For the Jacobians, we need to re-order slightly and get

$$\mathbf{J}_\theta(\mathbf{YK}(\theta)) = \mathrm{real}(\mathbf{F}(\mathrm{diag}(\mathbf{FQ}v)\mathbf{F}^*\mathbf{Y}^\top))^\top$$

and for the transpose we need to sum over examples

$$\mathbf{J}_\theta(\mathbf{YK}(\theta))\mathbf{W} = \mathrm{real}(\mathbf{Q}^\top\mathbf{F}((\mathbf{F}^*\mathbf{Y}^\top) \odot (\mathbf{F}\mathbf{W}^\top)\mathbf{e}_n))$$

Extension 2: 2D Convolution

Example: Let $\mathbf{y}, \mathbf{z}, \theta \in \mathbb{R}^{3\times 3}$ and assume periodic BCs then

$$\begin{aligned}
\mathbf{z}_{21} &= \theta_{33}\mathbf{y}_{13} + \theta_{32}\mathbf{y}_{11} + \theta_{31}\mathbf{y}_{12} \\
&\quad + \theta_{23}\mathbf{y}_{23} + \theta_{22}\mathbf{y}_{21} + \theta_{21}\mathbf{y}_{22} \\
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In matrix form, this gives

$$\begin{pmatrix} \mathbf{z}_{21} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{pmatrix} = \left(\begin{array}{ccc|ccc|ccc} \theta_{32} & \theta_{22} & \theta_{12} & \theta_{31} & \theta_{21} & \theta_{11} & \theta_{33} & \theta_{23} & \theta_{13} \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \\ &&&&&&&& \end{array}\right) \begin{pmatrix} \mathbf{y}_{11} \\ \mathbf{y}_{21} \\ \mathbf{y}_{31} \\ \mathbf{y}_{12} \\ \mathbf{y}_{22} \\ \mathbf{y}_{32} \\ \mathbf{y}_{13} \\ \mathbf{y}_{23} \\ \mathbf{y}_{33} \end{pmatrix}$$

good news: this matrix is BCCB (block circulant with circulant blocks)

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=
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\theta_{12} & \theta_{32} & \theta_{22} & \theta_{11} & \theta_{31} & \theta_{21} & \theta_{13} & \theta_{33} & \theta_{23} \\
\hline
\theta_{23} & \theta_{13} & \theta_{33} & \theta_{22} & \theta_{12} & \theta_{32} & \theta_{21} & \theta_{11} & \theta_{31} \\
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\begin{pmatrix} \mathbf{y}_{11} \\ \mathbf{y}_{21} \\ \mathbf{y}_{31} \\ \mathbf{y}_{12} \\ \mathbf{y}_{22} \\ \mathbf{y}_{32} \\ \mathbf{y}_{13} \\ \mathbf{y}_{23} \\ \mathbf{y}_{33} \end{pmatrix}
$$

good news: this matrix is BCCB (block circulant with circulant blocks)

Extension 2: 2D Convolution using FFTs

Since the 2D convolution operator is BCCB, we still have that

$$\mathbf{K}(\theta) = \mathbf{F}^* \mathrm{diag}(\lambda(\theta))\mathbf{F}, \quad \lambda(\theta) = \mathbf{F}(\mathbf{K}(\theta)\mathbf{u}_1).$$

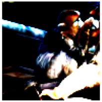
Differences:

- $\mathbf{F}$ now refers to the 2D Fourier transform (`fft2` and `ifft2`).
- need to find an efficient way to build first column of $\mathbf{K}(\theta)$ and encode that using $\mathbf{Q}$.

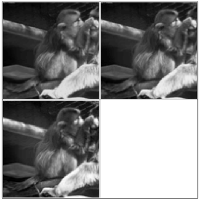
All else stays the same and extends also to higher dimensions (like for videos).

Extension 3: Width of CNNs

RGB image



input channels



output channels

Width of CNN can be controlled by number of input and output channels of each layer. Let $\mathbf{y} = (\mathbf{y}_R, \mathbf{y}_G, \mathbf{y}_B)$, then we might compute

$$\begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{z}_3 \\ \mathbf{z}_4 \end{pmatrix} = \begin{pmatrix} \mathbf{K}^{11}(\theta^{11}) & \mathbf{K}^{12}(\theta^{12}) & \mathbf{K}^{11}(\theta^{13}) \\ \mathbf{K}^{21}(\theta^{21}) & \mathbf{K}^{22}(\theta^{22}) & \mathbf{K}^{21}(\theta^{23}) \\ \mathbf{K}^{31}(\theta^{31}) & \mathbf{K}^{32}(\theta^{32}) & \mathbf{K}^{31}(\theta^{33}) \\ \mathbf{K}^{41}(\theta^{41}) & \mathbf{K}^{42}(\theta^{42}) & \mathbf{K}^{41}(\theta^{43}) \end{pmatrix} \begin{pmatrix} \mathbf{y}_R \\ \mathbf{y}_G \\ \mathbf{y}_B \end{pmatrix},$$

where $\mathbf{K}^{ij}$ is a 2D convolution operator with stencil θ^{ij}

Outlook: Extensions for Later

For now, we just introduced the very basic convolution layer. CNNs used in practice also use the following components (discussed later)

- *pooling:* reduce image resolution (e.g. by averaging over patches)
- *stride:* Example: stride of two reduces image resolution by computing $\mathbf{z}$ only at every other pixel.

Build your own parametric model (ideas for projects)

- $M-$matrix for convolution
- cheaper convolution models: separable kernels, doubly symmetric kernels
- Wavelet, ...
- other sparsity patterns