Regularization for Image Classification

Numerical Methods for Deep Learning

Motivation

Recall single layer

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

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

We saw that $m \gg n_f$ needed to fit training data.
Conservative example: Consider MNIST ($n_f = 28^2$) and use $m = n_f \rightsquigarrow 614,656$ unknowns for a single layer. Famous quote:

> *With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.*

Possible remedies:

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

Some Simple Parametric Models

- Diagonal scaling:

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

  Advantage: preserves size and structure of data.

- Antisymmetric kernel

$$\mathbf{K}(\boldsymbol{\theta}) = \begin{pmatrix} 0 & \boldsymbol{\theta}_1 & \boldsymbol{\theta}_2 \\ -\boldsymbol{\theta}_1 & 0 & \boldsymbol{\theta}_3 \\ -\boldsymbol{\theta}_2 & -\boldsymbol{\theta}_3 & 0 \end{pmatrix}$$

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

- M-matrix

$$\mathbf{K}(\boldsymbol{\theta}) = \begin{pmatrix} \boldsymbol{\theta}_1 + \boldsymbol{\theta}_2 & -\boldsymbol{\theta}_1 & -\boldsymbol{\theta}_2 \\ -\boldsymbol{\theta}_3 & \boldsymbol{\theta}_3 + \boldsymbol{\theta}_4 & -\boldsymbol{\theta}_4 \\ -\boldsymbol{\theta}_5 & -\boldsymbol{\theta}_6 & \boldsymbol{\theta}_5 + \boldsymbol{\theta}_6 \end{pmatrix} \qquad \boldsymbol{\theta} \geq 0$$

  Advantage: like differential operator

Differentiating Parametric Models

Need derivatives of model to optimize $\boldsymbol{\theta}$ in

$$E(\mathbf{W}\sigma(\mathbf{K}(\boldsymbol{\theta})\mathbf{Y} + \mathbf{b}), \mathbf{C})$$

(we can re-use previous derivatives and use chain rule)

Note that all previous models are linear in the following sense

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

Therefore, matrix-vector products with the Jacobian simply are

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

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

Example: Derivative of M-matrix

$$\mathbf{K}(\boldsymbol{\theta}) = \begin{pmatrix} \boldsymbol{\theta}_1 + \boldsymbol{\theta}_2 & -\boldsymbol{\theta}_1 & -\boldsymbol{\theta}_2 \\ -\boldsymbol{\theta}_3 & \boldsymbol{\theta}_3 + \boldsymbol{\theta}_4 & -\boldsymbol{\theta}_4 \\ -\boldsymbol{\theta}_5 & -\boldsymbol{\theta}_6 & \boldsymbol{\theta}_5 + \boldsymbol{\theta}_6 \end{pmatrix} \quad \boldsymbol{\theta} \geq 0$$

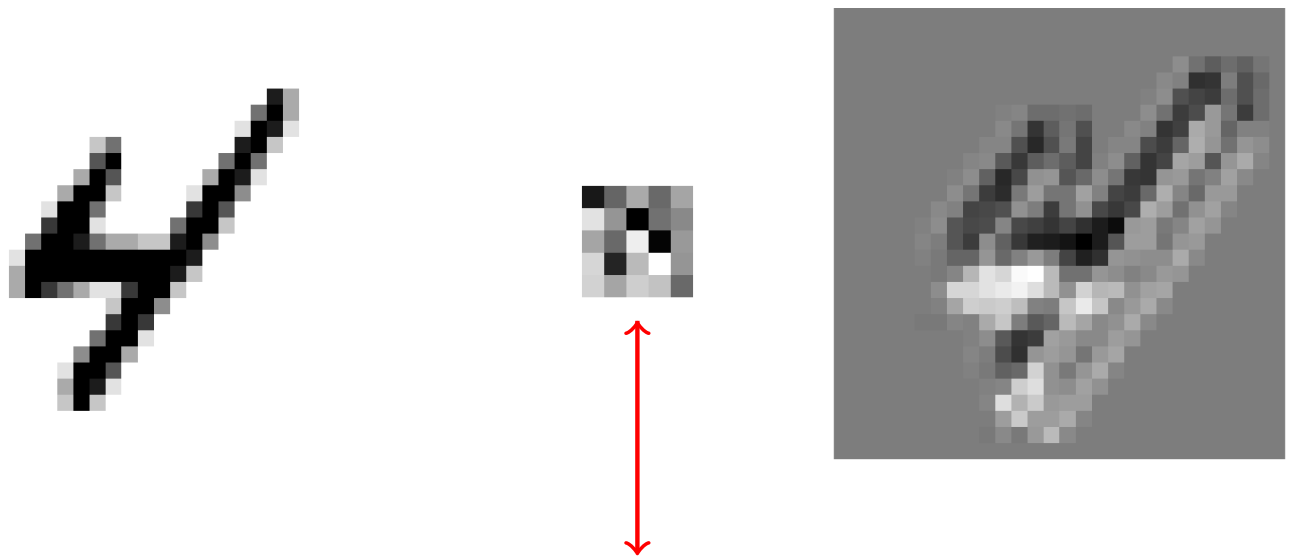
verify that this can be written as $K(\boldsymbol{\theta}) = \mathrm{mat}(\mathbf{Q}\,\boldsymbol{\theta})$ where

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

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

Convolutional Neural Networks [4]

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



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

- useful for speech, images, videos, ...
- efficient parameterization, efficient codes (GPUs, ...)
- later: CNNs as parametric model and PDEs, simple code
- see `E13Conv2D.m`

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).

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

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

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

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

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

- 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 $\mathbf{w}_2 = \mathbf{x}_1$

$$\begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{z}_3 \\ \mathbf{z}_4 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\theta}_2 & \boldsymbol{\theta}_1 & & \boldsymbol{\theta}_3 \\ \boldsymbol{\theta}_3 & \boldsymbol{\theta}_2 & \boldsymbol{\theta}_1 & \\ & \boldsymbol{\theta}_3 & \boldsymbol{\theta}_2 & \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_1 & & \boldsymbol{\theta}_3 & \boldsymbol{\theta}_2 \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix}$$

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

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

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

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

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

Coding: 1D Convolution using FFTs

Let $\boldsymbol{\theta} \in \mathbb{R}^3$ 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

$$\mathbf{J}_{\boldsymbol{\theta}}(\mathbf{K}(\boldsymbol{\theta})\mathbf{Y})\mathbf{v} \quad \text{and} \quad \mathbf{J}_{\boldsymbol{\theta}}(\mathbf{K}(\boldsymbol{\theta})\mathbf{Y})^{\top}\mathbf{w}, \quad (\mathbf{J}_{\boldsymbol{\theta}} \in \mathbb{R}^{m \times p})$$

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

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

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

Need to differentiate eigenvalues w.r.t. $\boldsymbol{\theta}$. Note linearity

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

Derivatives of 1D Convolution - 2

Assume we have

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

Then mat-vecs with Jacobian are easy to compute

$$\mathbf{J}_{\boldsymbol{\theta}}(\mathbf{K}(\boldsymbol{\theta})\mathbf{y})\mathbf{v} = \mathrm{real}(\mathbf{F}^*(\mathrm{diag}(\mathbf{F}\mathbf{y})\mathbf{F}\mathbf{Q}\mathbf{v}))$$

and (note that $\mathbf{F}^\top = \mathbf{F}$ and $(\mathbf{F}^*)^\top = \mathbf{F}^*$)

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

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

Extension 1: Many Examples

Let $n > 1$. In MATLAB must avoid for-loop over examples.

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

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

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

$$\mathbf{J}_{\boldsymbol{\theta}}(\mathbf{K}(\boldsymbol{\theta})\mathbf{Y}) = \mathrm{real}(\mathbf{F}^* \mathrm{diag}(\mathbf{F}\mathbf{Q}v)\mathbf{F}\mathbf{Y})$$

and for the transpose we need to sum over examples

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

Extension 2: 2D Convolution

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

$$\begin{aligned}\mathbf{z}_{21} = &\boldsymbol{\theta}_{33}\mathbf{y}_{13} + \boldsymbol{\theta}_{32}\mathbf{y}_{11} + \boldsymbol{\theta}_{31}\mathbf{y}_{12} \\ &+ \boldsymbol{\theta}_{23}\mathbf{y}_{23} + \boldsymbol{\theta}_{22}\mathbf{y}_{21} + \boldsymbol{\theta}_{21}\mathbf{y}_{22} \\ &+ \boldsymbol{\theta}_{13}\mathbf{y}_{33} + \boldsymbol{\theta}_{12}\mathbf{y}_{31} + \boldsymbol{\theta}_{11}\mathbf{y}_{32}\end{aligned}$$

In matrix form, this gives

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

Extension 2: 2D Convolution using FFTs

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

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

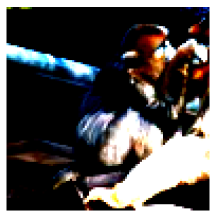
Differences:

- $\mathbf{F}$ and $\mathbf{F}^*$ now refer to 2D Fourier transform and its inverse (`fft2` and `ifft2`), respectively.
- need to find an efficient way to build first column of $\mathbf{K}(\boldsymbol{\theta})$ and encode that using $\mathbf{Q}$.

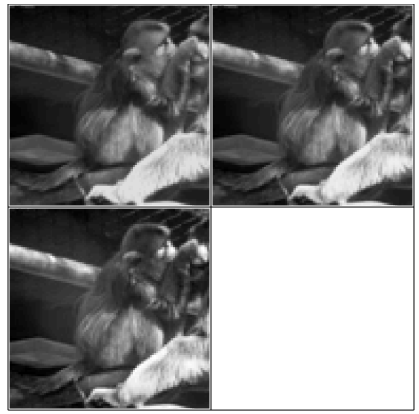
All else stays the same and extends also to higher dimensions (like for videos).
For more details on convolutions and structured matrices see [3]. For FFT-based implementations of CNNs see [5, 6].

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

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

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

Outlook: Possible Extensions

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

- *pooling:* reduce image resolution (e.g. average 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

Why use regularization?

We are attempting to train weights $\mathbf{W} \in \mathbb{R}^{n_c \times n_f}$ to express the relation between some data $\mathbf{Y} \in \mathbb{R}^{n_f \times n}$ and their labels $\mathbf{C} \in \mathbb{R}^{n_c \times n}$ by solving

$$\min_{\mathbf{W}} E(\mathbf{W}) = E(\mathbf{C}, \mathbf{W}, \mathbf{Y})$$

Recall: $\operatorname{rank}(\mathbf{Y}) \leq \min\{n_f, n\}$

- $n < n_f$: No unique solution
- $n > n_f$: $\mathbf{Y}$ may still be rank-deficient

Challenges in image classification:

- data is high dimensional ($n_f \approx$ number of pixels/voxels/frames)
- higher resolution $\rightsquigarrow$ need more examples?
- higher resolution $\rightsquigarrow$ larger rank?

Regularization

If Hessian $\nabla^2 E$ highly ill-conditioned, regularization is needed.

- Symptom: weights are large or oscillatory.
- Alternative: Estimate condition number (costly!)

Solution: require solution to be regular

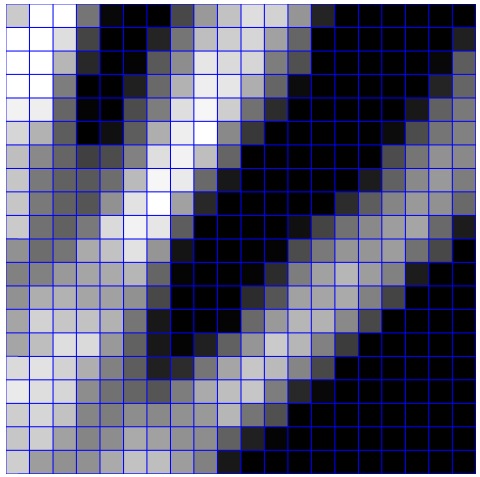
$$\min_{W} \ \phi(\mathbf{W}) = E(\mathbf{W}) + \lambda R(\mathbf{W}),$$

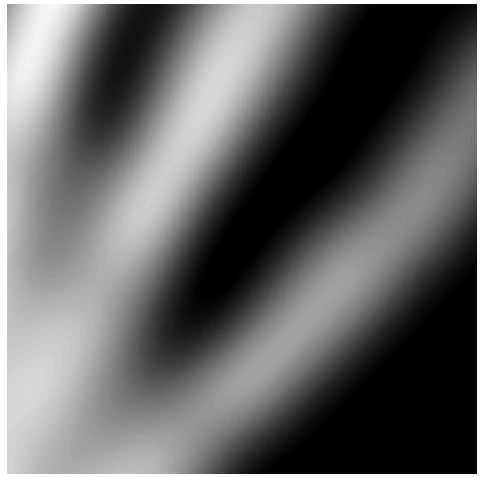
where

- R is a regularizer, $R(\mathbf{W})$ large when $\mathbf{W}$ is irregular and small otherwise
- λ is a regularization parameter (needs to be chosen)
- Mathematically: R makes sure $\mathbf{W}^*$ lies in desired function space (and is sufficiently *regular*).

Excellent references include [1, 2, 7].

What is an Image?





Digital images are arrays $\mathbf{U} = \mathbb{R}^{m_1 \times m_2 \times c}$ ($c = 1 \rightsquigarrow$ grey only).

- perhaps most common interpretation in image processing

Continuous point of view: Images are functions supported on a domain $\Omega \in \mathbb{R}^2$ $u : \Omega \to \mathbb{R}^c$.

- choose function space (e.g., continuous, differentiable)
- discretize on regular grids $\rightsquigarrow$ digital image
- apply operators to images (e.g., gradient in edge detection)

Type of Regularization

Classical Tikhonov (aka weight decay)

$$R(\mathbf{W}) = \frac{1}{2}\|\mathbf{W}\|_F^2$$

requires elements to be small.

When $\mathbf{Y}$ are images, also columns in $\mathbf{W}$ can be seen as images

$$\mathbf{w}^\top \mathbf{y} \approx \int_\Omega w(\boldsymbol{\xi}) y(\boldsymbol{\xi}) d\boldsymbol{\xi}.$$

General Tikhonov: Let $\mathbf{L}$ be a given matrix

$$R(\mathbf{W}) = \frac{1}{2}\|\mathbf{L}\mathbf{W}\|_F^2$$

If $\mathbf{L}$ is discrete derivative operator, entries need to be smooth.

Discretization of ∇^2

Idea: Ensure classifier is smooth by using $\mathbf{L} \approx \nabla^2$.

Finite difference in 1D: Let $\mathbf{u} \in \mathbb{R}^m$ be discretization of $u : [0, 1] \to \mathbb{R}$ on regular grid with pixel size $h = 1/m$

$$\nabla^2 u(x_j) \approx \frac{1}{h^2}(-2\mathbf{u}_j + \mathbf{u}_{j-1} + \mathbf{u}_{j+1}).$$

Code in 1D

```
L1D = @(m,h) 1/h^2 *...
 spdiags(ones(n,1)  * [1  -2  1],-1:1,m,m)
```

Finite difference in 2D: Let $\mathbf{U} \in \mathbb{R}^{m \times m}$ be discretization of $u : [0, 1]^2 \to \mathbb{R}$ on regular grid with pixel size $h = 1/m$

$$\nabla^2 I(x_{ij}) \approx \frac{1}{h^2}(-4\mathbf{I}_{ij} + \mathbf{I}_{i-1j} + \mathbf{I}_{i+1j} + \mathbf{I}_{ij-1} + \mathbf{I}_{ij+1}).$$

Discretization of ∇^2

In 2D $\quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

Use Kroneker products

$$\mathrm{vec}(\mathbf{LUI}) = (\mathbf{I}^\top \otimes \mathbf{L})\mathrm{vec}(\mathbf{U}).$$

Code in 2D

```
L = kron(speye(m2), L1D(m1,h1)) + ...
      kron(L1D(m2,h2),speye(m1) );
```

More about discrete ∇^2

Note that $\mathbf{L}$ can also be written as a convolution

$$\mathbf{L} = \frac{1}{h^2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix} * \mathbf{U}.$$

In general - any differential operator with constant coefficients can be written as convolution and vice versa.

Continuous interpretation allows re-computing a convolution kernel for different image resolutions.

Recap: Numerical Optimization

Require derivatives of the regularization to efficiently solve

$$\min_{\mathbf{W}} \ \phi(\mathbf{W}) = E(\mathbf{W}) + \lambda R(\mathbf{W})$$

Tip for Newton-CG: Use $\nabla^2 R$ as a preconditioner for the conjugate gradient solver in the Newton iteration.

Exercise: Setup smoothness regularizer and test it on MNIST and CIFAR-10

References

[1] P. C. Hansen. *Rank-deficient and discrete ill-posed problems*. SIAM Monographs on Mathematical Modeling and Computation. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1998.

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[3] P. C. Hansen, J. G. Nagy, and D. P. O'Leary. *Deblurring Images: Matrices, Spectra and Filtering*. Matrices, Spectra, and Filtering. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2006.

[4] Y. LeCun, B. E. Boser, and J. S. Denker. Handwritten digit recognition with a back-propagation network. In *Advances in neural information processing systems*, pages 396–404, 1990.

[5] M. Mathieu, M. Henaff, and Y. LeCun. Fast Training of Convolutional Networks through FFTs. *arxiv preprint 1312.5851*, 2013.

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[7] C. R. Vogel. *Computational Methods for Inverse Problems*. SIAM, Philadelphia, 2002.