Optimization Models

EECS 127 / EECS 227AT

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LECTURE 26

Implicit Deep Learning

The Matrix is everywhere. It is all around us.

Morpheus

Outline

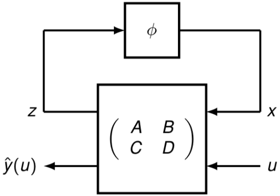
Collaborators

Joint work with:

- Armin Askari, Fangda Gu, Bert Travacca, Alicia Tsai (UC Berkeley);
- Mert Pilanci (Stanford);
- Emmanuel Vallod, Stefano Proto (`www.sumup.ai`).

Sponsors:

Implicit prediction rule



Equilibrium equation:

$$x = \phi(Ax + Bu)$$

Prediction:

$$\hat{y}(u) = Cx + Du$$

- Input $u \in \mathbb{R}^p$, predicted output $\hat{y}(u) \in \mathbb{R}^q$, hidden "state" vector $x \in \mathbb{R}^n$.
- Model parameter matrix:

$$M = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right).$$

- Activation: vector map $\phi : \mathbb{R}^n \to \mathbb{R}^n$, *e.g.* the ReLU: $\phi(\cdot) = \max(\cdot, 0)$ (acting componentwise on vectors).

Deep neural nets as implicit models

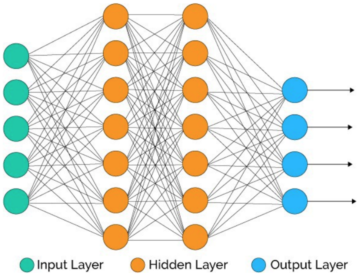


Figure: A neural network.

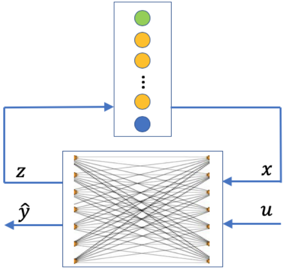


Figure: An implicit model.

Implicit models are more general: they allow loops in the network graph.

Example

Fully connected, feedforward neural network:

$$\hat{y}(u) = W_L x_L, \quad x_{l+1} = \phi_l(W_l x_l), \quad l = 1, \ldots, L-1, \quad x_0 = u.$$

Implicit model:

$$\left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right) = \left(\begin{array}{cccc|c} 0 & W_{L-1} & \ldots & 0 & 0 \\ & 0 & \ddots & \vdots & \vdots \\ & & \ddots & W_1 & 0 \\ & & & 0 & W_0 \\ \hline W_L & 0 & \ldots & 0 & 0 \end{array}\right), \quad \begin{array}{c} x = \\ \begin{pmatrix} x_L \\ \vdots \\ x_1 \end{pmatrix} \end{array}, \quad \begin{array}{c} \phi(z) = \\ \begin{pmatrix} \phi_L(z_L) \\ \vdots \\ \phi_1(z_1) \end{pmatrix} \end{array}.$$

The equilibrium equation $x = \phi(Ax + Bu)$ is easily solved via backward substitution (forward pass).

Example: ResNet20

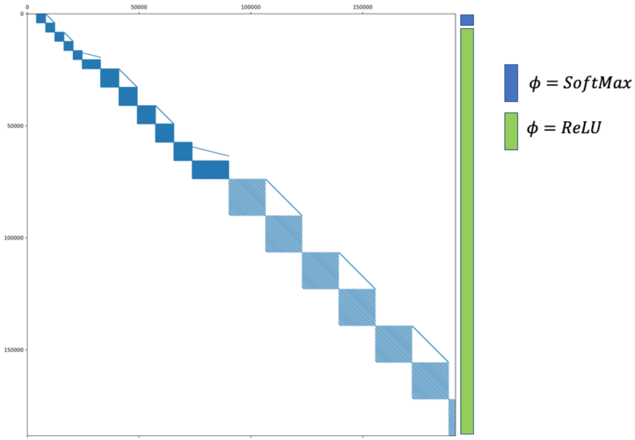


Figure: The A matrix for ResNet20.

- 20-layer network, implicit model of order $n \sim 180000$.
- Convolutional layers have blocks with Toeplitz structure.
- Residual connections appear as lines.

Neural networks as implicit models

Framework covers most neural network architectures:

- Neural nets have strictly upper triangular matrix A.
- Equilibrium equation solved by substitution, *i.e.* "forward pass".
- State vector x contains all the hidden features.
- Activation ϕ can be different for each component or blocks of x.
- Covers CNNs, RNNs, recurrent neural networks, (Bi-)LSTM, attention, transformers, etc.

Related concept: state-space models

The so-called "state-space" models for dynamical systems use the same idea to represent high-order differential equations . . .

Linear, time-invariant (LTI) dynamical system:

$$\dot{x} = Ax + Bu, \quad y = Cx + Du$$

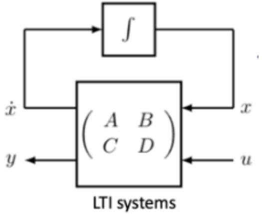


Figure: LTI system

Well-posedness

The matrix $A \in \mathbb{R}^{n \times n}$ is said to be well-posed for ϕ if, for every $b \in \mathbb{R}^n$, a solution $x \in \mathbb{R}^n$ to the equation

$$x = \phi(Ax + b),$$

exists, and it is unique.

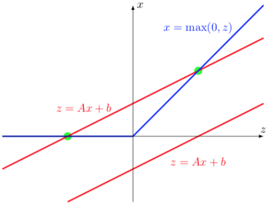


Figure: Equation has two or no solutions, depending on $\mathrm{sgn}(b)$.

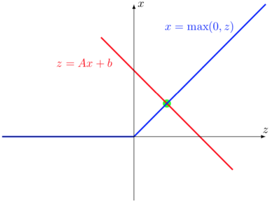


Figure: Solution is unique for every b.

Perron-Frobenius theory [1]

A square matrix P with non-negative entries admits a real eigenvalue λ with a non-negative eigenvector $v \neq 0$:

$$Pv = \lambda v.$$

The value λ dominates all the other eigenvalues: for any other (complex) eigenvalue $\mu \in \mathbf{C}$, we have $|\mu| \leq \lambda_{\mathrm{PF}}$.

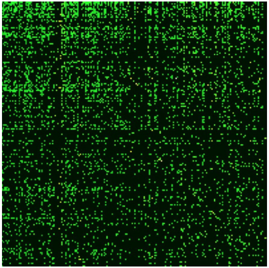


Figure: A web link matrix.

Google's Page rank search engine relies on computing the Perron-Frobenius eigenvector of the web link matrix.

PF Sufficient condition for well-posedness

Fact: Assume that ϕ is componentwise non-expansive (*e.g.*, $\phi =$ ReLU):

$$\forall\, u, v \in \mathbb{R}^n \;:\; |\phi(u) - \phi(v)| \leq |u - v|.$$

Then the matrix A is well-posed for ϕ if the non-negative matrix $|A|$ satisfies

$$\lambda_{pf}(|A|) < 1,$$

in which case the solution can be found via the fixed-point iterations:

$$x(t+1) = \phi(Ax(t) + b), \quad t = 0, 1, 2, \ldots$$

Covers neural networks: since then $|A|$ is strictly upper triangular, thus $\lambda_{pf}(|A|) = 0$.

Proof: existence

We have

$$|x(t+1) - x(t)| = |\phi(Ax(t)+b) - \phi(Ax(t-1)+b)| \leq |A||x(t) - x(t-1)|,$$

which implies that for every $t, h \geq 0$:

$$|x(t+\tau) - x(t)| \leq \sum_{k=t}^{t+\tau} |A|^k |x(1) - x(0)| \leq |A|^t \sum_{k=0}^{\tau} |A|^k |x(1) - x(0)| \leq |A|^t w,$$

where

$$w := \sum_{k=0}^{+\infty} |A|^k |x(1) - x(0)| = (I - |A|)^{-1} |x(1) - x(0)|,$$

since, due to $\lambda_{\mathrm{PF}}(|A|) < 1$, $I - |A|$ is invertible, and the series above converges.

Since $\lim_{t \to 0} |A|^t = 0$, we obtain that $x(t)$ is a Cauchy sequence, hence it has a limit point, x_∞. By continuity of ϕ we further obtain that $x_\infty = \phi(Ax_\infty + b)$, which establishes the existence of a solution.

Proof: unicity

To prove unicity, consider $x^1, x^2 \in \mathbb{R}^n_+$ two solutions to the equation. Using the hypotheses in the theorem, we have, for any $k \geq 1$:

$$|x^1 - x^2| \leq |A||x^1 - x^2| \leq |A|^k|x^1 - x^2|.$$

The fact that $|A|^k \to 0$ as $k \to +\infty$ then establishes unicity.

Norm condition

More conservative condition: $\|A\|_\infty < 1$, where

$$\lambda_{\mathrm{PF}}(|A|) \leq \|A\|_\infty := \max_i \sum_j |A_{ij}|.$$

Under previous PF conditions for well-posedness:

- we can always rescale the model so that $\|A\|_\infty < 1$, without altering the prediction rule;
- scaling related to PF eigenvector of $|A|$.

Hence during training we may simply use norm condition.

Composing implicit models

Cascade connection

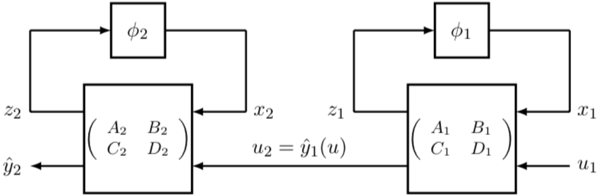


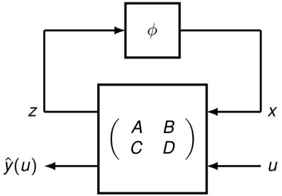
Figure: A cascade connection.

Class of implicit models closed under the following connections:

- Cascade
- Parallel and sum
- Multiplicative
- Feedback

Robustness analysis

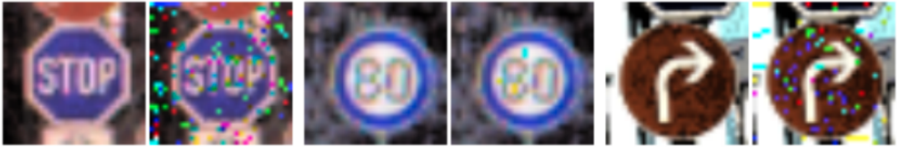
Goal: analyze the impact of input perturbations on the state and outputs.



Motivations:

- Diagnose a given (implicit) model.
- Generate adversarial attacks.
- Defense: modify the training problem so as to improve robustness properties.

Why does it matter?



stop	30m speed limit	80m speed limit	30m speed limit	go right	go straight

Changing a few carefully chosen pixels in a test image can cause a classifier to mis-categorize the image (Kwiatkowska *et al.*, 2019).

Robustness analysis

Input is unknown-but-bounded: $u \in \mathcal{U}$, with

$$\mathcal{U} := \left\{ u^0 + \delta \in \mathbb{R}^p \;:\; |\delta| \le \sigma_u \right\},$$

- $u^0 \in \mathbb{R}^n$ is a "nominal" input;
- $\sigma_u \in \mathbb{R}^n_+$ is a measure of componentwise uncertainty around it.

Assume (sufficient condition for) well-posedness:

- ϕ componentwise non-expansive;
- $\lambda_{\mathrm{PF}}(|A|) < 1$.

Nominal prediction:

$$x^0 = \phi(Ax^0 + Bu^0), \;\; \hat{y}(u^0) = Cx^0 + Du^0.$$

Component-wise bounds on the state and output

Fact: If $\lambda_{\mathrm{PF}}(|A|) < 1$, then $I - |A|$ is invertible, and

$$|\hat{y}(u) - \hat{y}(u^0)| \leq S|u - u^0|,$$

where

$$S := |C|(I - |A|)^{-1}|B| + |D|$$

is a "sensitivity matrix" of the implicit model.

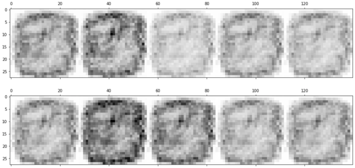
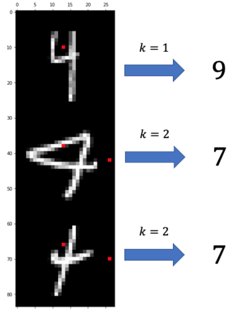


Figure: Sensitivity matrix of a classification network with 10 outputs (each image is a row).

Generate a sparse attack on a targeted output

Attack method:

- select the output to attack based on the rows (class) of sensitivity matrix;
- select top k entries in chosen row;
- randomly alter corresponding pixels.



Changing $k = 1$ (top) $k = 2$ (mid, bot) pixels, images are wrongly classified, and accuracy decreases from 99% to 74%.

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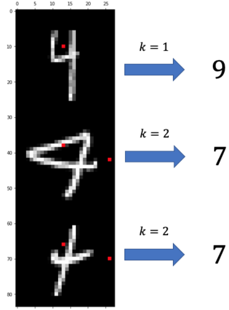


Changing $k = 1$ (top) $k = 2$ (mid, bot) pixels, images are wrongly classified, and accuracy decreases from 99% to 74%.

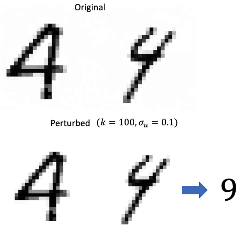
Generate a sparse bounded attack on a targeted output

Target a specific output with sparse attacks:

$$\mathcal{U} := \left\{ u^0 + \delta \in \mathbb{R}^p \ : \ |\delta| \leq \sigma_u, \ \ \textbf{Card}(\delta) \leq k \right\},$$

With $k \leq n$. Solve a linear program, with c related to chosen target:

$$\max_{x,\, u} \ c^\top x \ : \quad \begin{array}{l} x \geq Ax + Bu, \ \ x \geq 0, \ \ |x - x^0| \leq \sigma_x, \ \ |u - u^0| \leq \sigma_u \\ \|\mathrm{diag}\,(()\, \sigma_u)^{-1}(u - u^0)\|_1 \leq k. \end{array}$$



Changing $k = 100$ pixels by a tiny amount ($\sigma_u = 0.1$), targe images are wrongly classified a network with 99% nominal accuracy.

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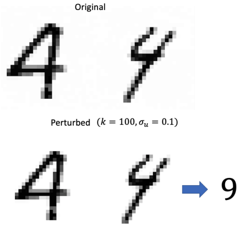

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Training problem

Setup

- Inputs: $U = [u_1, \ldots, u_m]$, with m data points $u_i \in \mathbb{R}^p$, $i \in [m]$.
- Outputs: $Y = [y_1, \ldots, y_m]$, with m responses $y_i \in \mathbb{R}^q$, $i \in [m]$.

Predictions: with $X = [x_1, \ldots, x_m] \in \mathbb{R}^{n \times m}$ the matrix of hidden feature vectors, and ϕ acting columnwise,

$$\hat{Y} = CX + DU, \quad X = \phi(AX + BU).$$

Training problem

Constrained problem

$$\begin{aligned}\min_{X,A,B,C,D} \quad & \mathcal{L}(Y,\hat{Y}) + \pi(A,B,C,D) \\ \text{s.t.} \quad & \hat{Y} = CX + DU, \;\; X = \phi(AX + BU), \;\; \|A\|_\infty \le \kappa.\end{aligned}$$

- Constraint on A with $\kappa < 1$ ensures well-posedness.
- $\pi(\cdot)$ is a (convex) penalty, *e.g.* one that encourages robustness:

$$\pi(A,B,C,D) \propto \frac{1}{2}\frac{\|B\|_\infty^2 + \|C\|_\infty^2}{1 - \|A\|_\infty} + \|D\|_\infty.$$

- May also incorporate penalties to encourage sparsity, low-rank, etc., *e.g.*:

$$\sum_{i\in[p]} \|Be_i\|_\infty$$

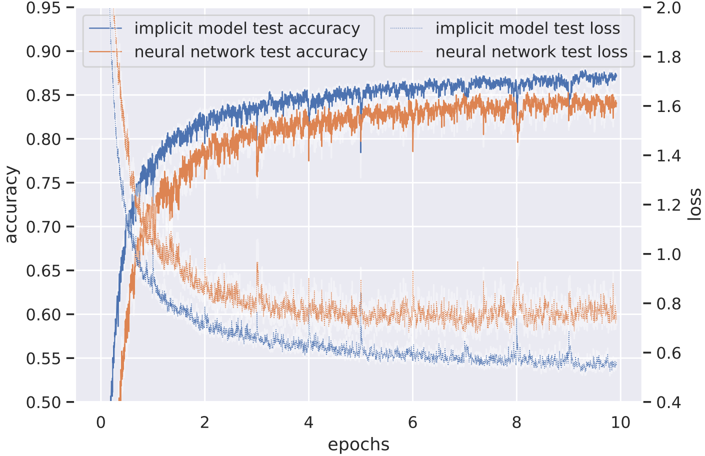
encourages entire columns of B to be zero, for feature selection.

Projected (sub) gradient

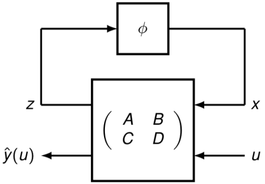
SGD can be adapted to the problem:

- Differentiating through the equilibrium equation is possible.
- Need to deal with the constraint of well-posedness via projection.
- Projection on constraint $\|A\|_\infty \leq \kappa$ can be done extremely fast using (vectorized) bisection, solving for each row of A in parallel.
- Can extend to Frank-Wolfe methods, which are suited to seeking sparse models.

Example: traffic sign data set

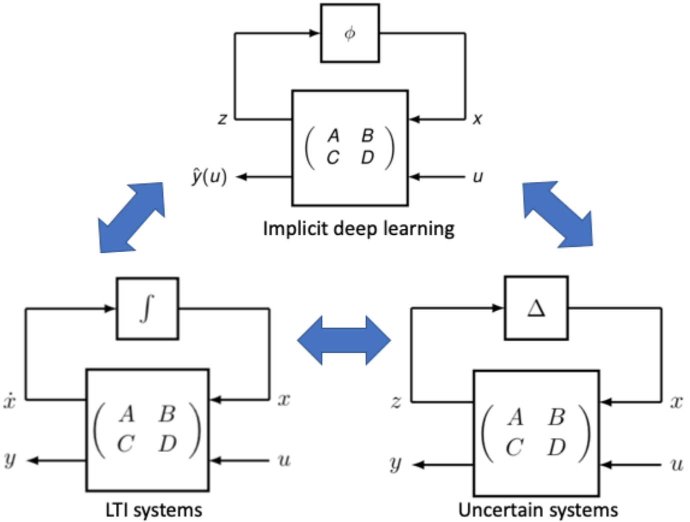


Take-aways



- Implicit models are more general than standard neural networks.
- Well-posedness is a key property that can be enforced via norm or eigenvalue conditions.
- Models can be composed together in modular fashion.
- The notationally very simple framework allows for rigorous analyses for robustness, model compression, architecture optimization, etc.
- The corresponding training problem is amenable to SGD methods.

Towards a general theory?



References

Stephen Boyd.
Perron-Frobenius theory, 2008.
Lecture slides for EE 363, Stanford University.

Geir E Dullerud and Fernando Paganini.
A course in robust control theory: a convex approach, volume 36.
Springer Science & Business Media, 2013.

L. El Ghaoui, F. Gu, B. Travacca, A. Askari, and A. Tsai.
Implicit deep learning.
Submitted to ICML, preliminary version at https://arxiv.org/abs/1908.06315, February 2020.