ECE209AS (Winter 2021)

Lecture 5: Learning with Irregularly Sampled Time Series Data

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Regularly and Irregularly Sampled Time Series





Multivariate irregularly sampled (unaligned)



 Availability of sensors energy, mobility, multi-tenancy, human operator



- Availability of sensors energy, mobility, multi-tenancy, human operator
- Samples are lost or dropped network outage, bit corruption



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- Sensors report asynchronous events ▶ e.g. motion sensors, event-oriented imagers



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- Sensors sampling intervals are adapted state of the process being sampled (e.g. patient's health)



Sampling Adaptively



- when the position of the motor changes sufficiently? sample more frequently if position changes more rapidly
- This sampling policy is called *Lebesgue* Sampling

Idea: Instead of sampling periodically as is traditionally done, could we sample only

Riemann Sampling vs. Lebesgue Sampling



From:Roy McCann, Anil Kumar Gunda, Suchit Reddy Damugatla, "Improved Operation of Networked Control Systems using Lebesgue Sampling"





Riemann Sampling vs. Lebesgue Sampling



From:Roy McCann, Ap Operation of Netw





Event-Triggered Control System



- Introduce an Event Controller that monitors the Position Encoder signal continuously and determines the optimal sampling time
- x(t) is the continuous-time analog position encoder signal
- $x[t_k]$ is the last sample produced by the ADC



Event-Triggered Control System



- if the Event Controller produces a sampling trigger whenever: $||x(t) - x[t_k]|| > \sigma ||x(t)||$
 - $\bullet \sigma$ is a design parameter that trades off average sampling rate and performance
 - Intuition: Lebesgue interval must be the "error" relative to size of signal

• Theorem [Anta-Tabuada]: Sampling is optimal and the system is guaranteed stability



- Event Controller needs to check the inequality at ALL times. Can one do better?
- Motor controller is designed with a model of the motor in mind
- Given the current state of the motor and the command input, control theory provides an estimate of the next state
- One can extend this estimation to predict when the state of the motor will violate the sampling inequality
- Thus, one can predict when the sample should be taken and schedule the ADC

- No continuous time check needed
- However, this does not work well when the model has uncertainties or when perturbations to the system cannot be bounded

 $CurrentMeasurement + SystemDynamics \Rightarrow NextSampleTime$





 $t_{k+1} = \alpha(\lambda, x[t_k])$







 $(t_{k+1}) = \alpha(\lambda, x[t_k])$































time























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- Sensors report asynchronous events • e.g. motion sensors, event-oriented imagers
- Sensors sampling intervals are adapted state of the process being sampled (e.g. patient's health)
- Compressive sampling of sensors

Sampling a Signal



Steve Brunton, "Shannon Nyquist Sampling Theorem" <u>https://www.youtube.com/watch?v=FcXZ28BX-xE&t=449s</u>



Sampling a Signal

- Shannon-Nyquist Sampling Theorem:
 - ► To resolve all frequencies in a function, it must be sampled at twice the highest frequency present
 - A function containing no frequency > ω Hz is completely

determined by sampling at 2ω Hz (Nyquist Rate) $\Delta t =$

• Aliasing if we sample at a rate lower than 2ω

 2ω



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- Aliasing if we sample at a rate lower than 2ω
- Beating Shannon-Nyquist Sampling Theorem
 - Advances in applied mathematics, statistics, and optimization have changed how we thinks about sampling
 - Technically, the Shannon-Nyquist Sampling Theorem is necessary only signals that are broadband, i.e. densely packed with energy in all the frequencies from 0 to ω
 - But if the signal is sparse in frequency domain, one can beat the 2ω sampling rate requirement

 2ω



Steve Brunton, https://www.youtube.com/watch?v=hmBTACBGWJs





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Real world signals are sparse in Fourier domain (or some other such universal domain, such as Wavelet)

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Real world signals are sparse in Fourier domain (or some other such universal domain, such as Wavelet)



Fourier basis $X = \Psi S$ Sparse



If we throw away most of the information during compression, why do we collect it to begin with? Can we not just starts with a massively downsampled signal?



Steve Brunton, https://www.youtube.com/watch?v=hmBTACBGWJs



If we throw away most of the information during compression, why do we collect it to begin with? Can we not just starts with a massively downsampled signal?



Inferring s from y



Steve Brunton, https://www.youtube.com/watch?v=hmBTACBGWJs



$y = Cx = C\Psi s = \Theta s$

Undetermined Inverse Problem Solution for s given y and Θ is not unique.

Adding the Sparsity Requirement to Infer s







 $y = Cx = C\Psi s = \Theta s$ $\hat{\mathbf{s}} = \operatorname{argmin}_{\mathbf{s}'} ||\mathbf{C}\Psi\mathbf{s}' - \mathbf{y}||_2 + \lambda ||\mathbf{s}'||_0$ alternatively: $\hat{s} = \operatorname{argmin}_{s'} ||s'||_0$, s.t. $||C\Psi s' - y||_2 < \epsilon_{17}$



Adding the Sparsity Requirement to Infer s







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Adding the Sparsity Requirement to Infer s





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A Big Applied Math Breakthrough to the Rescue (~ 2004-2005 @ CalTech, Rice, UCLA)

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Computationally Intractable



alternatively:

 $\hat{\mathbf{s}} = \operatorname{argmin}_{s'} ||\mathbf{s}'||_1$, s.t. $||\mathbf{C}\Psi\mathbf{s}' - \mathbf{y}||_2 < \epsilon$

Computationally Efficient (Convex Optimization)

Gives the exact solution for s with probability close to 1 if **certain conditions** are satisfied





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Computationally Intractable

C should be incoherent w.r.t. Ψ (i.e. rows of C should not be too parallel to columns of Ψ)
of measurements p ~ O(klog(n/k)) where k = ||s||₀ and n = |s| = |x|



alternatively:

 $\hat{\mathbf{s}} = \operatorname{argmin}_{s'} ||\mathbf{s}'||_1$, s.t. $||\mathbf{C}\Psi\mathbf{s}' - \mathbf{y}||_2 < \epsilon$

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Computationally Intractable

- C should be incoherent w.r.t. Ψ (i.e. rows of C should not be too parallel to columns of Ψ)
 - # of measurements $p \sim O(k \log(n/k))$ where $k = ||\mathbf{s}||_0$ and $n = |\mathbf{s}| = |\mathbf{x}|$

Restricted Isometry Property (RIP) i.e. $C\Psi$ acts like a unitary matrix on sparse vector s



alternatively:

 $\hat{\mathbf{s}} = \operatorname{argmin}_{s'} ||\mathbf{s}'||_1$, s.t. $||\mathbf{C}\Psi\mathbf{s}' - \mathbf{y}||_2 < \epsilon$

Computationally Efficient (Convex Optimization)

Gives the exact solution for s with probability close to 1 if **certain conditions** are satisfied





Example of Bad Measurement Matrix C

С

Θ

C has rows that are the same as a subset of columns of Ψ

Only picks up information only from a part of s

Steve Brunton, https://www.youtube.com/watch?v=hmBTACBGWJs



Measurement Matrix C in Practice

- Random 0-1 mask matrix: each element in y is a random sample picked from x rows of C have exactly one 1 to indicate the sample picked by that measurement • must be causal in case of real-time sampling of a time-series



commonly used: Gaussian, Bernoulli



Steve Brunton, https://www.youtube.com/watch?v=hmBTACBGWJs

• Random real-numbers: each element in y is an incoherent random projection of x

Causal Random Sampling of a Time Series



Signal to be acquired

Causal Random Sampling of a Time Series



Signal to be acquired

100 x 100 identity matrix with 75 rows uniformly randomly selected and thrown out

Causal Random Sampling of a Time Series



Signal to be acquired

100 x 100 identity matrix with 75 rows uniformly randomly selected and thrown out

> Measurements actually acquired

Taking Incoherent Projections of a Time Series - Gaussian



Signal to be acquired

Taking Incoherent Projections of a Time Series - Gaussian





25 x 100 matrix of Gaussian $\mathcal{N}(0, \frac{1}{n})$ **distributed random numbers**

Taking Incoherent Projections of a Time Series - Gaussian





25 x 100 matrix of Gaussian $\mathcal{N}(0, \frac{1}{n})$ **distributed random numbers**

> Measurements actually acquired

Taking Incoherent Projections of a Time Series - Bernoulli



Signal to be acquired



Taking Incoherent Projections of a Time Series - Bernoulli





25 x 100 Bernoulli distributed (p = 0.5**)** random numbers $\in \{-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}\}$





Taking Incoherent Projections of a Time Series - Bernoulli





25 x 100 Bernoulli distributed (p = 0.5**)** random numbers $\in \{-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}\}$

> **Measurements** actually acquired





Compressed Sensing Example







Compressive Sampling to Save Energy on Edge Devices



- In compressive sampling, the highest cost is random number generation
- To maximize benefit, may also need to duty cycle analog circuitry



Learning from Irregularly Sampled Time Series

Irregularly Sampled Time Series Data



 Present fundamental challenges to many classical models from machine learning and statistics

Consider supervised learning task where a model takes as input an irregularly sampled time series and must predict a scalar output

• Training set \mathscr{D} with samples (\mathbf{s}_i, y_i) where \mathbf{s}_i 's are irregularly

samples time series, and y_i 's are corresponding labels

• Problems:

Variable gaps between successive observation time points Variable number of observations: the total # of observations across dimensions can vary across samples Lack of alignment: Different dimensions of a single multivariate time series can be observed at a different collection of time points. The collection of observation times across dimensions can also differ between samples.







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Data Representations for Irregularly Sampled Time Series

- There are several possible data representime series.
- These representations are equivalent, b different approaches to modeling



There are several possible data representations for multivariate irregularly sampled

These representations are equivalent, but expose different properties and suggest

Series-based Representation

A *D*-dimensional multivariate irregularly sampled time series $\mathbf{s} = [\mathbf{s}_1, \dots, \mathbf{s}_D]$ is represented as a collection of univariate irregularly sampled time series, one per dimension.

- $\mathbf{s}_d = (\mathbf{t}_d, \mathbf{x}_d)$ indicates the time series for dimension *d*.
- \mathbf{t}_d indicates the collection of time points with observed values for dimension d.
- \mathbf{x}_d indicates the corresponding collection of observed values.



Data Representations for Irregularly Sampled Time Series

- time series.
- different approaches to modeling

Vector-based Representation



There are several possible data representations for multivariate irregularly sampled

These representations are equivalent, but expose different properties and suggest

In this representation, there is a single collection of time points **t**. At each time point t_i , there is a *D*-dimensional vector-valued observation \mathbf{x}_i .

In the general case, not all dimensions of \mathbf{x}_i are observed, leading to the need to explicitly represent which dimensions are observed and which are missing.

A *D*-dimensional binary response indicator vector \mathbf{r}_i at each time point t_i indicates which dimensions are observed and which are missing.





Data Representations for Irregularly Sampled Time Series

- time series.
- different approaches to modeling

Set-based Representation



There are several possible data representations for multivariate irregularly sampled

These representations are equivalent, but expose different properties and suggest

In this representation, a *D*-dimensional multivariate irregularly sampled time series is represented as a set of (*time*, *dimension*, *value*) tuples, one for each observation.





Inference Tasks

- **Detection:** Inferring prediction target values $\mathbf{y}[t_*]$ at time t_* conditioning on the observations $s[: t_*]$ available up to and including time t_* .
- **Prediction:** Inferring prediction target values $\mathbf{y}[t_* + \delta]$ at time $t_* + \delta$ (for $\delta > 0$) conditioning on the observations $\mathbf{s}[: t_*]$ available up to and including time t_*
- Forecasting: Inferring $\mathbf{x}[t_* + \delta]$ (for $\delta > 0$) by conditioning on the observations $\mathbf{s}[:t_*]$ up to an including time t_* .
- Filtering: Inferring missing variables $\mathbf{x}^m[t_*]$ at time t_* by conditioning on the observations $s[: t_*]$ up to an including time t_* .
- **Smoothing:** Inferring the values of $\mathbf{x}^m[t_*]$ at time t_* using the observed data in **S**.
- Interpolation: Inferring the values of $\mathbf{x}[t_*]$ at time t_* using the observed data in **S**.

y(t)

 $x_1(t)$

 $x_2(t)$

x₁(t)

 $x_2(t)$



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Modeling Primitives for Irregularly Sampled Time Series





Discretization





- Reduces to a regularly sampled multivariate time series with missing values vector-based representation with missing data indicator
- Approach: divide the time axis into equal sized non-overlapping intervals and define a value within each time interval based on the observed values falling within that interval ▶ e.g. average or median

Regularly sampled with missing values



Interpolation



- Approach:
 - 1. Define a set of K reference time points $\tau = [\tau_1, ..., \tau_K]$
 - 2. Use a a basic kernel smoother to produce interpolated values at the reference time points

 - deterministic: e.g., squared exponential kernel, stochastic: e.g., Gaussian process regression

- kernel typically puts higher weights (learnable parameters) to points that are closer to the reference points - for multivariate case, can account for both correlation in time and correlation across different dimensions



- Applies multiple semi-parametric interpolation schemes to obtain a regularly-sampled time series representation with samples at a set of reference time points The parameters of the interpolation network are trained with the classifier in an end-to-end setup
- Prediction Network can be any standard supervised neural network architecture such as fully-connected feedforward, convolutional, or recurrent network.





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capture where observations occur





Output of Interpolation Network





Recurrence



 Use a RNN cell with the ability to explicitly represent time to integrate the input at each time point with the latent state from the previous time point

• e.g. append the time points or inter-observation intervals to the vector-valued observations $[\mathbf{x}_{in}, t_{in}]$ or $[\mathbf{x}_{in}, t_{in} - t_{i-1n}]$

$$\mathbf{h}_i = f_{ heta}(\mathbf{h}_{i-1}, \mathbf{z}_{in})$$
 $\hat{\mathbf{y}}_{in} = q_{\phi}(\mathbf{h}_i)$

Recent work on ordinary differential equation (ODE) models in ML provides an alternative recurrence-based solution
In these ODE-RNN models, ODEs are used to evolve the hidden state between continuous time observations.

 Better properties than traditional RNNs in terms of their ability to accommodate irregularly sampled data.

$$\begin{aligned} \mathbf{h}'_i &= \text{ODESolve}(g_{\gamma}, \mathbf{h}_{i-1}, (t_{i-1n}, t_{in})) \\ \mathbf{h}_i &= f_{\theta}(\mathbf{h}'_i, \mathbf{x}_{in}) \end{aligned}$$



Attention



 Self-Attention module learns which regions of an input time series to attend to when computing outputs at different points in time by leveraging positional or time encodings.

$$\operatorname{Attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \operatorname{softmax}\left(\frac{\mathbf{Q} \mathbf{K}^T}{\sqrt{C}}\right) \mathbf{V}$$

 There is no recurrent structure, which allows parallel processing go the entire time series instead of sequentially as in RNN

• Time values can be converted into a vector representation using positional encoding and concatenated with the observation value (as in RNN)

Missing values in vector-valued observations are also problematic for attention-based modules, which (like standard RNNs) expect fully observed vectors as input imputation solutions can be used





Structural Invariance



Multivariate irregularly sampled (unaligned)

- function and then pools over the output of all such tuples
 - of pooling through one additional set of encoding layers g_{φ} to produce the final representation

$$\mathbf{h} = g_{\varphi}(\mathsf{pool}(f_{\theta}(t_{in}, d_{in}, t_{in})))$$

Inspired by the set-based view of a multivariate irregularly sampled time series $\mathbf{s}_n = (t_{in}, d_{in}, \mathbf{x}_{in}) \mid 1 \le i \le L_n$

• Set-based neural network approach processes individual (time, value, dimension) tuples via an encoding

• such approaches (i) produce an encoding of an input irregularly sampled time series by applying an initial encoder f_{θ} to individual time-dimension-value tuples, (ii) then perform a pooling operation (e.g. max, mean and sum) over all initial encodings in a way that is completely invariant to the temporal structure of the data, and (iii) map the output

 \mathbf{x}_{in}) $| 1 \leq i \leq L_n$)









Example Approach: Set Functions for Time Series (SeFT)



Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series

Challenge

Imputation requires solving the harder problem of learning the time series dynamics, and also sacrifices interpretability of the inference.

Problem Statement

Can we learn classification models on irregularlysampled time series without prior imputation?

Set Functions for Time Series Time series classification as set classification

> (based on recent advances in differentiable set function learning)



SeFT Architecture Overview



Irregularly Sampled Multivariate Time Series

Set Encoding

Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series

Embedding, Attention, and Aggregation

Classification


Key Idea in SeFT: Time Series as Set of Observations



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Background: Deep Sets Framework (Zaheer et. al., NeurIPS 2017)

- Neural network architectures that operate over sets • encountered in many applications: compute statistics over sets (e.g. sum of digits in a set of images), classify sets (e.g. LIDAR or RADAR point cloud classification)
- Key requirement:

 - permutation equivariance of the task is $f: \mathcal{X}^M \to \mathcal{Y}^M$ (i.e. transduction)
- Key Results

form $\rho(\sum_{x \in X} \phi(x))$, for suitable transformations ϕ and ρ .

 $\mathbf{f}_{\Theta}(\mathbf{x}) = \boldsymbol{\sigma}(\Theta \mathbf{x})$ is restricted to standard neural network layer **Lemma 3** The function $\mathbf{f}_{\Theta} : \mathbb{R}^M \to \mathbb{R}^M$ defined above is permutation equivariant iff all the offdiagonal elements of Θ are tied together and all the diagonal elements are equal as well. That is, $\Theta = \lambda \mathbf{I} + \gamma (\mathbf{1}\mathbf{1}^{\mathsf{T}}) \qquad \lambda, \gamma \in \mathbb{R} \quad \mathbf{1} = [1, \dots, 1]^{\mathsf{T}} \in \mathbb{R}^{M} \qquad \mathbf{I} \in \mathbb{R}^{M \times M}$ is the identity matrix

• permutation invariance if the task is $f: 2^{\mathscr{X}} \to \mathscr{Y}$ (i.e. regression or classification)

Theorem 2 A function f(X) operating on a set X having elements from a countable universe, is a valid set function, i.e., invariant to the permutation of instances in X, iff it can be decomposed in the





Background: Architecture of DeepSets Invariant Model



Zaheer, Manzil, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Ruslan Salakhutdinov, and Alexander Smola. "Deep sets." arXiv preprint arXiv:1703.06114 (2017). https://arxiv.org/pdf/1703.06114



Background: Architecture of DeepSets Equivariant Model



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Background: Architecture of DeepSets Equivariant Model



Using multiple permutation equivariant layers. (Since permutation equivariance compose we can stack multiple such layers.)

Zaheer, Manzil, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Ruslan Salakhutdinov, and Alexander Smola. "Deep sets." arXiv preprint arXiv:1703.06114 (2017). https://arxiv.org/pdf/1703.06114





Applying Deep Sets to SeFT

Sum-decompose the set function to achieve permutation invariance

 $f(\mathcal{S}) = g$

where $h: \Omega \to \mathbb{R}^d$ and $g: \mathbb{R}^d \to \mathbb{R}^c$ are neural networks

Problem Influence of an element shrinks as |S| grows!

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$$\left(\frac{1}{|S|}\sum_{s_j\in S}h(s_j)\right)$$

Time Encoding in SeFT

- Employs a variant of *positional encoding* seen earlier with transformer
- varying frequencies
- $x \in \mathbb{R}^{\tau}$, where

$$\begin{aligned} x_{2k}(t) &:= \sin\left(\frac{t}{\mathfrak{t}^{2k/\tau}}\right) \\ z_{2k+1}(t) &:= \cos\left(\frac{t}{\mathfrak{t}^{2k/\tau}}\right) \qquad \qquad k \in \{0, \dots, \tau/2\} \end{aligned}$$

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• The time encoding converts the 1-dimensional time axis into a multi-dimensional input by passing the time t of each observation through multiple trigonometric functions of

• Given a dimensionality $\tau \in \mathbb{N}^+$ of the time encoding, SeFT encodes the position as

Attention-based Aggregation



 $\mathcal{L}(\theta, \psi) =$

Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series

Keys:
$$K_{j,i} = [f(S), s_j]^T W_i$$

Queries: $Q \in \mathbb{R}^{m \times d}$
Preattentions: $e_{j,i} = \frac{K_{j,i} \cdot Q_i}{\sqrt{d}}$
Attentions: $a_{j,i} = \frac{\exp(e_{j,i})}{\sum_j \exp(e_{j,i})}$
Values: $V_i = \sum_j a_{j,i}h_{\theta}(s_j)$
 $= \mathbb{E}_{(S,y)\in\mathcal{D}} \left[\ell \left(y; g_{\psi} \left(\sum_{s_j \in S} a(S, s_j)h_{\theta}(s_j) \right) \right) \right]$



SeFT Evaluation

| Dataset | Model | Accuracy | AUPRC | AUROC | s/epoch |
|---------|-------------------------|----------------------------------|----------------------------------|----------------------------------|-----------------------------------|
| МЗМ | GRU-D | 77.0 ± 1.5 | $\textbf{52.0} \pm \textbf{0.8}$ | $\textbf{85.7} \pm \textbf{0.2}$ | 133 ± 8 |
| | GRU-SIMPLE | 78.1 ± 1.3 | 43.6 ± 0.4 | 82.8 ± 0.0 | 140 ± 7 |
| | IP-NETS | 78.3 ± 0.7 | 48.3 ± 0.4 | 83.2 ± 0.5 | 81.2 ± 8.5 |
| | Phased-LSTM | 73.8 ± 3.3 | 37.1 ± 0.5 | 80.3 ± 0.4 | 166 ± 7 |
| | TRANSFORMER | 77.4 ± 5.6 | 42.6 ± 1.0 | 82.1 ± 0.3 | 20.1 ± 0.1 |
| | Latent-ODE [†] | 72.8 ± 1.7 | 39.5 ± 0.5 | 80.9 ± 0.2 | 4622 |
| | SeFT-Attn | $\textbf{79.0} \pm \textbf{2.2}$ | 46.3 ± 0.5 | 83.9 ± 0.4 | $\textbf{14.5} \pm \textbf{0.5}$ |
| P12 | GRU-D | 80.0 ± 2.9 | 53.7 ± 0.9 | $\textbf{86.3} \pm \textbf{0.3}$ | 8.67 ± 0.49 |
| | GRU-SIMPLE | 82.2 ± 0.2 | 42.2 ± 0.6 | 80.8 ± 1.1 | 30.0 ± 2.5 |
| | IP-NETS | 79.4 ± 0.3 | 51.0 ± 0.6 | 86.0 ± 0.2 | 25.3 ± 1.8 |
| | Phased-LSTM | 76.8 ± 5.2 | 38.7 ± 1.5 | 79.0 ± 1.0 | 44.6 ± 2.3 |
| | TRANSFORMER | $\textbf{83.7} \pm \textbf{3.5}$ | $\textbf{52.8} \pm \textbf{2.2}$ | $\textbf{86.3} \pm \textbf{0.8}$ | $\textbf{6.06} \pm \textbf{0.06}$ |
| | LATENT- ODE^{\dagger} | 76.0 ± 0.1 | 50.7 ± 1.7 | 85.7 ± 0.6 | 3500 |
| | SeFT-Attn | 75.3 ± 3.5 | 52.4 ± 1.1 | 85.1 ± 0.4 | 7.62 ± 0.10 |

Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series



SeFT Result: Performance vs. Runtime



Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series

SeFT's Outputs are Explainable



Allows a per-observation quantification of importance

Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020. http://proceedings.mlr.press/v119/horn20a/horn20a.pdf & https://slideslive.com/38928275/set-functions-for-time-series



Combining Compressed Sensing and Machine Learning

Recall: Compressed Sensing







Combining Compressive Sensing and Machine Learning



Option 1



Combining Compressive Sensing and Machine Learning





Option 1

Option 2





Could we Combine Compressive Sensing and Deep Learning?



Compressed Learning with Deep Neural Networks

Adler, Amir, Michael Elad, and Michael Zibulevsky. "Compressed learning: A deep neural network approach." arXiv preprint arXiv:1610.09615 (2016). https://arxiv.org/pdf/1610.09615



Compressed Learning with Deep Neural Networks

- with high classification accuracies
 - Calderbank, Jafarpour, and Schapire. "Compressed learning: Universal sparse
 - the best linear threshold classifier operating in the signal domain x

• Compressed Learning: direct inference from compressive measurements is feasible

dimensionality reduction and learning in the measurement domain." preprint (2009). Proved that under certain conditions the performance of a linear SVM classifier operating in the compressed sensing domain y = Cx is almost equivalent to the performance of



Compressed Learning with Deep Neural Networks

- with high classification accuracies
 - Calderbank, Jafarpour, and Schapire. "Compressed learning: Universal sparse
 - the best linear threshold classifier operating in the signal domain x
- (same shape as x) as the input to a convolutional neural network Showed pretty good results on MNIST and ImageNet classification by training on projected measurement z = C'y instead of on the original signal x

Adler, Amir, Michael Elad, and Michael Zibulevsky. "Compressed learning: A deep neural network approach." arXiv preprint arXiv:1610.09615 (2016). https://arxiv.org/pdf/1610.09615

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dimensionality reduction and learning in the measurement domain." preprint (2009). Proved that under certain conditions the performance of a linear SVM classifier operating in the compressed sensing domain y = Cx is almost equivalent to the performance of

• Subsequent work combined CL with DNNs: projected measurement vector $z = C^{T}y$ Lohit, Kulkarni, and Turaga. "Direct inference on compressive measurements using convolutional neural networks." IEEE Intl Conf on Image Proc. (ICIP), pp. 1913-1917.



Direct Inference on Compressive Measurements using CNN



| Measurement | Number of | Test Error | |
|-------------|--------------|-------------|--------|
| Rate (MR) | Measurements | Smashed | Our |
| | | Filters [4] | Method |
| 1 (Oracle) | 784 | 13.86% | 0.89% |
| 0.25 | 196 | 27.42% | 1.63% |
| 0.10 | 78 | 43.55% | 2.99% |
| 0.05 | 39 | 53.21% | 5.18% |
| 0.01 | 8 | 63.03% | 41.06% |

| Measurement Rate | No. |
|------------------|-----|
| 1 (Oracle) | |
| 0.25 | |
| 0.10 | |

MNIST Classification

ImageNet Classification

Lohit, Suhas, Kuldeep Kulkarni, and Pavan Turaga. "Direct inference on compressive measurements using convolutional neural networks." In 2016 IEEE International Conference on Image Processing (ICIP), pp. 1913-1917. IEEE, 2016. https://ieeexplore.ieee.org/iel7/7527113/7532277/07532691.pdf

Convergence of Test Error

End-to-end Deep Learning Solution for Compressed Learning

- Idea: jointly optimize the sensing matrix Cand the inference operator (i.e. the CNN)
 - Adler, Amir, Michael Elad, and Michael Zibulevsky. "Compressed learning: A deep neural network approach." arXiv preprint arXiv:1610.09615 (2016).
- Approach
 - The first layer learns and performs the sensing matrix C

 - The first and second layers are followed by ReLU
 - The two components of end-to-end CL detached after training



The subsequent layers (a fully-connected layer followed by a CNN) perform the non-linear inference stage • The second fully-connected layer performs operation similar to $z = C^T y$ but a different matrix \tilde{C} is learnt

End-to-end Deep Learning Solution for Compressed Learning

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| Sensing Rate | No. of Measurements | Smashed Filters [12] | Random Sensing + CNN [4] | Proposed |
|--------------|---------------------|----------------------|--------------------------|---------------|
| 0.25 | 196 | 27.42% | 1.63% | 1.56% |
| 0.1 | 78 | 43.55% | 2.99% | 1.91% |
| 0.05 | 39 | 53.21% | 5.18% | 2.86 % |
| 0.01 | 8 | 63.03% | 41.06% | 6.46 % |

Adler, Amir, Michael Elad, and Michael Zibulevsky. "Compressed learning: A deep neural network approach."

The subsequent layers (a fully-connected layer followed by a CNN) perform the non-linear inference stage • The second fully-connected layer performs operation similar to $z = C^T y$ but a different matrix \tilde{C} is learnt

Classification Error (%) for the MNIST handwritten digits dataset vs. sensing rate R = M/N (averaged over 10,000 test images)



Compressed Sensing Using Generative Models

- Instead of relying on sparsity, one can use structure from a generative model. GANs and VAEs



Generative Adversarial Networks

Bora, Ashish, Ajil Jalal, Eric Price, and Alexandros G. Dimakis. "Compressed sensing using generative models." In International Conference on Machine Learning, pp. 537-546. PMLR, 2017. http://proceedings.mlr.press/v70/bora17a/bora17a.pdf

• CS compresses by taking random linear projections (measurement matrix) of the original signal, and reconstructs by exploiting sparsity present in "natural" signals

Variational Auto Encoder





Compressed Sensing Using Generative Models

- CS compresses by taking random linear projections (measurement matrix) of the original signal, and reconstructs by exploiting sparsity present in "natural" signals
- Instead of relying on sparsity, one can use structure from a generative model. GANs and VAEs
 - A generative model is given by a deterministic function $G: \mathbb{R}^k \to \mathbb{R}^n$, and a distribution P_Z over $z \in \mathbb{R}^k$.
 - To generate a sample from the generator, we draw $z \sim P_z$ and the sample then is G(z)
- Approach: find a vector in representation space s.t. the corresponding vector in the sample space matches the observed measurements, i.e. optimize $loss(z) = ||AG(z) - y||_2^2$ (highly non-convex, approximated using gradient descent) If the optimization procedure gives \hat{z} , then reconstruct by computing $\hat{x} = G(\hat{z})$

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Compressed Sensing Using Generative Models



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References

- Alexander Smola. "Deep sets." arXiv preprint arXiv:1703.06114 (2017).
- equations." arXiv preprint arXiv:1806.07366 (2018).
- time series." arXiv preprint arXiv:1909.07782 (2019).
- arXiv preprint arXiv:1907.03907 (2019).
- series." In International Conference on Machine Learning, pp. 4353-4363. PMLR, 2020.
- Shukla, Satya Narayan, and Benjamin M. Marlin. "A Survey on Principles, Models and Methods for preprint arXiv:2012.00168 (2020).
- Time Series." arXiv preprint arXiv:2101.10318 (2021).

Zaheer, Manzil, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Ruslan Salakhutdinov, and

Chen, Ricky TQ, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. "Neural ordinary differential

• Shukla, Satya Narayan, and Benjamin M. Marlin. "Interpolation-prediction networks for irregularly sampled

Rubanova, Yulia, Ricky TQ Chen, and David Duvenaud. "Latent ODEs for irregularly-sampled time series."

Horn, Max, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. "Set functions for time

Learning from Irregularly Sampled Time Series: From Discretization to Attention and Invariance." arXiv

Shukla, Satya Narayan, and Benjamin M. Marlin. "Multi-Time Attention Networks for Irregularly Sampled



The End