Gaussian Process Generative Models for Language and Robotics

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Self introduction

- PhD NAIST, 2005
- B.Sc. University of Tokyo, 1998
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 Research fields: Natural Language Processing and Bayesian Machine Learning

Overview

- Brief introduction to Gaussian processes (GP)
 - Very flexible nonlinear regression from Bayesian point of view
- Recognizing "Motion" (run, throw, bend, ...) through a combination of:
 - Gaussian processes + semi-Markov HMM + Hierarchical Dirichlet processes (IROS 2018)
 - Variational Antoencoder for high-dimensional signals (IROS 2019)
- GP Neural Networks for Text Visualization

Part 1: What is a Gaussian process?

Gaussian processes

Gaussian process ··· stochastic process to generate random functions



- function : mapping from $\mathbf{x} \mapsto y$
- As a function of time t, it represents a trajectory

Gaussian processes (2)



- Gaussian process on two-dimensional inputs =Random surface function
- Similarly for higher-dimensional inputs *x*

Gaussian processes (3)

• Bayesian learning of a function: given datapoint, posterior distribution of functions is obtained



- Blue: Expectation
- High variance (light blue) for area with no data
- Ordinary model cannot represent variances of prediction

GPML

• GPML ("Gaussian Processes for Machine Learning")



Carl Edward Rasmussen and Christopher K. I. Williams

- Published in 2006
- For intermediate and expert users who need more mathematical constructions
- Textbook is downloadable for free: http://www.gaussianproce ss.org/gpml/

Introductory textbook



- "Gaussian process and Machine Learning", Kodansha MLP series, 2019 in Japan
 - 55 Amazon Ratings so far
- From linear model to Gaussian processes
- Also covers unsupervised learning and variational inference
- Why deer?

Simple regression

- Simplest prediction: y = a + bx
- How to determine *a* and *b*?



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Minimization of error

• Minimize error ϵ between the observation y_n and prediction $\hat{y}_n = a + b x_n$: $\epsilon = y_n - \hat{y}_n = y_n - (a + b x_n)$



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Simple regression (2)

- Given data $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$,
- Prediction \hat{y}_n for each x_n is a linear function

$$\hat{y}_n = a + bx_n$$

Difference between the observation is

$$y_n - \hat{y}_n = y_n - (a + bx_n)$$

- We want to minimize this error!

Simple regression (3)

• For
$$n=1,2,...,N$$
,
error = $y_n - \hat{y}_n \rightarrow \text{Minimize sum of errors}$

 Errors can be negative, thus take a square of errors (Least squares):

$$E = \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 = \sum_{n=1}^{N} (y_n - (a + bx_n))^2$$

We want *a*,*b* to minimize this E

Simple regression

• Since derivative of E is zero at minimal point,

$$\frac{\partial E}{\partial a} = \frac{\partial}{\partial a} \sum_{\substack{n=1\\N}}^{N} (y_n - (a + bx_n))^2$$
$$= \frac{\partial}{\partial a} \sum_{\substack{n=1\\n=1}}^{N} (y_n^2 + a^2 + b^2 x_n^2 - 2ay_n - 2abx_n + 2bx_n y_n) = 0$$

$$\frac{\partial E}{\partial b} = \frac{\partial}{\partial b} \sum_{\substack{n=1\\N}}^{N} (y_n - (a + bx_n))^2$$

$$= \frac{\partial}{\partial b} \sum_{\substack{n=1\\N}}^{N} (y_n^2 + a^2 + b^2 x_n^2 - 2ay_n - 2abx_n + 2bx_n y_n) = 0$$
Yields
$$a = \frac{\sum_n x_n^2 \sum_n y_n - \sum_n x_n \sum_n x_n y_n}{N \sum_n x_n^2 - (\sum_n x_n)^2}$$

$$b = \frac{N \sum_n x_n y_n - \sum_n x_n \sum_n y_n}{N \sum_n x_n^2 - (\sum_n x_n)^2}$$

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Simple regression (example)



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Multiple regression

• x is multi-dimensional? \rightarrow Multiple regression

When
$$\mathbf{x} = (x_1, x_2, \cdots, x_D)^T$$
,
 $y = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_D x_D$

Squared error is

$$(y - \hat{y})^2 = (y - (w_0 + w_1 x_1 + w_2 x_2 + \dots + w_D x_D))^2$$

- Minimize this error:
 - → Take gradients of $E = \sum_{n=1}^{N} (y_n \hat{y}_n)^2$ w.r.t. w_0, w_1, \cdots, w_D to equate 0 and solve linear equations.

Vector-Matrix form

• When we set
$$\mathbf{x} = (1, x_1, x_2, \cdots, x_D)$$

and $\mathbf{w} = (w_0, w_1, w_2, \cdots, w_D)$,
 $\hat{y} = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_D x_D$
 $= (w_0, w_1, w_2, \cdots, w_D) \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_D \end{pmatrix}$
 $= \mathbf{w}^T \mathbf{x}$

Vector-Matrix form (2)

Aligning vertically over n=1,2,...,N gives



Vector-Matrix form (3)

$$E = \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 = (y_1 - \hat{y}_1, \cdots, y_N - \hat{y}_N) \begin{pmatrix} y_1 - \hat{y}_1 \\ \vdots \\ y_N - \hat{y}_N \end{pmatrix}$$

Therefore

$$E = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

= $\mathbf{y}^T (\mathbf{y} - \mathbf{X}\mathbf{w}) - (\mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$
= $\mathbf{y}^T \mathbf{y} - 2\mathbf{w}^T (\mathbf{X}^T \mathbf{y}) + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w}$

Analytical solution of multiple regression

$$E = \mathbf{y}^T \mathbf{y} - 2\mathbf{w}^T (\mathbf{X}^T \mathbf{y}) + \mathbf{w}^T \mathbf{X}^T \mathbf{X} \mathbf{w}$$

• taking derivative wrt w,

$$\frac{\partial E}{\partial \mathbf{w}} = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{0}$$

Thus

$$\mathbf{X}^T \mathbf{X} \mathbf{w} = \mathbf{X}^T \mathbf{y} \quad \text{(Normal equation)}$$

$$\therefore \quad \mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$$

Solution of multiple regression

Multiple regression example

• Given data below: $\mathcal{D} = \{((1,2),4), ((-1,1),2), ((3,0),1), ((-2,-2),-1)\}$



Multiple regression example (2)

• Therefore, optimal weight vector is



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More complex regression?



Data often exhibit nonlinear relationships
 More complex regression function!

Linear regression



- Both written as linear function of weights w – $y = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) \cdots$ Linear regression
- Combining this with sigmoid function yields logistic regression:

$$y = \sigma(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}))$$

Linear regression

$$y = \mathbf{w}^T \phi(\mathbf{x}) + \epsilon$$

• For explanation, assume no noise:

$$y = \mathbf{w}^T \phi(\mathbf{x}) = w_1 \phi_1(\mathbf{x}) + w_2 \phi_2(\mathbf{x}) + \dots + w_M \phi_M(\mathbf{x})$$

• For given pairs $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N), \}$ this gives $\mathbf{y} = \mathbf{\Phi} \mathbf{w}$

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_M(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_M(\mathbf{x}_2) \\ \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_M(\mathbf{x}_N) \end{pmatrix}}_{\mathbf{y}} \underbrace{\begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_M \end{pmatrix}}_{\mathbf{w}}$$

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From Linear regression to Gaussian processes

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_M(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_M(\mathbf{x}_2) \\ \vdots & & & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_M(\mathbf{x}_N) \end{pmatrix}}_{\mathbf{y}} \underbrace{\begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_M \end{pmatrix}}_{\mathbf{w}}$$

• When we assume $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{I})$ like a ridge regression,

 $\mathbf{y} = \boldsymbol{\Phi} \mathbf{w}$ also obeys Gaussian distribution

$$\mathbf{y} = \mathbf{\Phi} \mathbf{w} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$$

• What are μ, Σ ?

From Linear regression to Gaussian processes (2)

$$\mathbf{y} = \mathbf{\Phi} \mathbf{w} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- $\mu = \mathbb{E}[\mathbf{y}] = \mathbb{E}[\mathbf{\Phi}\mathbf{w}] = \mathbf{\Phi}\mathbb{E}[\mathbf{w}] = \mathbf{0}$ • $\mathbf{\Sigma} = \mathbb{E}[\mathbf{y}\mathbf{y}^T] - \mathbb{E}[\mathbf{y}]\mathbb{E}[\mathbf{y}]^T$ $= \mathbb{E}[(\mathbf{\Phi}\mathbf{w})(\mathbf{\Phi}\mathbf{w})^T] = \mathbb{E}[\mathbf{\Phi}\mathbf{w}\mathbf{w}^T\mathbf{\Phi}^T]$ $= \alpha\mathbf{\Phi}\mathbf{\Phi}^T$
- Therefore,

$$\mathbf{y} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{\Phi} \mathbf{\Phi}^T)$$

This is called a Gaussian process!
(y is jointly Gaussian)

From Linear regression to Gaussian processes (3)

$$\mathbf{y} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{\Phi} \mathbf{\Phi}^T) = \mathcal{N}(\mathbf{0}, \mathbf{K})$$



 $K_{ij} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) = k(\mathbf{x}_i, \mathbf{x}_j)$: kernel function

Now, w are integrated out in a Bayesian way

Random draw from a Gaussian process



• Why such smooth functions?

Multivariate Gaussian distribution



Random draws from MVN



If correlation is high, similar values are sampled
 Minus for negative correlation, 0 for independent

Random draws from MVN (2)



Three dimensional case

Intuitive explanation

• Assume grid of input points

$$\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)$$

and create a covariance matrix \mathbf{K} between them:
 $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$
e.g.

		x_1	x_2	x_3	x_4
$\mathbf{K} =$	x_1	(1.0000)	0.3679	0.0183	0.0001
	x_2	0.3679	1.0000	0.3679	0.0183
	x_3	0.0183	0.3679	1.0000	0.3679
	x_4	(0.0001)	0.0183	0.3679	1.0000

kernel function

• $k(x_i, x_j)$: kernel function. For example:

$$k(\mathbf{x}, \mathbf{x}') = \exp(-|\mathbf{x} - \mathbf{x}'|^2/\theta)$$

(RBF kernel)

 Same as those used in SVM or others (GP is a Bayesian version of the kernel methods)

Intuitive explanation (2)

Draw from correlated multivariate Gaussian:



Intuitive explanation (3)

• Draw from correlated multivariate Gaussian:


Intuitive explanation (4)

Draw from correlated multivariate Gaussian:



Kernels and random draws from GP



Ordinary usage: GPR

- Gaussian process regression (GPR)
 - Given a set of pairs (x,y), predict y for new x^*



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Part 2: Language, Robotics, and Gaussian processes

Language and Robotics

- (Intellectual) Robotics is not only around physical movements, but symbolic actions are necessary for high-level behavior
 - Closely tied with languages

What is "word"?

 Children are not taught about "words" : learn only from experiences



- Robots should be flexible enough to learn "words" automatically from their environment
- Novel words, colloquial expressions, dialects, and child languages .. should be robust in a practical viewpoint

What is "word"?

 Problem: want to find "words" from a sequence of acoustic signals



 \rightarrow "she sings the song"

 Easier version: find words from phonological sequences of child's speech (Goldwater+ 2006)

```
WAtsDIs \rightarrow WAts DIs
WAtIzIt \rightarrow WAt Iz It
yuwanttusiD6bUk \rightarrow yu want tu si D6 bUk
```

(CHILDES corpus)

Word segmentation

• Word segmentation and morpheme analysis are crucial tool to analyze Asian languages

山花貞夫・新民連会長は十六日の記者会見で
→山花貞夫・新民連会長は十六日の記者会見で
今后一段时期,不但居民会更多地选择国债
→今后一段时期,不但居民会更多地选择国债

 Usually done by supervised learning, but can be made unsupervised (Mochihashi+ ACL 2009, Uchiumi+ ACL 2015)!

Western languages

• Case of Latin (Scripta continua)

- English was also originally written without spaces

KOALINS ATVALINS DATA ANTERBERATAMNI AUAPHINSPELAGOQAUIVSTRAHITVAHDALINA IVMILERINGORMOARCVIMILAMAIINASERRAE NAMPRIMICVN HISSCINDEBANTEISSILLIGNNAI IVMNARIAEVENEREARTES[ABOROMNIAVICH] INIPROFILDVRISSVRGENSIN REFINEGESIAS PRIMACERISEISROMORIALISVERTERHERRAM INSTITUTIOVAIIAMGIANDISAIQARDVIASACIBM DELICERENTSHIVAELIVICIVAHDODONANLGNRE MONFIFRYMENTISLABORADDIIVSVIMALNEWMS ISSUROBICOSECNISO/HORREREUNINGVISIUM CARDVVSINTERIVNISIGEHSSV6HASPHRXSINA LAPPARQ 13 IBOLIQ IN HRON HEN PLACYLEN I / IN HUXLOUVMEISURILISDOMIN'ANIVR NOTING QVODNISHIADSIDVISHRRAMINSECIABERERASIA HSONAINTERREDISANTSURWRISOPACE

Vergil text, around AD 141

Unsupervised word segmentation (Mochihashi+ ACL 2009)



first, shedreamed of littlealice herself, and once again the tiny hands were clasped up on herknee, and the bright eager eyes were looking up into hers she could hear the very tones of hervoice, and see that queer little toss of her head to keep back the wandering hair that would always get into here yes and still as she listened, or seemed to listen, the whole place around herbe came alive the strange creatures of herlittlesister's dream. The long grass rust led at herfeet as the white rabbit hurried by the fright end mouses plashe dhis way through the neighbouring pools he could hear the ratt leof the teacups as the maintenance.

first, she dream ed of little alice herself ,and once again the tiny hand s were clasped upon her knee ,and the bright eager eyes were looking up into hers -- shecould hearthe very tone s of her voice , and see that queer little toss of herhead to keep back the wandering hair that would always get into hereyes -- and still as she listened , or seemed to listen , thewhole place a round her became alive the strange creatures of her little sister 'sdream. thelong grass rustled ather feet as thewhitera bbit hurried by -- the frightened mouse splashed his way through the neighbour ing pool -- shecould hearthe rattle ofthe tea cups...



Arabic unsupervised segmentation

• Arabic AFP news, 40,000 sentences





Inference with Dynamic Programming



各国的朋友们 "friends of each country"

- "Inducing Word and Part-of-speech with Pitman-Yor Hidden Semi-Markov models", ACL 2015
- Forward filtering-backward sampling MCMC to escape from local minima

Learning with Multimodal information



"Mutual Learning of an Object Concept and Language Model based on MLDA and NPYLM",

Nakamura et al., IROS 2014

Word discovery from acoustic signals



Word discovery from acoustic signals (2)

- Five artificial words {aioi, aue, ao, ie, uo} prepared by connecting five Japanese vowels.
- 30 sentences (25 two-word and 5 three-word sentences) are prepared and each sentence is recorded twice by four Japanese speakers.
- MFCC (frame size =25ms, shift = 10ms, frame rate 100hz)

* HDP-HLM are trained separately for each speaker.





uo aue ie ie ie uo aue ao ie ao ie ao aioi uo ie

ex) ao-ie-ao



Part 2: Motion segmentation and Gaussian processes

Learning "Motion" from Movements



- Crucial for high-level recognition and planning of actions of robots .. word segmentation for robots
 - Planning for preparing dishes: wash->cut->boil->...

Model of movements



- Observations are continuous
 Stochastic models for trajectories are necessary
- We leverage the Gaussian processes

Actual data of movements



- Time series from two angles (knee and shoulder)
- How to induce "motion" from this data?

Gaussian process hidden semi-Markov model



- Hidden state (motion class): $c_j \sim \text{Mult}(c|c_{j-1})$
- Generate trajectory: $\mathbf{x}_j \sim \operatorname{GP}(\mathbf{x} | \mathbf{X}_{c_j})$
- a kind of HMM, but segmentations are unknown

Application to Robotics

- Hidden semi-Markov model with Gaussian process observations to model the time series of joint angles, Forward-Backward Bayesian learning (infer "words")
- Segmentation results using simple arm motions :



Segmentation result

Dynamic programming MCMC

- Forward filtering:
- $\alpha[t][k][c] = GP(\mathbf{s}_{t-k:k}|\mathbf{X}_c) \sum_{k} \sum_{c} p(c|c')\alpha[t-k][k'][c']$
- Backward sampling:





Draw high-probability path via dynamic programming

The first experiment

- Unsupervised segmentation of arm movements measured by Kinect
- 2D coordinates (x,y) of the right hand
 - Assume x and y are independently generated:
 x ~ GP(c), y ~ GP(c)
- Motions involved:
 - Move the hand to right
 - Raise the hand high
 - Raise the hand slightly



Results

 Correctly recovered the three motions

х

y



Learned Gaussian processes:





Motion segmentation



Correctly recognized Karate motions from observations

Inferred motions (excerpt)

Class 0: Right punch with an additional step



• Class 6: Left lower guarding



Comparison with other methods

• GP-HSMM vs. HDP-HMM, HDP-HMM+NPYLM



Number of Motions

 Number of hidden states (motions) can also be estimated using hierarchical Dirichlet processes

– HDP-GP-HSMM

 - "Sequence Pattern Extraction by Segmenting Time Series Data Using GP-HSMM with Hierarchical Dirichlet Process", Nagano+, IROS 2018

TABLE V

SEGMENTATION RESULTS FOR THE EXERCISE MOTION.

	Hamming distance	Precision	Recall	F-measure	# of estimater classes
HDP-GP-HSMM	0.31	0.38	0.95	0.55	10
HDP-HMM	0.82	0.070	1.0	0.13	14
HDP-HMM+NPYLM	0.63	0.61	1.0	0.76	26
BP-HMM	0.23	0.25	1.0	0.40	18
Autoplait	0.61	0.67	0.18	0.28	5

Ground

truth: 11

Number of Motions (2)

- We leveraged infinite HMM (Beal+ 2001, Teh+ 2006) with our semi-Markov structure
- Since the state space is infinite-dimensional, also used a Beam sampling (van Gael+2007) for slice sampling+dynamic programming
 - Internally, using a stick-breaking representation for possibly infinite state spaces

High-dimensional regime

- Actually, robot movements are quite highdimensional
 - In our case, # of joint angles = 93
 - Cannot apply the method to whole data



Strategy (Our work at IROS 2019)

- Solution: dimensionality reduction
- Linear PCA \rightarrow NG
- GPLVM (Gaussian process LVM) → OK, but inference is not stable
- Using VAE as a surrogate of GPLVM



Fig. 3. Variational autoencoder (VAE) to obtain the latent low-dimensional representation z_j of observed time series x_j .



Simultaneous optimization



Note

In this case, each cluster (=motion) has its own VAE for compression

- VAE priors are different for each cluster



Graphical model

• We observe only **s** (high-dimensional time series)



Hierarchical Dirichlet process-variational autoencoder-Gaussian process-hidden semi-Markov model (Long!) = HVGH
Experiments

 Dance exercises which include four and seven unit motions (labels are not used in learning)



Seven unit motions included in the exercise motion1:
(a) jumping jack, (b) twist, (c) arm circle, (d) bend over,
(e) knee raise, (f) squatting, and (g) jogging

Results (1)

• Exercise containing four unit motions:

表 1: Segmentation results for the chicken dance.

		Hamming				# of estimated
1		distance	Precision	Recall	F-measure	classes
	HVGH	0.23	0.86	0.86	0.86	4
VAE+HDP-G	P-HSMM	0.31	1.0	0.71	0.83	4
VAE+HDP-HMM		0.74	0.15	1.0	0.26	11
VAE+						
HDP-HMM+NPYLM		0.48	1.0	0.86	0.92	7
VAE+BP-HMM		0.34	1.0	0.86	0.92	3
VAE+.	Autoplait	0.66	0.0	0.0	0.0	1

VAE as a preprocessing

Results (2)

Exercise containing seven unit motions:

\cancel{x} 2: Segmentation results for the exercise motion.						
		Hamming				# of estimated
		distance	Precision	Recall	F-measure	classes
	HVGH	0.16	0.66	0.93	0.75	11
VAE+HDP-GP-HSMM		0.24	0.53	0.93	0.67	12
VAE+HDP-HMM		0.75	0.05	1.0	0.09	10
VAE+		121271		09102	202200	
HDP-HMM+NPYLM		0.61	0.30	1.0	0.45	28
VAE+BP-HMM		0.58	0.29	0.97	0.44	7
VAE+Autoplait		0.76	0.0	0.0	0.0	2

t a a 1, 6, 11



Estimated latent space in VAE



- VAE is separately learned for compression
- Motions (in color) are mixed and not separated

Estimated latent space in VAE (2)



- Simultaneous learning in HVGH
- Motions (in color) are clearly separated

Zoology and Brain science (Marmoset)

class06



Can recognize ape's motions *automatically*joint work with Koki Mimura (NCAP), JSAI 2019

Part 3: Nonparametric Bayesian Deep Visualization (NPDV)

Joint work with Bridgestone Corporation; appeared at IBISML 43 (2021)

Data Visualization

- Visualize high-dimensional data by mapping them into 2D or 3D
 - Important first step for exploratory data analysis



 Principal Component Analysis (PCA) has a strong limitation → Data often have nonlinear structures

NPDV: NP Bayesian Deep Visualization



Simultaneously optimize $Y \rightarrow X, X \rightarrow V$ • $Y \rightarrow X$: NN-iWMM Neural network using GP +infinite mixture (no NN weights) • $X \rightarrow V$: visualization via t-SNE (van der Maaten 2009)

Infinite Warped Mixture Model (iWMM) (Iwata+ 2013)



- Infinite Gaussian mixture in latent space
 → Map to observation through Gaussian process
- d'th dimension of observation Y distributes according to GP on X: Y_d ~ GP(µ, K_X)

Neural network = Gaussian process

- Single hidden-layer NN with input layer \boldsymbol{x}
- *i*'th output $z_i^1(x)$ is written as :

$$z_i^1(x) = b_i^1 + \sum_{j=1}^{N_1} W_{ij}^1 x_j^1(x), \quad x_j^1(x) = \phi \left(b_j^0 + \sum_{k=1}^{N_0} W_{jk}^0 x_k \right)$$



Connection $W_{ij}^{\ell} \sim \mathcal{N}(0, \sigma_w/N_{\ell})$ Bias $b_i^{\ell} \sim \mathcal{N}(0, \sigma_b)$

Neural network = Gaussian process (2)

$$z_i^1(x) = b_i^1 + \sum_{j=1}^{N_1} W_{ij}^1 x_j^1(x), \quad x_j^1(x) = \phi \left(b_j^0 + \sum_{k=1}^K W_{jk}^0 x_k \right)$$

- Sum of independent weights W^ℓ_{ij} and biases b^ℓ_i
 → Joint probability p(z¹₁(x), z¹₂(x), · · · , z¹_{N₂}(x)) has a multivariate Gaussian distribution by Central Limit Theorem … Gaussian process
 - Mean: clearly 0
 - Covariance is

$$K^{1}(x, x') \equiv \mathbb{E}\left[z_{i}^{1}(x)z_{i}^{1}(x')\right]$$
$$= \sigma_{b}^{2} + \sigma_{w}^{2}\mathbb{E}\left[x_{i}^{1}(x)x_{i}^{1}(x')\right] = \sigma_{b}^{2} + \sigma_{w}^{2}C(x, x')$$

NNGP (Neural Network Gaussian process)

- Assume $\ell 1$ layer output $z_j^{\ell-1}$ is GP: $z_i^{\ell}(x) = b_i^{\ell} + \sum_{j=1}^{N_{\ell}} W_{ij}^{\ell} x_j^{\ell}(x), \quad x_j^{\ell}(x) = \phi(z_j^{\ell-1}(x))$
- ℓ -layer Mean is 0, variance is

$$\begin{split} K^{\ell}(x,x') &\equiv \mathbb{E}\left[z_{i}^{\ell}(x)z_{i}^{\ell}(x')\right] \\ &= \sigma_{b}^{2} + \sigma_{w}^{2} \mathbb{E}_{z_{i}^{\ell-1} \sim \mathrm{GP}(0,K^{\ell-1})}\left[\phi(z_{i}^{\ell-1}(x))\phi(z_{i}^{\ell-1}(x'))\right] \end{split}$$

This expectation can be computed by:
(1) GP regression (2) Numerical approximation
(3) Analytical solution for specific φ like ReLU

NNGP (Neural Network Gaussian process) When φ is ReLU (Cho&Saul 2009, Lee+ 2017) :

$$\begin{aligned} K^{\ell}(x,x') &= \sigma_b^2 + \frac{\sigma_w^2}{2\pi} \sqrt{K^{\ell-1}(x,x)K^{\ell-1}(x',x')} \\ &\times \left(\sin\theta_{x,x'}^{\ell-1} + (\pi - \theta_{x,x'}^{\ell-1})\cos\theta_{x,x'}^{\ell-1}\right) \\ \theta_{x,x'}^{\ell} &= \cos^{-1}\left(\frac{K^{\ell}(x,x')}{\sqrt{K^{\ell}(x,x)K^{\ell}(x',x')}}\right) \end{aligned}$$

Generative model of NN-iWMM

- ∞-Gaussian mixture ∞-mixture of Gaussians generates latents
- $oldsymbol{X} \equiv \{oldsymbol{x}_i\}_{i=1}^N$ • From $oldsymbol{X}$ and kernel parameters σ_b, σ_w , compute NNGP kernel matrix K_{NN}^L
- Generate data Y

 for each dimension d
 from NNGP



Unsupervised NN with no units, no numerical weights

Joint modeling with *t*-SNE



Problem: *t*-SNE has no clear generative model
 → How to combine NN-iWMM and *t*-SNE?

Joint modeling with t-SNE: RegBayes

Posterior *p*(θ|Y) equals to following optimization:
 (A. Zellner, 1988)

$$\min_{q(\boldsymbol{\theta})} \quad \operatorname{KL}[q(\boldsymbol{\theta}) \| p(\boldsymbol{\theta})] - \int q(\boldsymbol{\theta}) \log p(\boldsymbol{Y} | \boldsymbol{\theta}) d\boldsymbol{\theta}$$
s.t. $q(\boldsymbol{\theta}) \in \mathcal{P}$

 $\boldsymbol{\theta}$: parameters

 \mathcal{P} : probability distribution

- RegBayes : Bayesian model with posterior constraint (J. Zhu+. 2014) $\begin{cases} \min_{q(\theta)} & \operatorname{KL}[q(\theta) \| p(\theta)] - \int q(\theta) \log p(\boldsymbol{Y} | \theta) d\theta & \mathcal{R}(\theta, \boldsymbol{Y}) : \operatorname{Regularization term} \\ \text{s.t.} & E_{q(\theta)}[\mathcal{R}(\theta, \boldsymbol{Y})] \leq 0, \ q(\theta) \in \mathcal{P} \end{cases}$
 - Optimal distribution $q^*(\theta) \propto p(Y|\theta)p(\theta) \exp(-\lambda \mathcal{R}(\theta, Y))$ under the given constraint Joint distribution of θ and Y

NPDV Formulation

Joint distribution of NPDV (q*(θ) and NN-iWMM, t-SNE)

 $q^{*}(\boldsymbol{\theta}) \propto \underline{p(\boldsymbol{Y}|\boldsymbol{\theta})p(\boldsymbol{\theta})} \exp(-\lambda \mathcal{R}(\boldsymbol{\theta}, \boldsymbol{Y}))$ NN-iWMM *t*-SNE

Specifically,

 $p(\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{z}, \{\boldsymbol{m}_k, \boldsymbol{R}_k \pi_k\}_{k=1}^{\infty} | \boldsymbol{V})$

 $\propto p(\boldsymbol{Y}|\boldsymbol{X})p(\boldsymbol{X}|\boldsymbol{z}, \{\boldsymbol{m}_k, \boldsymbol{r}_k, \pi_k\}_{k=1}^{\infty})p(\boldsymbol{z}|\{\pi_k\}_{k=1}^{\infty}) \succ \mathsf{NN-iWMM}$

 $\times p(\{m{m}_k\}_{k=1}^\infty) p(\{m{r}_k\}_{k=1}^\infty) p(\{m{\pi}_k\}_{k=1}^\infty)$

 $\times \exp(-\lambda \operatorname{KL}[\boldsymbol{p}^X \| \boldsymbol{p}^V])$ *t*-SNE between *X* and *V*

- *V*: visual coordinates, σ_w , σ_b : NNGP kernel hyperparameter
- λ : hyperparameter $\approx \lambda = ND$ in this study

NPDV training

• Objective : lower bound of likelihood using variational distribution Q

$$\mathcal{L} = \mathbb{E}_{q(\boldsymbol{X})}[\log p(\boldsymbol{Y}|\boldsymbol{X})] - \mathbb{E}_{q(\boldsymbol{X})}[\log q(\boldsymbol{X})] + \mathbb{E}_{q(\boldsymbol{X},\boldsymbol{z},\boldsymbol{m},\boldsymbol{\Sigma},\boldsymbol{\phi})}\left[\log \frac{p(\boldsymbol{X},\boldsymbol{z},\{\boldsymbol{m}_{k},\boldsymbol{r}_{k},\boldsymbol{\pi}_{k}\}_{k=1}^{K})}{q(\boldsymbol{z},\{\boldsymbol{m}_{k},\boldsymbol{R}_{k}\}_{k},\boldsymbol{\pi})}\right] - \lambda \mathbb{E}_{q(\boldsymbol{X})}[\mathrm{KL}[\boldsymbol{p}^{X} \| \boldsymbol{p}^{V}]] \\= \underbrace{\mathcal{L}_{1} + \mathcal{L}_{2} - \lambda \mathcal{R}}_{(*)} + \underbrace{\mathcal{H}(q(\boldsymbol{X}))}_{\text{Gauss Entropy}}$$

- Re-parametrization trick to generate randomly from $q(x_n) = \mathcal{N}(x_n | \mu_n, S_n)$ to approximate (*)
- Gradient base learning from the approximation

GP Neural Networks and ARD

 Since there is no NN weights in NPDV, we can directly optimize hidden X for observation Y



- determination) prior on X \rightarrow We can learn hidden dimensionality of X!
- This is impossible for ordinary neural networks with numerous weights to learn



GP Neural Networks and ARD

- Input: "mammoth" 3D data mapped non-linearly for high dimensions
 - NPDV correctly recovered mammoth, with effectively three dimensions!



(d) NN-iWMM

(e) NN-iWMM+PCA



(f) ARD weights rch Organization of Information and Systems

Experiments

- Text corpus: 20newsgroups (English)、 Livedoor News corpus (Japanese)
 - 20newsgroups: USENET internet news text on 20 newsgroups, 18000 documents
 - Livedoor: Livedoor news articles, 9 categories, 7300 documents
- tf.idf preprocessing, compress into 1000 dims to visualize in 2D
- Baseline: t-SNE (Maaten+ 2009), Deep K-means (Phard+ 2020)

Results (20newsgroups: English)



k-NN classification accuracy (Bold: SOTA, *: Next to SOTA)

近傍数	Deep k-means	GPLVM	t-SNE	t-SNE-GPLVM	提案手法(次点との差分)
<i>k</i> = 10	0.383	0.527	0.559	0.593 *	0.599 (+0.6%)
<i>k</i> = 20	0.347	0.496	0.512	0.529 *	0.552 (+ 2.3%)
<i>k</i> = 30	0.330	0.487	0.492	0.500 *	0.529 (+ 2.9%)

Clearer idendification of clusters & SOTA accuracy

Results (Livedoor: Japanese)



k-NN classification accuracy (Bold: SOTA, *: Next to SOTA)

近傍数	Deep k-means	t-SNE-GPLVM	t-SNE	GPLVM	提案手法(次点との差分)
<u>k = 10</u>	0.755	0.793	0.793	0.809 *	0.844 (+ 3.5%)
<i>k</i> = 20	0.746	0.767	0.767	0.798 *	0.822 (+ 2.4%)
<i>k</i> = 30	0.742	0.747	0.747	0.790 *	0.809 (+ 1.9%)

Unsupervised visualization of sentences (*t*-SNE)

- Directly visualize sentences via t-SNE
 - \rightarrow Prone to noise, cannot consider meanings



× Unrelated clustering of sentences that belong to "cooking" cluster under NPDV

Unsupervised visualization of sentences (NPDV)

Internally estimates ∞-GMM to give "label" on each sentence

Clusters obtained through NPDV

Simultaneously estimates latent clustering and visualization



NPDV estimates semantically meaningful clusters

Data: Kyoto corpus (5000 articles from Mainichi newspaper 1995)

Summary

- Gentle introduction to Gaussian processes
- Learning "Motions" from movements through a Gaussian process generative model for robots (from research on NLP)
 - GP+HDP+Hidden semi-Markov Model (IROS 2018)
 - HVGH: GP+HDP+Hidden SMM+VAE (IROS 2019) for high-dimensional observations (segmentation on latent Gaussian processes)
- Analytical Gaussian process neural network with no neural weights
 - NPDV: Visualization w/ combination with t-SNE

"Language and Robotics"

 Advanced Robotics (2019), "Survey on frontiers of language and robotics".
 T. Taniguchi, D. Mochihashi, T. Nagai, et al.

https://www.tandfonline.com/doi/full/10.1080/01691864.2019.1632223

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