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From Gaussian Processes to the Mixture of Gaussian Processes A Survey

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Abstract Gaussian process GP model is a paradigmatic machine learning model that combines the advantages of both kernel learning method and Bayesian inference mechanism and thus has become a very popular area in machine learning in recent years. As an extension of the GP model the Mixture of Gaussian Processes MGP fits datasets more effectively and thus it has a better ability of learning and generalization. However

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[6] GP

GP

Tresp[7] 2000

Mixture of Gaussian Processes MGP

MGP

GP

1996 SVM 1992

Rasmussen[8] GP

20 GP

GP

[9] [10]

[9,11]

GP [12] GP MGP

GP

GP

MGP MGP

GP MGP

2

[1,2,6,10]

1 GP

N $\boldsymbol{x}_1\ \boldsymbol{x}_2\ \dots\ \boldsymbol{x}_N$

$t_1\ t_2\ \dots\ t_N$ $f(\boldsymbol{x})$

$\boldsymbol{x}_{N+1}$ $f(\boldsymbol{x}_{N+1})$ GP

$f(\boldsymbol{x})$ $\boldsymbol{t}_N=$

$(t_1\ t_2\ \dots\ t_N)^{\mathrm{T}}$ $t(\boldsymbol{x})$ $\boldsymbol{X}_N=(\boldsymbol{x}_1\ \boldsymbol{x}_2\ \dots\ \boldsymbol{x}_N)^{\mathrm{T}}$ $f(\boldsymbol{x})$ $t(\boldsymbol{x})$

$t(\boldsymbol{x})=f(\boldsymbol{x})+\mathrm{e}(\boldsymbol{x})$ $\mathrm{e}(\boldsymbol{x})$

σ_ν^2 $f(\boldsymbol{x})$ H

$$f(\boldsymbol{x})=\sum_{h=1}^{H}w_h\Phi_h(\boldsymbol{x})$$

$\boldsymbol{w}=(w_1\ w_2\ \dots\ w_H)^{\mathrm{T}}$ $\boldsymbol{w}\sim N(0,\sigma_w^2\boldsymbol{I}_H)$ $f(\boldsymbol{x})$

$t(\boldsymbol{x})$ $\boldsymbol{t}_N\sim N(0,\boldsymbol{C}_N)$

$\boldsymbol{C}_N$

$$C(\boldsymbol{x}_n,\boldsymbol{x}_m)=\sigma_w^2\sum_{h=1}^{H}\Phi_h(\boldsymbol{x}_n)\Phi_h(\boldsymbol{x}_m)+\sigma_\nu^2\delta_{nm}\quad(1)$$

$n=m$ $\delta_{nm}=1$ $\delta_{nm}=0$

$\boldsymbol{x}_{N+1}$ t_{N+1}

$$P(t_{N+1}|\boldsymbol{t}_N)=P(t_{N+1},\boldsymbol{t}_N)/P(\boldsymbol{t}_N)\quad(2)$$

GP

$$P(t_{N+1},\boldsymbol{t}_N)\propto\exp\left\{-\frac{1}{2}\left(\boldsymbol{t}_N^{\mathrm{T}}\ \ t_{N+1}\right)\boldsymbol{C}_{N+1}^{-1}\begin{bmatrix}\boldsymbol{t}_N\\ t_{N+1}\end{bmatrix}\right\}\quad(3)$$

$\boldsymbol{C}_{N+1}$ $\boldsymbol{k}$ $\boldsymbol{k}^{\mathrm{T}}$ κ

t_{N+1}

$$P(t_{N+1}|\boldsymbol{t}_N)\sim N(\hat{t}_{N+1},\sigma_{t_{N+1}}^2)\quad(4)$$

$\hat{t}_{N+1}=\boldsymbol{k}^{\mathrm{T}}\boldsymbol{C}_N^{-1}\boldsymbol{t}_N$ $\sigma_{\hat{t}_{N+1}}^2=\kappa-\boldsymbol{k}^{\mathrm{T}}\boldsymbol{C}_N^{-1}\boldsymbol{k}$ $f(\boldsymbol{x}_{N+1})=\hat{t}_{N+1}$ GP $\boldsymbol{x}_{N+1}$

2 GP

GP 2

$P(t_{N+1}|\boldsymbol{t}_N)$ $P(t_{N+1}|\boldsymbol{t}_N)$ $P(t_{N+1}|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)$

$$P(t_{N+1}=1|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)=\int P(t_{N+1}=1|f(\boldsymbol{x}_{N+1}))\,P(f(\boldsymbol{x}_{N+1})|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)\,\mathrm{d}f(\boldsymbol{x}_{N+1})\quad(5)$$

$$P(t_{N+1}=1|f(\boldsymbol{x}_{N+1}))=\frac{1}{1+\mathrm{e}^{-f(\boldsymbol{x}_{N+1})}}\quad(6)$$

$$P(f(\boldsymbol{x}_{N+1})|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)=\int P(f(\boldsymbol{x}_{N+1}),\boldsymbol{f}_N|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)\,\mathrm{d}\boldsymbol{f}_N=\int P(\boldsymbol{f}_{N+1}|\boldsymbol{X}_{N+1},\boldsymbol{t}_N)\,\mathrm{d}\boldsymbol{f}_N\quad(7)$$

$\boldsymbol{f}_N=(f(\boldsymbol{x}_1)\ f(\boldsymbol{x}_2)\ \dots\ f(\boldsymbol{x}_N))^{\mathrm{T}}$ $P(\boldsymbol{f}_{N+1}|\boldsymbol{X}_{N+1}$

$$t_N \propto P\ f_{N+1} \mid X_{N+1} \prod_{n=1}^{N+1} P\ t_n \mid f\ x_n \qquad P\ f_{N+1} \mid$$

$$X_{N+1} \propto \exp\left(-\frac{1}{2} f_{N+1}^{\mathrm{T}} K_{N+1}^{-1} f_{N+1}\right)$$

6 6 7

5 5 GP

[4] [13] [14]

[15] 5

3

GP

1 GP

GP

GP

GP

[16]

GP

GP

[10]

Seeger [17]

Schwaighofer [18]

GP

Sundararajan [19] Geisser

2 GP

GP

Chatzis [20] GP

Soh GP

[21] Snelson [22] GP

Boyle [23]

GP

Law-rence [24] [25] GP

Pillonetto [26] GP

Gilboa E. GP

[27] GP

Zhao [28]

Dallaire [29]

GP

3 GP

GP

Williams [30] GP

Opper [31]

Opper-Vivarelli OU

Sollich [32]

Malzahn [33]

Kakade [34] GP

4 GP

GP

GP

Mackay [6]

[35]

GP KD [36]

Nyström[37] GP

GP

[4,13]

[14]

[15] Chalupka

[38] GP

GP

[39]

[39] Snelson [40]

Quiñonero-Candela [39] GP

5 GP

GP

GP

GP

RBF SVM

Rasmussen [10] 6 GP

Kriging

[6]

Mackay[6] GP RBF

GP

RBF Sollich[41] GP

SVM SVM

GP

Gestel[42]

GP SVM

6 GP

Rasmussen[43] GP

[12]

GP

Engel[44]

Ko[45]

GP

GP

Wang[46] GPDM

[47]

GPDM Deisenroth[48]

GPDP

Amoto [49]

GP

7

GPLVM GP

[50]

GPLVM PPCA

Lawrence[51] PPCA

GPLVM GPLVM

GPLVM

Lawrence [52]

GPLVM

GPLVM

Urtasun [53] GPLVM

8 GP

GP

Cheng [54] JAFFE

GP

GP

[55] GP

[56]

[57] [58] [59]

9 GP

GP

GP

GP

GP

GP

GP

$\boldsymbol{\mu}$ x_i $z_i=j$ | θ_j $\boldsymbol{Q}$ x_i $z_i=j$ x_i $z_i=j$ |

θ_j j

$\boldsymbol{\mu}=0$ 10

GP

ME MGP

MGP

GP

ME GP ME

ME [66]

6

MGP

MGP

6.1 MGP

MGP 9

10

[7 61 67-81] [60 62-65 82-88]

[62]

MGP [62]

$$P\ t_N \mid X_N\ \boldsymbol{\mu} = \sum_{z_N}\prod_i \Pr\ z_i \mid x_i\ \tilde{\theta}$$

$$\prod_j P\ t_k\ z_k=j \mid x_k\ z_k=j\ \theta_j^{GP} \quad 11$$

$$P\ X_N\ t_N \mid \boldsymbol{\theta} = \sum_{z_N}\prod_i \Pr\ z_i \mid \tilde{\theta}\ \prod_j P\ t_k\ z_k=j \mid$$

$$x_k\ z_k=j\ \theta_j^{GP}\ P\ x_k\ z_k=j \mid \tilde{\theta}_j \quad 12$$

j P t_i $z_i=j$ | x_i z_t $=j$ θ_j^{GP} 10 Yuan [60] Sun [82]

Pr $z_i \mid x_i$ $\tilde{\theta}$ Pr $z_i \mid \tilde{\theta}$ [63-65 73 75 84 86-88]

Dirichlet [60 67-69 78 85 89] Dirichlet

Pitman-Yor [62 70 74 77 79 82-83]

j P x_i $z_t=j$ | $\tilde{\theta}_j$

[62-65 82-88] Yuan [60]

MGP

9 Wang Khardon [67]

GP GP

Kapoor [75] GP

Fox Dunson [90]

GP

MGP

[63-65 67-68 71-72 79 86-88]

[60-62 83 85]

Wishart [60-62 69 82-83 85]

Gamma [60-62 69 74 82-83]

6.2 MGP

MGP

MCMC

VB EM

MGP

MCMC

VB MCMC

[61-62 68-69 77-79 83 85 89]

M-H Gibbs MCMC

[60] MGP

MCMC MGP

[60 71 82] [60]

VB [70 74-75]

[86]

EM

MGP Q

MGP EM

EM

EM EM EM

MCMC-EM

EM E VB

M Q
[60,71,82] [67]

Sun Xu[82] EM

EM M
Tresp[7]
Stachniss Plagemann[91]

Yang Ma[63-64]
Schiegg[76] M Q

EM E
M

Yang Ma[63-64]
EM EM
Nguyen Bo-
nilla[71] E

Yu Chen[84] E

Chen
[65,86] EM

MC-
MC-EM Wu[86] 2015 Chen
[65] E
MCMC

MGP
1
Dong[72] GP MGP

2 Tuong[80]
Liu[81]
GP

GP 3
EP Kapoor[75] MGP

EP

MGP 5

6.3 MGP

MGP

1 ME [66]

[67,74-76,86,91]

2
EM

GP
[65,67,71,84,86,88] Nguyen Bo-
nilla[71,86]
EM

3 MCMC
MCMC

[68-69,83,86]
Meeds Osindero[62]
MCMC
4
Yuan[60] Sun[82] EM

6.4 MGP

MGP

2014 Chen[64] MGP

—— EM Chen
[86] [64] Zhao[88]
[64] Wu[86] E
MCMC

MGP MGP

3

1 GP MGP

MGP MGP

K

MGP

K[7,61,63-65,67-69,71,91] Huang[73] [60,67,82,91] Nguyen Bonil-

Akaike la[71] MGP 3

Zhao[88] 1 5

K K

K

Dirichlet Pitman-Yor

MGP

Rasmussen[92]

Dirichlet Motorcycle

K

MGP

Shi[93] MCMC

2015 Qiang Ma[89]

K

MGP

MGP

MGP

2

MGP

[60,65]

GPFR

7 и и

GMM

96 GMM

GP GMM MGP

2 IMGP

MGP

Dirichlet Pitman-Yor

IGMM GMM

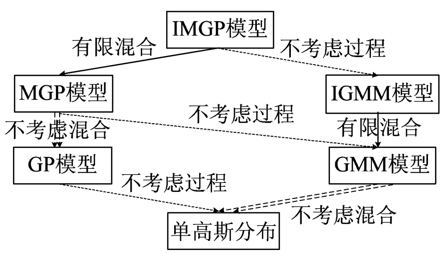
MGP

GP GMM

IMGP IGMM

“ ” IGMM

MGP GMM GP



2 GP MGP GMM

Fig. 2 The hierarchical relationship of GP MGP and GMM models where the arrows denote the direction of degeneration

IMGP

IGMM MGP GMM

1 MGP

GMM GP

IMGP MGP GP

IGMM GMM

GP MGP IMGP

8

GP

GP MGP

MGP

GP MGP GMM GP

MGP

GP

MGP

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