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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

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Tresp [7] 2000

Mixture of Gaussian Processes MGP

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1996 SVM 1992

Rasmussen [8] GP

20 GP

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[9] [10]

[9,11]

GP [12] GP MGP

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MGP MGP

GP MGP

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1 2 6 10

1 GP

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

t_1 t_2 … 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

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

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

t_{N+1}

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

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

2 GP

GP 2

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

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

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

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

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

$$t_N \propto P \; f_{N+1} \mid X_{N+1} \; \prod_{n=1}^{N+1} P \; t_n \mid f \; x_n \qquad P \; f_{N+1} \mid X_{N+1} \propto \exp\left(-\frac{1}{2} f_{N+1}^{\mathrm{T}} K_{N+1}^{-1} f_{N+1}\right)$$

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5 5 GP

[4 13] [14]

[15] 5

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GP

1 GP

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GP

GP

[16]

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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

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[55] GP

[56]

[57] [58] [59]

9 GP

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$\boldsymbol{\mu}$ 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]

$$P(\boldsymbol{t}_N \mid \boldsymbol{X}_N, \boldsymbol{\mu}) = \sum_{\boldsymbol{z}_N} \prod_i \Pr(z_i \mid x_i, \tilde{\theta}) \prod_j P(t_k, z_k=j \mid x_k, z_k=j, \theta_j^{GP}) \quad (11)$$

$$P(\boldsymbol{X}_N, \boldsymbol{t}_N \mid \boldsymbol{\theta}) = \sum_{\boldsymbol{z}_N} \prod_i \Pr(z_i \mid \tilde{\theta}) \prod_j P(t_k, z_k=j \mid x_k, z_k=j, \theta_j^{GP}) P(x_k, z_k=j \mid \tilde{\theta}_j) \quad (12)$$

j $P(t_i, z_i=j \mid x_i, z_t=j, \theta_j^{GP})$ 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 $P(x_i, z_t=j \mid \tilde{\theta}_j)$

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

MGP

9 Wang Khardon [67]

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

1

MGP

K

K [7,61,63-65,67-69,71,91] Huang [73]

Akaike

Zhao [88]

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]

MGP

3

GP MGP

MGP

MGP

[60,67,82,91] Nguyen Bonil-

la [71] MGP 3

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GPFR

MGP

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GP MGP GMM GP

MGP

GMM

[96] GMM

GP GMM MGP

2 IMGP GP

MGP MGP

Dirichlet Pitman-Yor

IGMM GMM

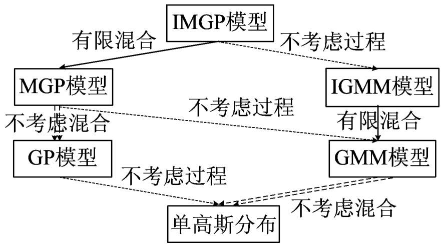
MGP

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

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