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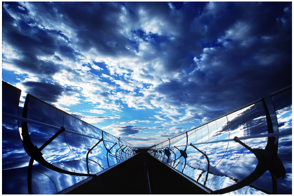

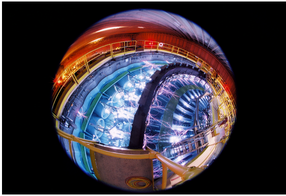

Integrated computational materials engineering with monotonic Gaussian process

ASME IDETC-CIE 2022. August 14–17, 2022. St. Louis, Missouri.

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Theron Rodgers

Nomenclature

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- $\mathbf{X} = \{\mathbf{x}^{(i)}\}_{i=1}^{N}$: training dataset of size N, $\mathbf{X} \in \mathbb{R}^{N \times D}$
- $\mathbf{x} = [\mathbf{x}_1, \ldots, \mathbf{x}_D]$: training input of D dimensionality
- $\mathbf{X}_m$: derivative inducing points, $\mathbf{X}_m \in \mathbb{R}^{m \times D}$
- $\mathbf{y}$: noisy observation $\mathbf{y}(\mathbf{x}) = \mathbf{f}(\mathbf{x}) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- $\mathbf{f}$: noiseless output $\mathbf{f}(\mathbf{x})$
- $\mathbf{f}'$: first derivative of $\mathbf{f}$
- x^*: testing input
- f^*: testing output
- N: number of data points
- M: number of inducing data points for derivatives
- D: input dimensionality
- i, j: dummy data point index
- d, g, h: dummy dimensionality index

Classical GP

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Assume a zero-mean GP,

$$\mathbf{f}|\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{f},\mathbf{f}}), \tag{1}$$

with covariance matrix defined by the squared exponential kernel

$$\text{Cov}\left[f^{(i)}, f^{(j)}\right] = \mathbf{K}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \eta^2 \exp\left[-\frac{1}{2}\sum_{d=1}^{D}\frac{(x_d^{(i)} - x_d^{(j)})^2}{\rho_d^2}\right], \tag{2}$$

Assume observations are Gaussian

$$\mathbf{y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \sigma^2\mathbf{I}), \tag{3}$$

then the testing distribution is also Gaussian

$$\begin{aligned} \mathbb{E}\left[f^*|x^*, \mathbf{y}, \mathbf{X}, \theta\right] &= \mathbf{K}_{*,\mathbf{f}}[\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}]^{-1}\mathbf{y}, \\ \mathbb{V}\left[f^*|x^*, \mathbf{y}, \mathbf{X}, \theta\right] &= \mathbf{K}_{*,*} - \mathbf{K}_{*,\mathbf{f}}[\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}]^{-1}\mathbf{K}_{\mathbf{f},*}. \end{aligned} \tag{4}$$

Trained by maximizing log likelihood

$$\log p(\mathbf{y}|\mathbf{X}, \theta) = -\frac{1}{2}\mathbf{y}^\top[\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}]^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}| - \frac{N}{2}\log(2\pi) \tag{5}$$

Classical GP: What about derivatives?

Derivative is a linear operator

$$\mathbb{E}\left[\frac{\partial f^{(i)}}{\partial x_d^{(i)}}\right] = \frac{\partial \mathbb{E}\left[f^{(i)}\right]}{\partial x_d^{(i)}}, \tag{6}$$

$$\text{Cov}\left[\frac{\partial f^{(i)}}{\partial x_d^{(i)}}, f^{(j)}\right] = \frac{\partial}{\partial x_d^{(i)}} \text{Cov}\left[f^{(i)}, f^{(j)}\right], \tag{7}$$

and

$$\text{Cov}\left[\frac{\partial f^{(i)}}{\partial x_d^{(i)}}, \frac{\partial f^{(j)}}{\partial x_g^{(j)}}\right] = \frac{\partial^2}{\partial x_d^{(i)} \partial x_g^{(j)}} \text{Cov}\left[f^{(i)}, f^{(j)}\right]. \tag{8}$$

Classical GP: What about derivatives?

. . . plug-in the squared exponential kernel

$$\text{Cov}\left[\frac{\partial f^{(i)}}{\partial x_g^{(i)}}, f^{(j)}\right] = -\eta^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{D} \rho_d^{-2}(x_d^{(i)} - x_d^{(j)})^2\right) \rho_g^{-2}\left((x_g^{(i)} - x_g^{(j)})\right), \tag{9}$$

and

$$\text{Cov}\left[\frac{\partial f^{(i)}}{\partial x_d^{(i)}}, \frac{\partial f^{(j)}}{\partial x_h^{(j)}}\right] = \eta^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{D} \rho_d^{-2}(x_d^{(i)} - x_d^{(j)})^2\right) \rho_g^{-2}\left(\delta_{gh} - \rho_h^{-2}(x_g^{(i)} - x_g^{(j)})(x_h^{(i)} - x_h^{(j)})\right), \tag{10}$$

respectively. The derivatives are analytical:

$$\mathbb{E}\left[\frac{\partial f^*}{\partial x_d^*}\right] = \frac{\partial \mathbf{K}_{*,\mathbf{f}}}{\partial x_d^*}[\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}]^{-1}\mathbf{y}, \tag{11}$$

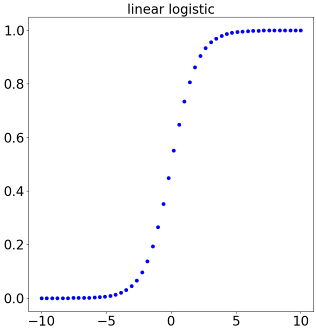
and

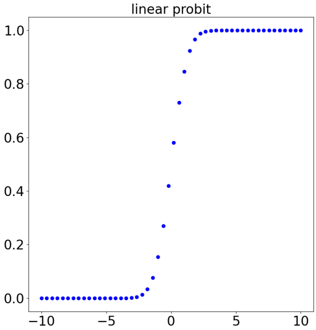
$$\mathbb{V}\left[\frac{\partial f^*}{\partial x_d^*}\right] = \frac{\partial^2 \mathbf{K}_{*,*}}{\partial x_d^* \partial x_d^*} - \frac{\partial \mathbf{K}_{*,\mathbf{f}}}{\partial x_d^*}[\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}]^{-1}\frac{\partial \mathbf{K}_{\mathbf{f},*}}{\partial x_d^*}. \tag{12}$$

Classical GP: Binary classification

$f : (-\infty, +\infty) \to (0, 1)$

- linear logistic regression: $f(x) = \frac{1}{1+\exp(-x)}$
- linear probit regression: standard normal cdf: $f(x) = \int_{-\infty}^{x} \mathcal{N}(z|0,1)dz$





Classical GP: A Bayesian perspective

A conditional of a Gaussian is also Gaussian.

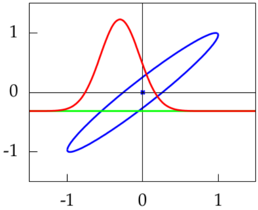


Figure: Photo courtesy of from Lawrence 2016.

If

$$P(\mathbf{f}, \mathbf{f}^*) = \mathcal{N}\left(\begin{bmatrix} \mu_{\mathbf{f}} \\ \mu_{\mathbf{f}*} \end{bmatrix}, \begin{bmatrix} A & C \\ C^\top & B \end{bmatrix}\right) \tag{13}$$

then by Bayes' rule

$$P(\mathbf{f}|\mathbf{f}^*) = \mathcal{N}(\mu_{\mathbf{f}} + CB^{-1}(f^* - \mu_{\mathbf{f}*}), A - CB^{-1}C^\top) \tag{14}$$

(cf. App. A, Quiñonero-Candela and Rasmussen 2005).

Monotonic Gaussian process: Formulation

Monotonic GP

Jaakko Riihimäki and Aki Vehtari (2010). "Gaussian processes with monotonicity information". In: *Proceedings of the thirteenth international conference on artificial intelligence and statistics*. JMLR Workshop and Conference Proceedings, pp. 645–652

Main ideas:

- augment covariance matrix with block structure (closely related to multi-fidelity and gradient-enhanced GP)

$$\mathbf{K}_{\text{joint}} = \begin{bmatrix} \mathbf{K}_{\mathbf{f},\mathbf{f}} & \mathbf{K}_{\mathbf{f},\mathbf{f}'} \\ \mathbf{K}_{\mathbf{f}',\mathbf{f}} & \mathbf{K}_{\mathbf{f}',\mathbf{f}'} \end{bmatrix} \tag{15}$$

- the augmentation constrains the derivatives w.r.t. certain variables
- binary (and numerically) classify the derivatives of whether monotonic or not with probit likelihood $\Phi(\cdot)$

Monotonic Gaussian process: Formulation

- monotonicity is imposed at M inducing locations $\mathbf{X}_m \in \mathbb{R}^{M \times D}$.
- at location $\mathbf{x}^{(i)} \in \mathbf{X}_m$, derivative of $\mathbf{f}$ is non-negative w.r.t. input dimension d_i. assume a probit likelihood at the location $\mathbf{x}^{(i)}$ as

$$p\left(m_{d_i}^{(i)} \middle| \frac{\partial f^{(i)}}{\partial x_{d_i}^{(i)}}\right) = \Phi\left(\frac{\partial f^{(i)}}{\partial x_{d_i}^{(i)}} \frac{1}{\nu}\right), \tag{16}$$

where

$$\Phi(z) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{z}{\sqrt{2}}\right)\right] = \int_{-\infty}^{z} \mathcal{N}(t|0,1)dt, \text{ small } \nu = 10^{-6} \left(\lim_{\nu \to 0} \Phi = \text{Heavyside function}\right) \tag{17}$$

- joint prior for $\mathbf{f}$ and its derivatives $\mathbf{f}'$ is given by

$$p(\mathbf{f}, \mathbf{f}'|\mathbf{X}, \mathbf{X}_m) = \mathcal{N}\left(\mathbf{f}_{\text{joint}}|\mathbf{0}, \mathbf{K}_{\text{joint}}\right), \quad \mathbf{f}_{\text{joint}} = \begin{bmatrix} \mathbf{f} \\ \mathbf{f}' \end{bmatrix}, \quad \mathbf{K}_{\text{joint}} = \begin{bmatrix} \mathbf{K}_{\mathbf{f},\mathbf{f}} & \mathbf{K}_{\mathbf{f},\mathbf{f}'} \\ \mathbf{K}_{\mathbf{f}',\mathbf{f}} & \mathbf{K}_{\mathbf{f}',\mathbf{f}'} \end{bmatrix}. \tag{18}$$

- by Bayes' rule, the joint posterior is

$$p(\mathbf{f}, \mathbf{f}'|\mathbf{y}, \mathbf{m}) = \frac{1}{Z} p(\mathbf{f}, \mathbf{f}'|\mathbf{X}, \mathbf{X}_m) p(\mathbf{y}|\mathbf{f}) p(\mathbf{m}|\mathbf{f}'), \quad p(\mathbf{m}|\mathbf{f}') = \prod_{i=1}^{M} \Phi\left(\frac{\partial f^{(i)}}{\partial x_{d_i}^{(i)}} \frac{1}{\nu}\right). \tag{19}$$

Monotonic Gaussian process: Formulation

Expectation propagation

"best Gaussian by moment matching": Thomas P Minka (2001). "Expectation propagation for approximate Bayesian inference". In: UAI'01, pp. 362–369

- the posterior is analytically intractable, local likelihood approximations are given by the expectation propagation (EP) algorithm, allowing the approximation of the posterior distribution

$$\begin{aligned} p(\mathbf{f}, \mathbf{f}' | \mathbf{y}, \mathbf{m}) &\approx q(\mathbf{f}, \mathbf{f}' | \mathbf{y}, \mathbf{m}) \\ &= \frac{1}{Z_{\text{EP}}} p(\mathbf{f}, \mathbf{f}' | \mathbf{X}, \mathbf{X}_m) p(\mathbf{y}|\mathbf{f}) \prod_{i=1}^{M} t_i(\tilde{Z}_i, \tilde{\mu}_i, \tilde{\sigma}_i^2), \end{aligned} \tag{20}$$

  where $t_i(\tilde{Z}_i, \tilde{\mu}_i, \tilde{\sigma}_i^2) = \tilde{Z}_i \mathcal{N}(f_i' | \tilde{\mu}_i, \tilde{\sigma}_i^2)$ are local likelihood approximations with site parameters $\tilde{Z}_i, \tilde{\mu}_i, \tilde{\sigma}$ from the EP algorithm.
- approximate posterior is analytically tractable as a product of Gaussian distributions and can be simplified to

$$q(\mathbf{f}, \mathbf{f}' | \mathbf{y}, \mathbf{m}) = \mathcal{N}(\mathbf{f}_{\text{joint}} | \mu, \Sigma), \tag{21}$$

$$\mu = \Sigma \tilde{\Sigma}_{\text{joint}}^{-1} \tilde{\mu}_{\text{joint}}, \quad \Sigma = [\mathbf{K}_{\text{joint}}^{-1} + \tilde{\Sigma}_{\text{joint}}^{-1}]^{-1}, \tilde{\mu}_{\text{joint}} = \begin{bmatrix} \mathbf{y} \\ \tilde{\mu} \end{bmatrix}, \quad \tilde{\Sigma}_{\text{joint}} = \begin{bmatrix} \sigma^2 \mathbf{I} & 0 \\ 0 & \tilde{\Sigma} \end{bmatrix}, \tag{22}$$

- why approximate? reduce cost complexity for computing moments of posterior from $\mathcal{O}\left(2^{N+M}\right)$ to $\mathcal{O}(N+M)$
- how? minimize KL divergence from the approximate to the true – similar to variational inference

Monotonic Gaussian process: Formulation

Training the monotonic Gaussian process with $\mathcal{O}\left((N+M)^3\right)$:

$$\log Z_{\mathrm{EP}} = -\frac{1}{2}\log|\mathbf{K}_{\text{joint}} + \tilde{\Sigma}_{\text{joint}}| - \frac{1}{2}\tilde{\mu}_{\text{joint}}^{\top}[\mathbf{K}_{\text{joint}} + \tilde{\Sigma}_{\text{joint}}]^{-1}\tilde{\mu}_{\text{joint}} + \sum_{i=1}^{M}\frac{(\mu_{-i}-\tilde{\mu}_i)^2}{2(\sigma_{-i}^2+\tilde{\sigma}_i^2)} + \sum_{i=1}^{M}\log\Phi\left(\frac{\mu_{-i}}{\nu\sqrt{\frac{1+\sigma_{-i}^2}{\nu^2}}}\right) + \frac{1}{2}\sum_{i=1}^{M}\log(\sigma_{-i}^2+\tilde{\sigma}_i^2), \tag{23}$$

Predictions:

$$\mathbb{E}\left[f^*|x^*, \mathbf{y}, \mathbf{X}, \mathbf{m}, \mathbf{X}_m\right] = \mathbf{K}_{*,\text{joint}}[\mathbf{K}_{\text{joint}} + \tilde{\Sigma}_{\text{joint}}]^{-1}\tilde{\mu}_{\text{joint}} \tag{24}$$

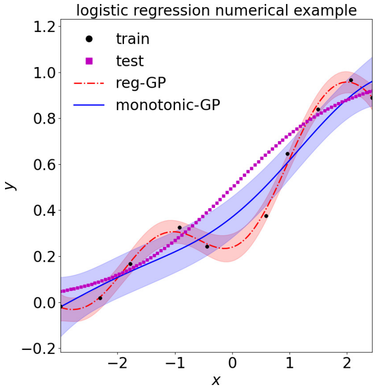
and

$$\mathbb{V}\left[f^*|x^*, \mathbf{y}, \mathbf{X}, \mathbf{m}, \mathbf{X}_m\right] = \mathbf{K}_{*,*} - \mathbf{K}_{*,\text{joint}}[\mathbf{K}_{\text{joint}} + \tilde{\Sigma}_{\text{joint}}]^{-1}\mathbf{K}_{*,\text{joint}}. \tag{25}$$

Numerical example 1

$$y = \frac{1}{1 + e^{-x}} + \varepsilon, \qquad (26)$$

- large homoscedastic noise $\varepsilon \sim \mathcal{N}(0, 0.1^2)$
- $x \in [-3, 3]$
- 10 samples
- true / test
- monotonic GP
- classical GP



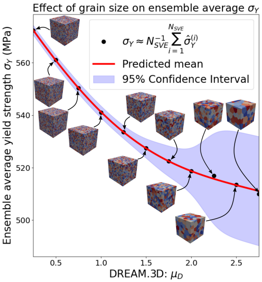
better approximation by the monotonic GP over the classical GP.

Semi-numerical example 2

Hall-Petch by CPFEM: smaller grain is stronger

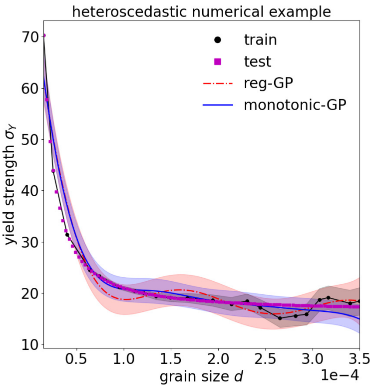
$$\sigma_Y = 16.47 + \varepsilon(d) + 0.0000288 \frac{1}{(10^{-6} \cdot d)^{1.3}} \quad (27)$$

- large heteroscedastic noise $\varepsilon(d) \sim \mathcal{N}(0, 2.2 \cdot 10^{10} \cdot d^3)$
- $d \in [15\mu m, 350\mu m]$



Tran and Wildey 2020 JOM

Hall-Petch relationship

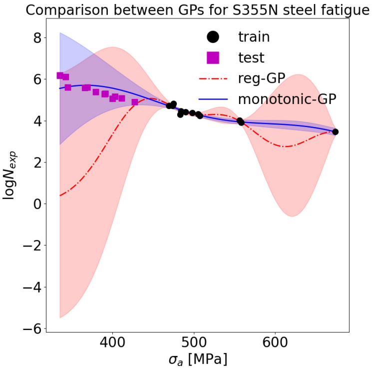


constrain GP to physics

Fatigue life prediction under multiaxial loading

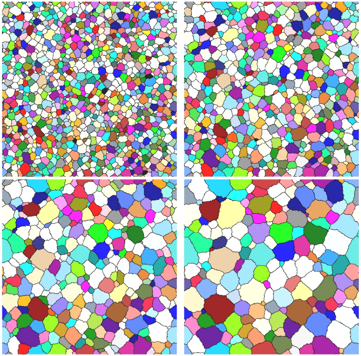
- dataset from Karolczuk and Słoński Karolczuk and Słoński 2022; Karolczuk and Kluger 2020
- 12 training data points
- 13 testing data points (extrapolatory)
- SN-curve

$$\log N_{\text{exp}} = A - B \log \sigma_a, \quad (28)$$

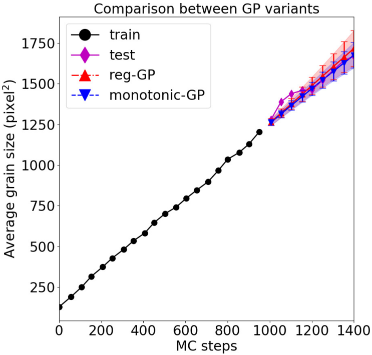


Monotonic GP can extrapolate (in short range).

Kinetic Monte Carlo for grain growth simulations (SNL/SPPARKS)

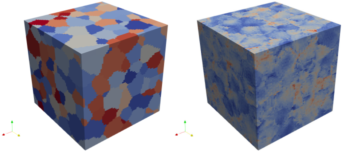


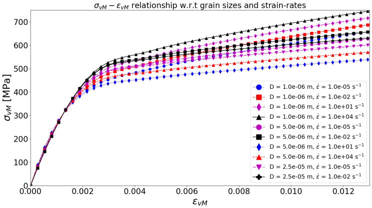
Grain growth simulation via kinetic Monte Carlo (SPPARKS).



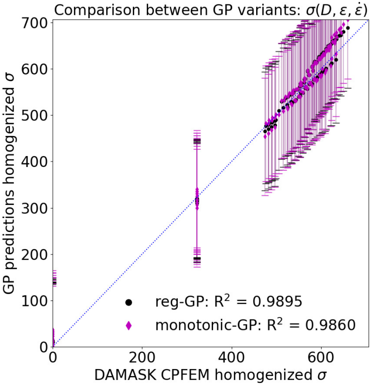
comparable performance between classical and monotonic GPs.

$\dot{\varepsilon}$-dependent $\sigma - \varepsilon$ with crystal plasticity FEM





$\sigma - \varepsilon$ compilation as a function of D and $\dot{\varepsilon}$



comparable performance between classical and monotonic GPs.

Conclusion

In this talk, we

- summarize the monotonic GP formulations(Riihimäki and Vehtari 2010)
- demonstrate with 2 numerical examples + 3 engineering models

Monotonic GP:

- works well for sparse + (very) noisy dataset,
- performs (slightly) worse with already monotonic dataset,
- might be useful for short-range extrapolation if physics support.

Thank you for listening.

Methodology:

- Anh Tran et al. (Aug. 2020c). "srMO-BO-3GP: A sequential regularized multi-objective constrained Bayesian optimization for design applications". In: *Proceedings of the ASME 2020 IDETC/CIE*. vol. Volume 1: 40th Computers and Information in Engineering Conference. International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. American Society of Mechanical Engineers
- Anh Tran et al. (2022). "aphBO-2GP-3B: a budgeted asynchronous parallel multi-acquisition functions for constrained Bayesian optimization on high-performing computing architecture". In: *Structural and Multidisciplinary Optimization* 65.4, pp. 1–45
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- Anh Tran et al. (2019a). "pBO-2GP-3B: A batch parallel known/unknown constrained Bayesian optimization with feasibility classification and its applications in computational fluid dynamics". In: *Computer Methods in Applied Mechanics and Engineering* 347, pp. 827–852

Applications:

- Anh Tran and Tim Wildey (2020). "Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning". In: *JOM* 73, pp. 72–89
- Anh Tran et al. (2020b). "Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys". In: *The Journal of Chemical Physics* 153 (7), p. 074705
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- Anh Tran et al. (2019b). "WearGP: A computationally efficient machine learning framework for local erosive wear predictions via nodal Gaussian processes". In: *Wear* 422, pp. 9–26
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