- 400 for initial design, via LHS
- 800 for the BO process.

To make significant, the comparison between the two schemes, penalty and SVM-CBO, they share the same initial design. They also share all the other choices, more precisely the probabilistic surrogate model (GP) and the acquisition function (LCB), so that the difference in the result can be only motivated by the usage, or not, of the estimate of the feasible region. Since the value $f(x^*)$ is not known for this case study, the Gap metrics cannot be used as metric, differently from the test functions reported in Chap. 5. The minimum value of the objective function observed at the end of the approaches, that is the energy cost associated to the best seen pump schedule, has been directly considered as metric.

As already reported by the authors in their previous work (Candelieri et al. 2018), assigning a penalty to function evaluations outside the feasible region has the aim to move towards feasible points/regions. Although this is usual the usual solution adopted, it is quite naïve in this problem especially when the penalty cannot be made dependent on the entity of violation. This leads to almost "flat" objective functions, especially when the unknown feasible region results extremely narrow with respect to the overall search space. As already reported, the real-life PSO case study seems to be characterized by this kind of situation.

BO with penalty was not able to provide any improvement with respect to the energy cost identified on the initial design that is 172.89€. On the contrary, SVM-CBO was able to further reduce the energy to 168.60€, by identifying a new and more efficient pump schedule. A significantly relevant result is that the improvement has been registered exactly at the starting of phase 2, just shown for the test functions in Chap. 5. This result proves that solving feasibility determination and constraining the following sequential optimization process to an accurate estimate of the feasible region can significantly improve the effectiveness and efficiency of the BO process.

A comment is due about the optimal value which is significantly lower than the average pumping cost because the pilot zone was equipped with VSP's and monitored and maintained specifically for the european project.

References

Aggarwal, C.C.: Recommender systems, pp. 1–28. Springer International Publishing, Cham (2016)

Archetti, F., Giordani, I., Vanneschi, L.: Genetic programming for QSAR investigation of docking energy. Appl. Soft Comput. **10**(1), 170–182 (2010)

Ashmaig, O., Connolly, M., Gross, R.E., Mahmoudi, B.: Bayesian optimization of asynchronous distributed microelectrode theta stimulation and spatial memory. In: 2018 40th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC), pp. 2683–2686 (2018)

Azimi, J., Jalali, A., Fern, X.: Hybrid batch Bayesian optimization 1–12 (2012). doi:10.1.1.467.8687. arXiv preprint arXiv:1202.5597

Baheri, A., Vermillion, C.: Combined plant and controller design using batch Bayesian optimization: a case study in airborne wind energy systems. J. Dyn. Syst. Meas. Control (2019)

Balachandran, P.V., Xue, D., Theiler, J., Hogden, J., Lookman, T.: Adaptive strategies for materials design using uncertainties. Scientific Reports. **6** (2016). https://doi.org/10.1038/srep19660

Bansal, S., Calandra, R., Xiao, T., Levine, S., Tomiin, C.J.: Goal-driven dynamics learning via Bayesian optimization. In: 017 IEEE 56th Annual Conference on Decision and Control (CDC), pp. 5168–5173. IEEE (2017)

Bogunovic, I., Scarlett, J., Jegelka, S., Cevher, V.: Adversarially Robust Optimization with Gaussian Processes. In: Advances in Neural Information Processing Systems, pp. 5760–5770 (2018)

Candelieri, A., Giordani, I., Archetti, F.: Automatic configuration of Kernel-based clustering: an optimization approach. In: International Conference on Learning and Intelligent Optimization, pp. 34–49. Springer, Cham (2017, June)

Candelieri, A., Soldi, D., Archetti, F.: Cost-effective sensors placement and leak localization—The Neptune pilot of the ICeWater project. J. Water Supply Res. Technol. AQUA. 567–582 (2015)

Candelieri, A., Perego, R., Archetti, F.: Bayesian optimization of pump operations in water distribution systems. J. Global Optim. **71**, 213–235 (2018). https://doi.org/10.1007/s10898-018-0641-2

Chaudhuri, A., Marques, A.N., Lam, R., Willcox, K.: Reusing Information for Multifidelity Active Learning in Reliability-Based Design Optimization. AIAA Scitech 2019 Forum. 1–12 (2019). https://doi.org/10.2514/6.2019-1222

Cheng, L.-F., Darnell, G., Dumitrascu, B., Chivers, C., Draugelis, M.E., Li, K., Engelhardt, B.E.: Sparse multi-output gaussian processes for medical time series prediction (2017). arXiv preprint arXiv:1703.09112

Colopy, G.W., Pimentel, M.A.F.F., Roberts, S.J., Clifton, D.A.: Bayesian optimisation of Gaussian processes for identifying the deteriorating patient. In: 2017 IEEE EMBS International Conference on Biomedical and Health Informatics, BHI 2017. pp. 85–88 (2017)

Colopy, G.W., Roberts, S.J., Clifton, D.A.: Bayesian optimization of personalized models for patient vital-sign monitoring. IEEE J. Biomed. Health Inform. **22**, 301–310 (2018). https://doi.org/10.1109/JBHI.2017.2751509

Cooper, J., Cervenansky, F., De Fabritiis, G., Fenner, J., Friboulet, D., Giorgino, T., Manos, S., Martelli, Y., Villá-Freixa, J., Zasada, S., Lloyd, S., Mccormack, K., Coveney, P.V.: The virtual physiological human toolkit. Philos. Trans. Royal Soc. A Mathe. Phys Eng. Sci. **368**, 3925–3936 (2010). https://doi.org/10.1098/rsta.2010.0144

Crespo-Vazquez, J.L., Carrillo, C., Diaz-Dorado, E., Martinez-Lorenzo, J.A., Noor-E-Alam, M.: A machine learning based stochastic optimization framework for a wind and storage power plant participating in energy pool market. Appl. Energy **232**, 341–357 (2018). https://doi.org/10.1016/j.apenergy.2018.09.195

Dolatnia, N., Fern, A., Fern, X.: Toward embedding Bayesian optimization in the lab: reasoning about resource and actions. In: AAAI Fall Symposium—Technical Report (2015)

Dong, G., Chen, Z.: Data-driven energy management in a home microgrid based on Bayesian optimal algorithm. IEEE Trans. Industr. Inf. **15**(2), 869–877 (2019)

Fersini, E., Messina, E., Archetti, F.: A p-median approach for predicting drug response in tumour cells. BMC Bioinform. **15** (2014). https://doi.org/10.1186/s12859-014-0353-7

Galuzzi, B.G., Perego, R., Candelieri, A., Archetti, F.: Bayesian optimization for full waveform inversion. In: Daniele P., S.L. (eds.) New Trends in Emerging Complex Real Life Problems, pp. 257–264. Springer International Publishing, Taormina (2018)

Garnett, R., Osborne, M.A., Roberts, S.J.: Bayesian optimization for sensor set selection. In: Proceedings of the 9th ACM/IEEE International Conference on Information Processing in Sensor Networks—IPSN'10, pp. 209–219. Stockholm (2010)

Ghoreishi, S.F., Allaire, D.: Multi-information source constrained Bayesian optimization. Struct. Multidisciplinary Optim. 1–15 (2018). https://doi.org/10.1007/s00158-018-2115-z

Ghosh, S., Berkenkamp, F., Ranade, G., Qadeer, S., Kapoor, A.: Verifying Controllers Against Adversarial Examples with Bayesian Optimization. In: IEEE International Conference on Robotics and Automation (ICRA). pp. 7306–7313, Brisbane (2018)

Golovin, D., Solnik, B., Moitra, S., Kochanski, G., Karro, J., Sculley, D.: Google Vizier: A Service for Black-Box Optimization. In: Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. pp. 1487–1495. ACM (2017)

Gonzalvez, J., Lezmi, E., Roncalli, T., Xu, J.: Financial applications of Gaussian processes and Bayesian optimization (2019). arXiv preprint arXiv:1903.04841

Gordon, D.F.N.N., Matsubara, T., Noda, T., Teramae, T., Morimoto, J., Vijayakumar, S.: Bayesian Optimisation of Exoskeleton Design Parameters. In: Proceedings of the IEEE RAS and EMBS International Conference on Biomedical Robotics and Biomechatronics, pp. 653–658 (2018)

Griffiths, R.-R., Hernández-Lobato, J.M.: Constrained Bayesian optimization for automatic chemical design (2017). arXiv preprint arXiv:1709.05501

Ju, S., Shiga, T., Feng, L., Hou, Z., Tsuda, K., Shiomi, J.: Designing nanostructures for phonon transport via Bayesian optimization. Phys. Rev. X **7**(2), 021024 (2017)

Kim, M., Ding, Y., Malcolm, P., Speeckaert, J., Siviy, C.J., Walsh, C.J., Kuindersma, S.: Human-in-the-loop Bayesian optimization of wearable device parameters. PloS one. **12**(9), e0184054 (2017)

Kitchen, D.B., Decornez, H., Furr, J.R., Bajorath, J.: Docking and scoring in virtual screening for drug discovery: methods and applications. Nat. Rev. Drug Discov. **3**(11), 935 (2004)

Kiyohara, S., Oda, H., Tsuda, K., Mizoguchi, T.: Acceleration of stable interface structure searching using a kriging approach. Japanese J. Appl. Phys. **55** (2016). https://doi.org/10.7567/jjap.55.045502

Lam, R., Willcox, K., Wolpert, D.H.: Bayesian optimization with a finite budget: an ap-proximate dynamic programming approach. Adv. Neural. Inf. Process. Syst. **30**, 883–891 (2016). https://doi.org/10.1186/1471-2407-4-76

Lancaster, J., Lorenz, R., Leech, R., Cole, J.H.: Bayesian optimization for neuroimaging pre-processing in brain age classification and prediction. Front. Aging Neuro. **10**, 28 (2018)

Letham, B., Karrer, B., Ottoni, G., Bakshy, E.: Constrained Bayesian optimization with noisy experiments. Bayesian Anal. **14**(2), 495–519 (2019)

Liang, X.: Image-based post-disaster inspection of reinforced concrete bridge systems using deep learning with Bayesian optimization. Comput.-Aided Civil Infrastruct. Eng (2018). https://doi.org/10.1111/mice.12425

Li, C., Pan, Q.: Adaptive optimization methodology based on Kriging modeling and a trust region method. Chinese J. Aeronaut. (2019). https://doi.org/10.1016/j.cja.2018.11.012

Liu, S., Yue, Y., Krishnan, R.: Adaptive collective routing using gaussian process dynamic congestion models. In: Proceedings of the 19th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp. 704–712. ACM (2013, August)

Lookman, T., Balachandran, P.V., Xue, D., Yuan, R.: Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design. Computat. Mater. **5**, 21 (2019). https://doi.org/10.1038/s41524-019-0153-8

Lorenz, R., Monti, R.P., Violante, I.R., Anagnostopoulos, C., Faisal, A.A., Montana, G., Leech, R.: The automatic neuroscientist: a framework for optimizing experimental design with closed-loop real-time fMRI. NeuroImage **129**, 320–334 (2016). https://doi.org/10.1016/j.neuroimage.2016.01.032

Lorenz, R., Simmons, L.E., Monti, R.P., Arthur, J.L., Limal, S., Laakso, I., Leech, R., Violante, I.R.: Efficiently searching through large tACS parameter spaces using closed-loop Bayesian optimization. Brain Stimul. (2019)

Mala-Jetmarova, H., Sultanova, N., Savic, D.: Lost in optimisation of water distribution systems? A literature review of system operation. Environ. Model Softw. **93**, 209–254 (2017)

Marco, A., Berkenkamp, F., Hennig, P., Schoellig, A. P., Krause, A., Schaal, S., Trimpe, S.: Virtual versus real: trading off simulations and physical experiments in reinforcement learning with bayesian optimization. In: 2017 IEEE International Conference on Robotics and Automation (ICRA), pp. 1557–1563. IEEE (2017, May)

Meldgaard, S.A., Kolsbjerg, E.L., Hammer, B.: Machine learning enhanced global optimization by clustering local environments to enable bundled atomic energies. J. Chem. Phys. **149** (2018). https://doi.org/10.1063/1.5048290

Moustakis, N., Mulders, S. P., Kober, J., van Wingerden, J.W.A.: Practical Bayesian optimization approach for the optimal estimation of the rotor effective wind speed (2019)

Naoum-Sawaya, J., Ghaddar, B., Arandia, E., Eck, B.: Simulation-optimization approaches for water pump scheduling and pipe replacement problems. Eur. J. Oper. Res. **246**, 293–306 (2015). https://doi.org/10.1016/j.ejor.2015.04.028

Negoescu, D.M., Frazier, P.I., Powell, W.B.: The knowledge-gradient algorithm for sequencing experiments in drug discovery. INFORMS J. Comput. **23**, 346–363 (2011). https://doi.org/10.1287/ijoc.1100.0417

Neumann-brosig, M., Marco, A., Schwarzmann, D., Trimpe, S.: Data-efficient Auto-tuning with Bayesian optimization: an industrial control study (2018). arXiv preprint arXiv:1812.06325

Olofsson, S., Mehrian, M., Calandra, R., Geris, L., Deisenroth, M., Misener, R.: Bayesian multi-objective optimisation with mixed analytical and black-box functions: application to tissue engineering, (2018)

Packwood, D.: Bayesian Optimization for Materials Science. Springer (2017)

Palar, P.S., Dwianto, Y.B., Regis, R.G., Oyama, A., Zuhal, L.R.: Benchmarking Constrained Surrogate-based Optimization on Low Speed Airfoil Design Problems (2019)

Pecci, F., Abraham, E., Stoianov, I.: Quadratic head loss approximations for optimisation problems in water supply networks, J. Hydroinformatics. **19**, 493–506 (2017). ISSN: 1464-7141

Pirot, G., Krityakierne, T., Ginsbourger, D., Renard, P.: Contaminant source localization via Bayesian global optimization. Hydrol. Earth Syst. Sci. **23**(1) (2019)

Polymenakos, K., Abate, A., Roberts, S.: Safe policy search using Gaussian process models. In: Proceedings of the 18th International Conference on Autonomous Agents and MultiAgent Systems, pp. 1565–1573. International Foundation for Autonomous Agents and Multiagent Systems (2019, May)

Przystałka, P.: Performance optimization of a leak detection scheme for water distribution networks. IFAC-PapersOnLine **51**(24), 914–921 (2018)

Pyzer-Knapp, E.O.: Bayesian optimization for accelerated drug discovery. IBM J. Res. Develop. 1–1 (2018). https://doi.org/10.1147/jrd.2018.2881731

Sano, S., Kadowaki, T., Tsuda, K., Kimura, S.: Application of bayesian optimization for pharmaceutical product development. J. Pharmaceutical Innov. 1–11 (2019)

Schillinger, M., Hartmann, B., Skalecki, P., Meister, M., Nguyen-Tuong, D., Nelles, O.: Safe active learning and safe Bayesian optimization for tuning a PI-controller. IFAC-PapersOnLine **50**, 5967–5972 (2017). https://doi.org/10.1016/j.ifacol.2017.08.1258

Seko, A., Maekawa, T., Tsuda, K., Tanaka, I.: Machine learning with systematic density-functional theory calculations: Application to melting temperatures of single- and binary-component solids. Phys. Rev. B Condens. Matter Mater. Phys. **89** (2014). https://doi.org/10.1103/physrevb.89.054303

Seko, A., Togo, A., Hayashi, H., Tsuda, K., Chaput, L., Tanaka, I.: Prediction of low-thermal-conductivity compounds with first-principles anharmonic lattice-dynamics calculations and bayesian optimization. Phys. Rev. Lett. **115** (2015). https://doi.org/10.1103/physrevlett.115.205901

Solomou, A., Zhao, G., Boluki, S., Joy, J.K., Qian, X., Karaman, I., Arroyave, R., Lagoudas, D.C.: Multi-objective bayesian materials discovery: Application on the discovery of precipitation strengthened NiTi shape memory alloys through micromechanical modeling. Mater. & Des. **160**, 810–827 (2018)

Tsai, Y.-A., Pedrielli, G., Mathesen, Logan Zabinsky, Z.B., Huang, H., Candelieri, Antonio Perego, R.: Stochastic optimization for feasibility determination: an application to water pump operation in water distribution network. In: Proceedings of the 2018 Winter Simulation Conference, pp. 1945–1956. IEEE, Gothenburg, Sweden (2018)

Turchetta, M., Makarova, A., Beyeler, S.: Calibration of agent based transport simulations with multi-fidelity Bayesian optimization. In: 18th Swiss Transport Research Conference (STRC 2018) (2018)

Vanchinathan, H.P., Nikolic, I., De Bona, F., Krause, A.: Explore-exploit in top-N recommender systems via Gaussian processes. In: Proceedings of the 8th ACM Conference on Recommender systems—RecSys'14, pp. 225–232 (2014)

Wang, H., Jin, Y.: A random forest-assisted evolutionary algorithm for data-driven constrained multiobjective combinatorial optimization of trauma systems. IEEE Trans. Cybern (2018). https://doi.org/10.1109/tcyb.2018.2869674

Zhan, H., Gomes, G., Li, X.S., Madduri, K., Wu, K.: Efficient online hyperparameter optimization for Kernel ridge regression with applications to traffic time series prediction. **89**, 1–19 (2018). arXiv preprint arXiv:1811.00620