Machine Learning in Healthcare

#L17-Neural Networks III

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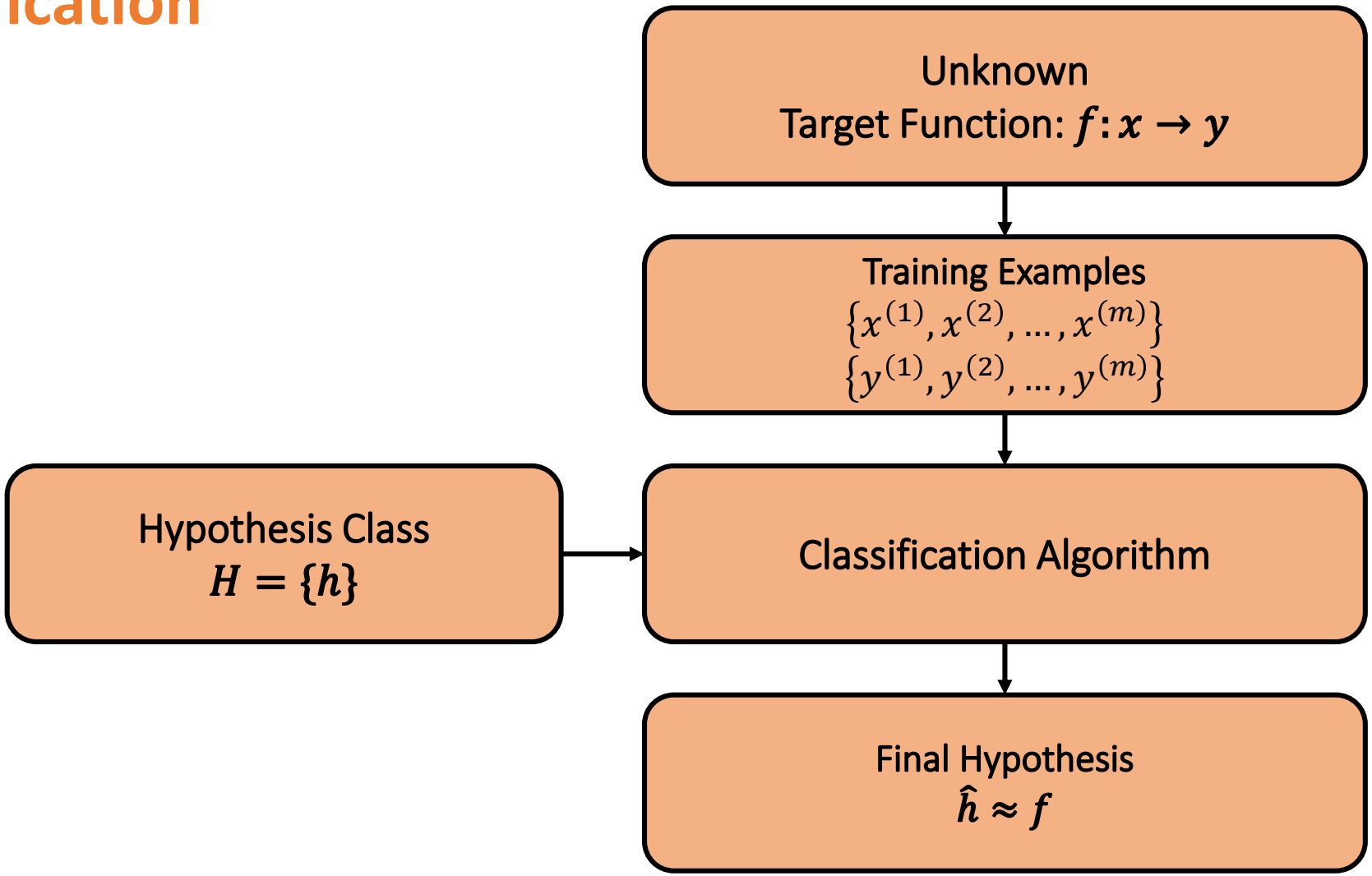
Classification



Hyperparameters tuning

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Hyperparameters versus parameters

- **Parameters:** are the parameters that define the model and that we want to learn through the training process with gradient descent.
  - $\forall\, l \in [1: L], W^{[l]}, b^{[l]}$
- **Hyperparameters:** other parameters that are set before the learning process is started but that have an influence on the classifier performances.
  - E.g. α, L
  - Need to search for these hyperparameters values to ensure a good model architecture.

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Hyperparameters

- With SVM we have a few typical hyperparameters C and γ.
- However, ***lots*** of hyperparameters in deep learning models. Some examples:

Symbol	
α	Learning rate.
β	Momentum
p	Mini batch size
K	Number of iterations for gradient descent.
$n_h^{[l]}$	Number of hidden units of the l^{th} layer.
L	Number of layers in a neural network.
$g^{[l]}$	Activation function for layer l.
k	Learning rate decay
	Features scaling method
	Other model specific hyperparameters (e.g. convolution kernel width in CNN.)

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Hyperparameters

- We will denote θ the set of hyperparameters we want to optimize for.
- Our goal is to find the values of θ that gives the best performance on the validation set.
- How do we find the best configuration of these hyperparameters in such a high dimensional search space?
  - Baby sitting,
  - Grid search,
  - Random search,
  - Bayesian optimization.

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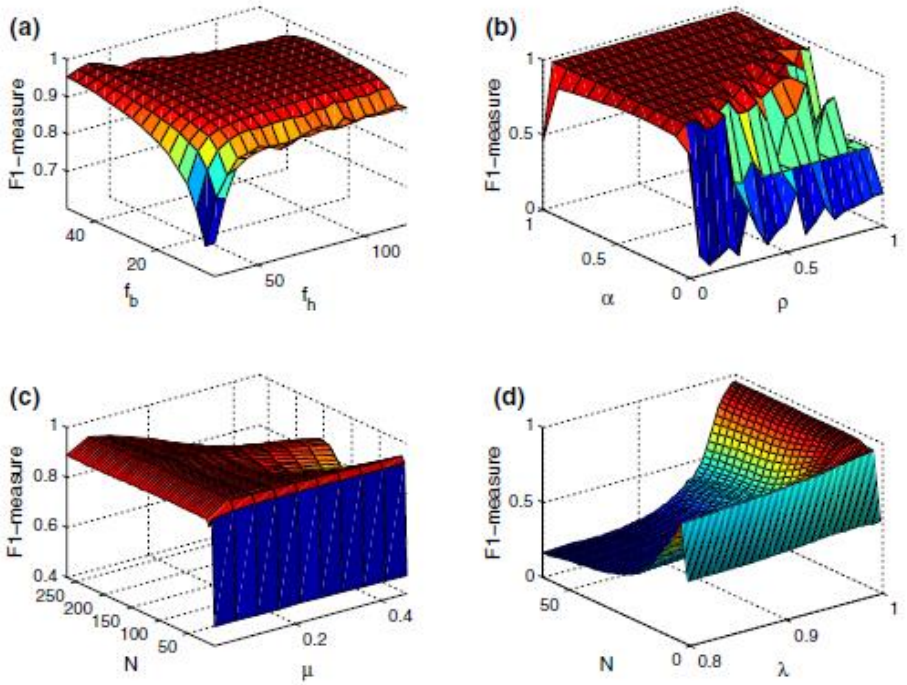
Babysitting

- Also known as the “Grad Student Descent”!
  - Iterate sequentially,
  - Manual.
- Usually keep doing that until you are running out of time for your assignment!
- This is meaningful in an initial stage of development to get a feel of what hyperparameters are particularly important for example. But then you need to quickly move to some more clever search algorithms.

Grid search

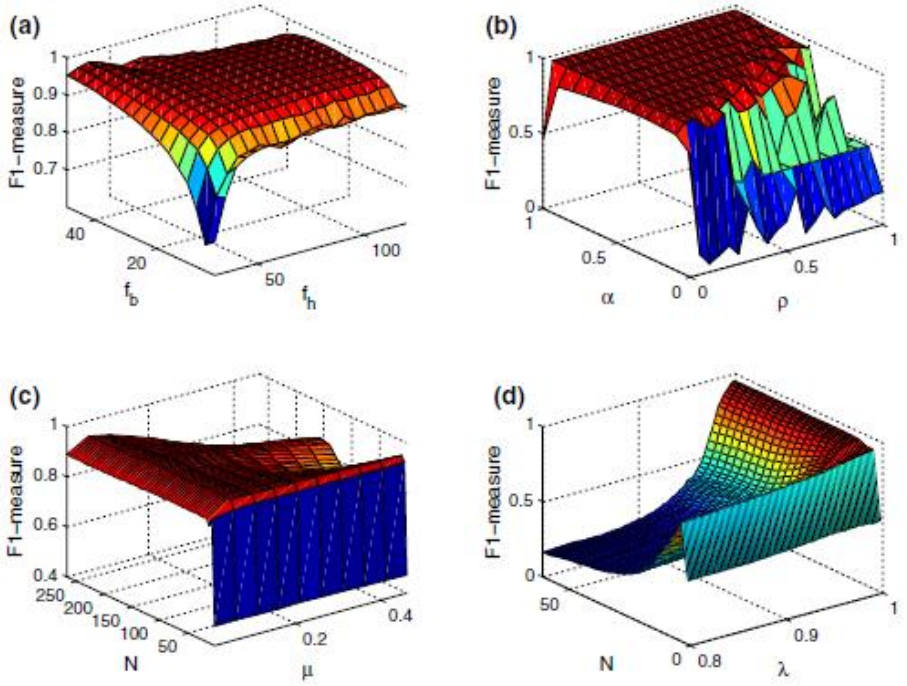
- The “just try everything” approach.
- Grid-search steps:
  - Define the p hyper-parameters,
  - For each one, define the range of possible values,
  - Search all possible configurations and report the performance.



Behar, Joachim, et al. "A comparison of single channel fetal ECG extraction methods." Annals of biomedical engineering 42.6 (2014): 1340-1353.

Grid search

- Pluses:
  - Will find a good combination of hyperparameters.
  - Can perform the search in parallel.
- Minuses:
  - Does not take into account the computation history.
  - Search space increases exponentially with the number of dimension: *curse of dimensionality*.
    - E.g. p hyperparameters, search of 5 values in a given range will require $5p$ iterations.



Behar, Joachim, et al. "A comparison of single channel fetal ECG extraction methods." Annals of biomedical engineering 42.6 (2014): 1340-1353.

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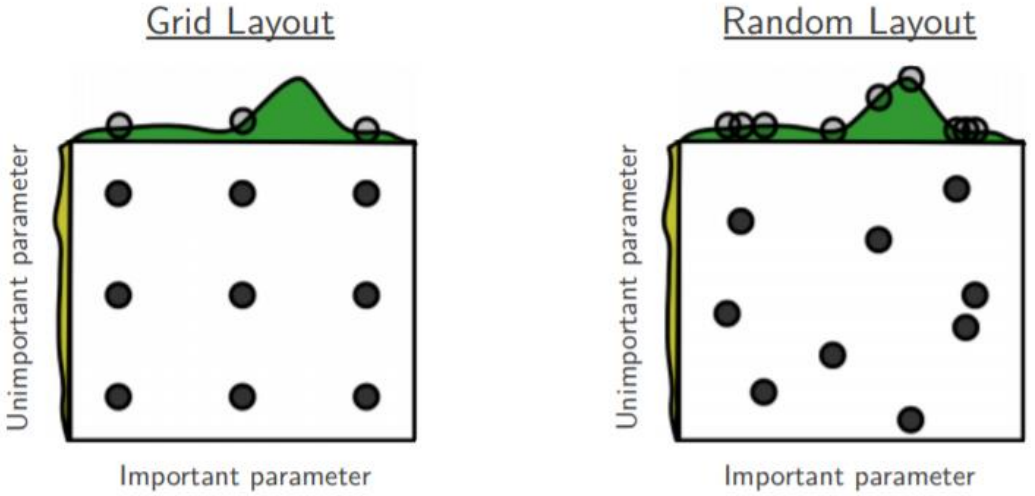
Random search

- Random-search steps:
  - Define the p hyper-parameters,
  - For each one, define the range of possible values,
  - ~~Search all possible configurations~~ sample randomly from the hyperparameters space and report the performance.



Bergstra, James, and Yoshua Bengio. "Random search for hyper-parameter optimization." Journal of Machine Learning Research 13.Feb (2012): 281-305.

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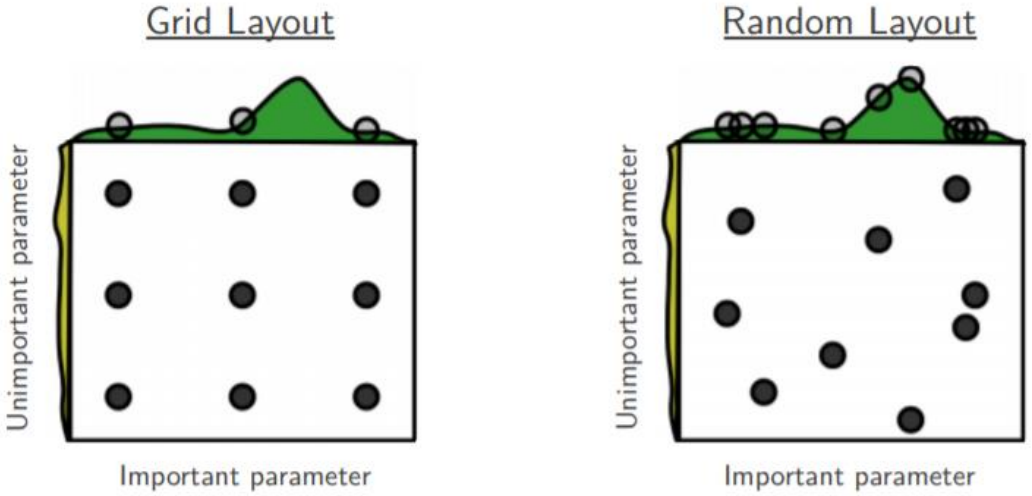
Random search

- Pluses:
  - Explore the hyperparameters space more widely in a given number of iterations than grid search. This will help find a good configuration with fewer iteration.
  - Enables the inclusion of prior knowledge by specifying the distribution from which you are sampling from.
  - Can perform the search in parallel.
- Minuses:
  - Still does not take into account the computation history.



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Hyperparameters versus parameters

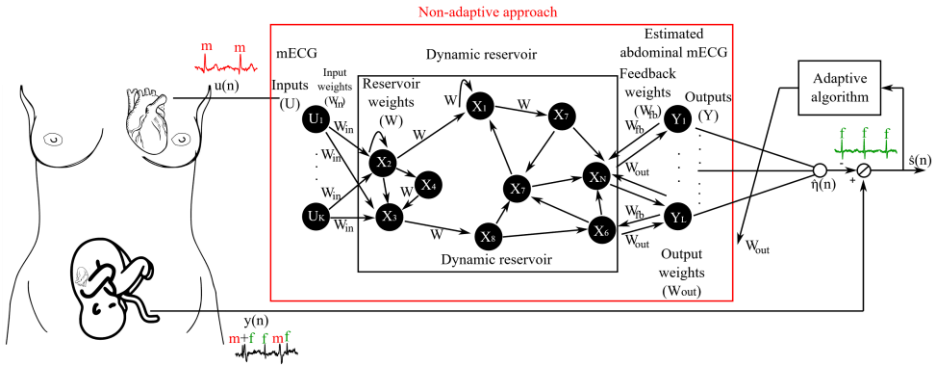
- Random search:

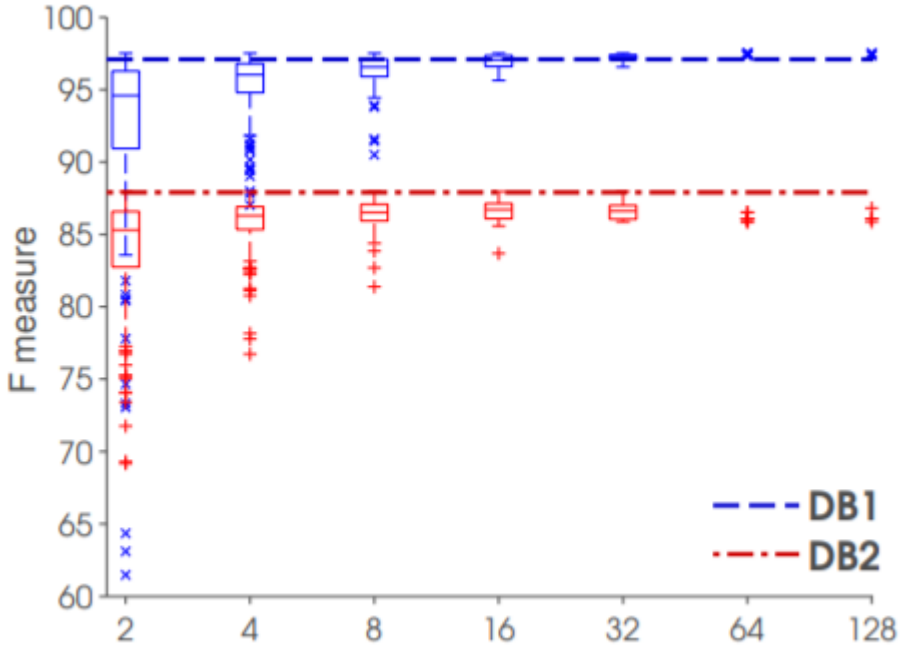
Table 1: Parameters search range and optimal parameters found for the preprocessing step and the ESN. GS: grid search. RS: random search. $\mathcal{U}$: uniform distribution.

Parameter	Search GS (step size)	Search RS	Optimal parameters GS	Optimal parameters RS
Low pass filter cut-off, f_b	[1, 49] (3)	$\mathcal{U} \sim [1, 50]$	20	26
High pass filter cut-off, f_h	[50, 120], (5)	$\mathcal{U} \sim [50, 120]$	95	87
Leakage, α	[0, 1] (0.1)	$\mathcal{U} \sim [0, 1]$	0.4	0.974
Spectral radius of W, ρ	[0, 1] (0.1)	$\mathcal{U} \sim [0, 1]$	0.4	0.821
Units in the reservoir, M	[10, 250] (20)	$\mathcal{U} \sim [10, 250]$	90	135
Scaling of W_{in}, γ	1	$\mathcal{U} \sim [0, 1]$	1	0.622
Seed value, s^1	–	$\mathcal{U} \sim [0, 10000]$	–	1588

Table 2: Performance comparison of the optimal parameters obtained by grid search (GS), random search (RS, best across 32 iterations $\pm$ 1 standard error), and template subtraction (TS).

Method — Statistics	DB_1 ESN-GS	DB_1 ESN-RS	DB_1 TS	DB_2 ESN-GS	DB_2 ESN-RS	DB_2 TS
Se	97.1	97.3 ± 0.29	90.3	87.6	87.6 ± 0.73	86.4
PPV	97.3	97.5 ± 0.28	90.0	86.5	85.5 ± 0.53	85.2
F_1	97.2	97.4 ± 0.27	90.1	87.9	86.5 ± 0.62	85.8





Behar, Joachim, et al. "An echo state neural network for foetal ECG extraction optimised by random search." Proc. Adv. Neural Inf. Process. Syst (2013).

Bayesian optimization

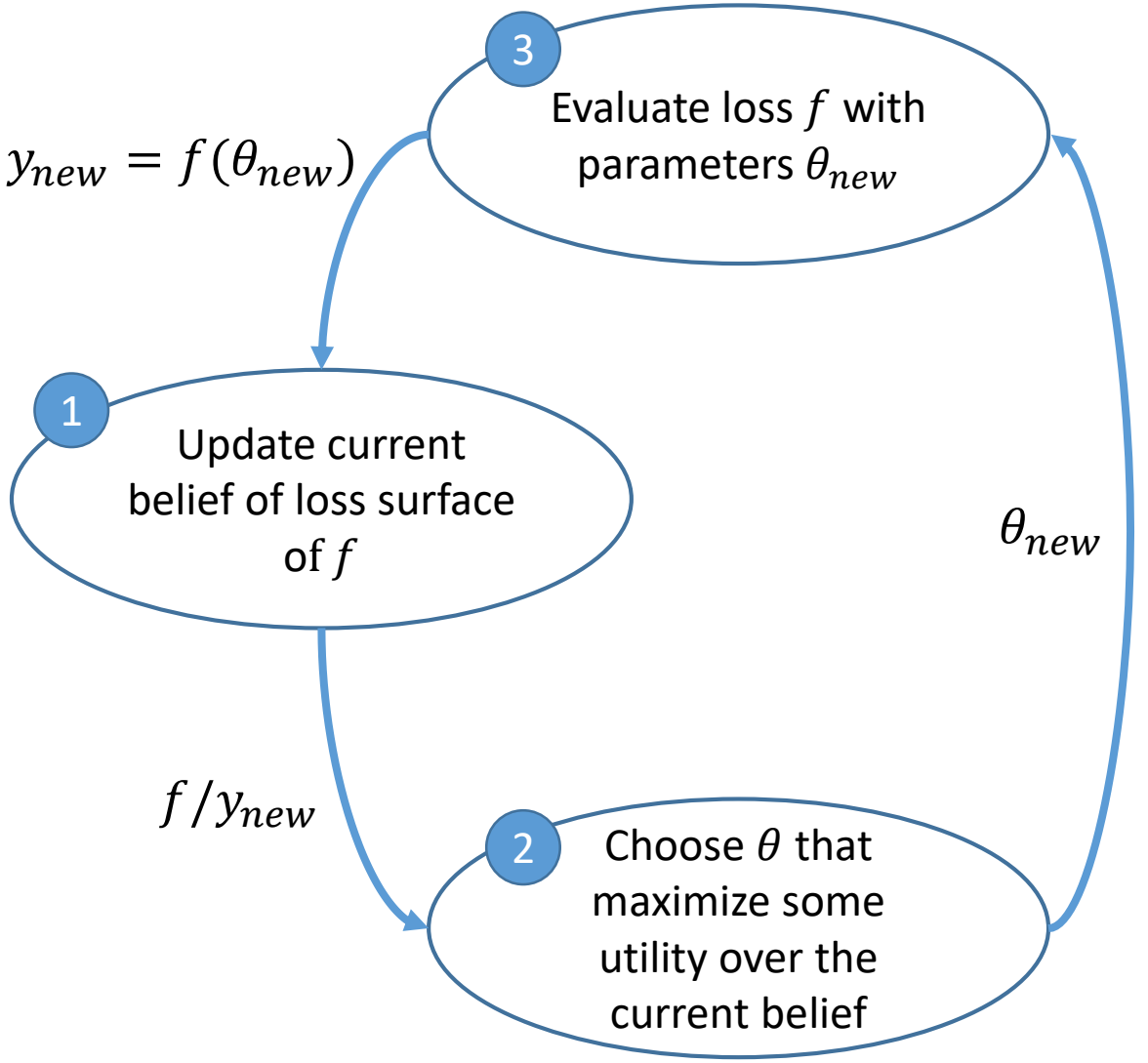
- Bayesian optimization: probability model for the loss function and sequentially move in that region of better performance.
  - It is a type of sequential model-based optimization (SMBO).
- We define the performance/cost function $f(\theta)$ given a dataset D.
  - We seek $\theta^* = argmin_{\theta \in \chi}(f(\theta))$
  - We can evaluate f for any θ but we do not have an easy functional form for it or gradients.
  - We seek to use Gaussian Processes (GP) to estimate f based on the points $\theta_{1:n}$ it was explicitly evaluated for and return the marginal means and variances.

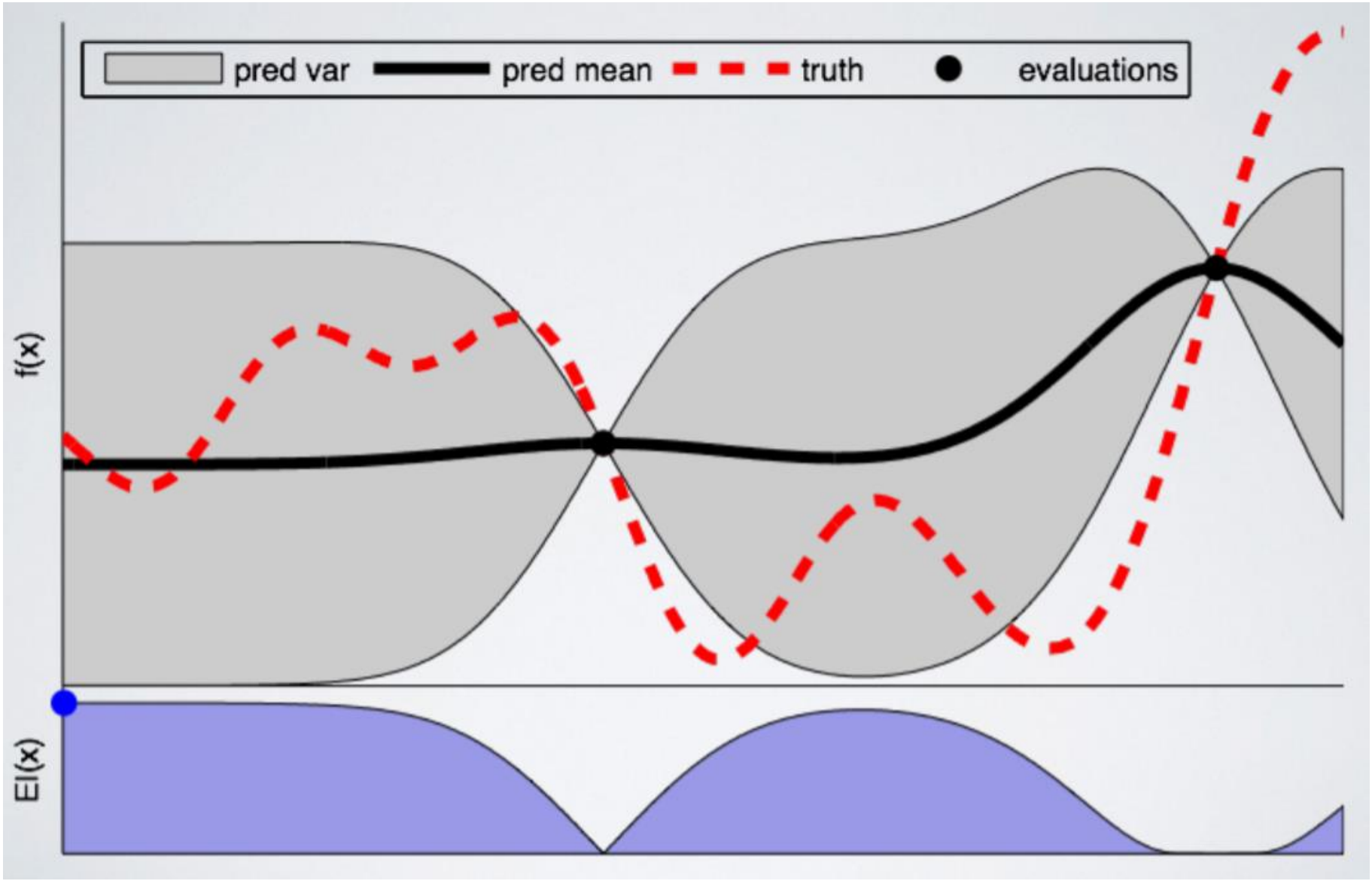
Bayesian optimization

- Bayesian optimization steps:
  - Use previous observations of the loss f to evaluate it,
  - Find the next (optimal) point to sample f for.
- In Bayesian optimization, we are building a probabilistic model for the performance metric f. Implicitly this is introducing computational overhead.
- So when does it makes sense to invest in this approach versus grid/random search?
  - The number of hyperparameters is very high.

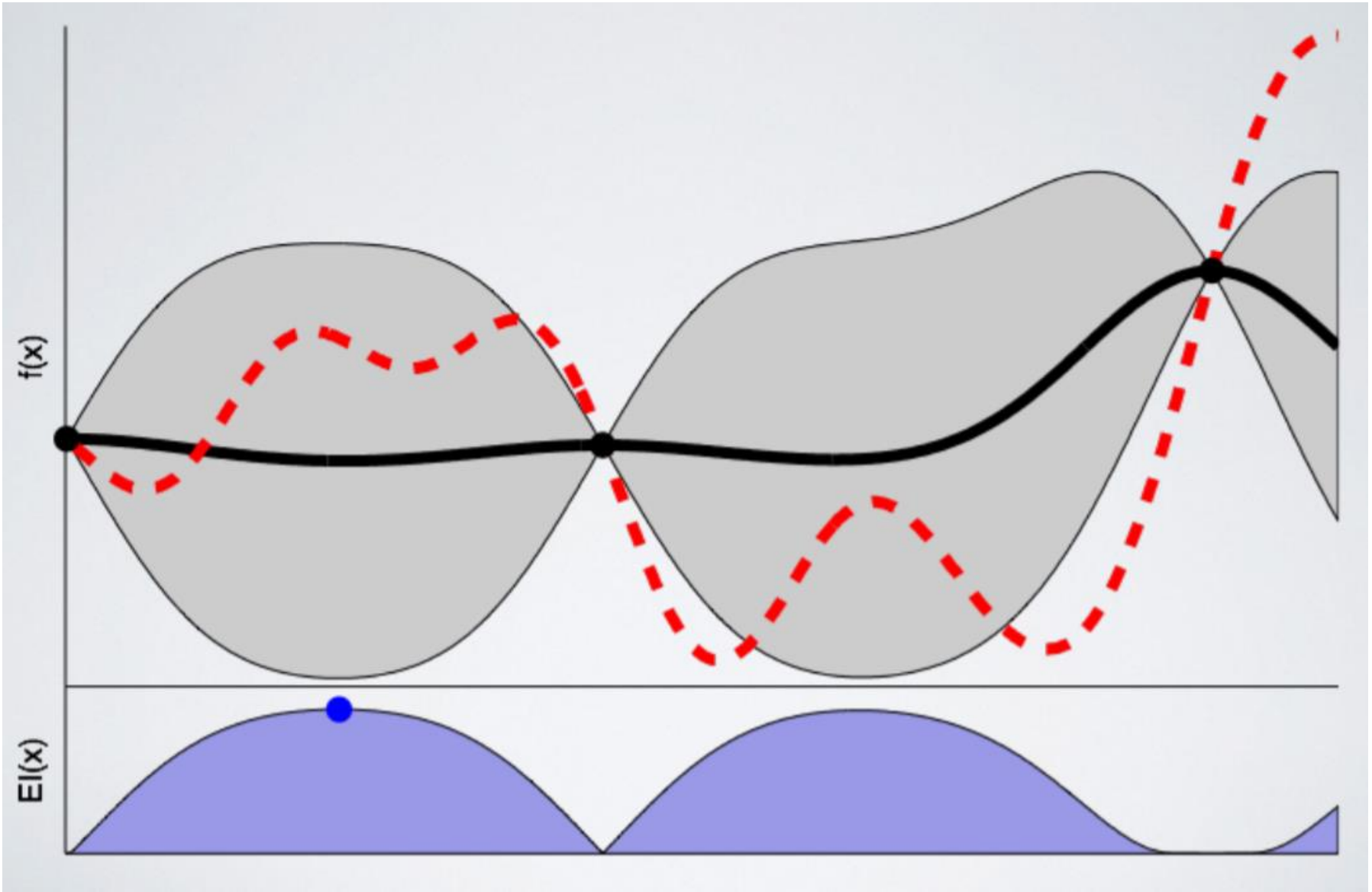
Bayesian optimization

- Steps:
  1. Using the points that were evaluated $\theta_{1:n}$, compute the posterior expectation of the loss f.
  2. Choose new point θ_{new} to sample by maximizing some utility of the expectation of f. The utility specifies which regions of the domain of f are optimal to sample from.
  3. Evaluate f at a new point θ_{new}.
- Gaussian processes used to represent the loss function f and evaluate its utility.





(Example from Ryan P. Adams)



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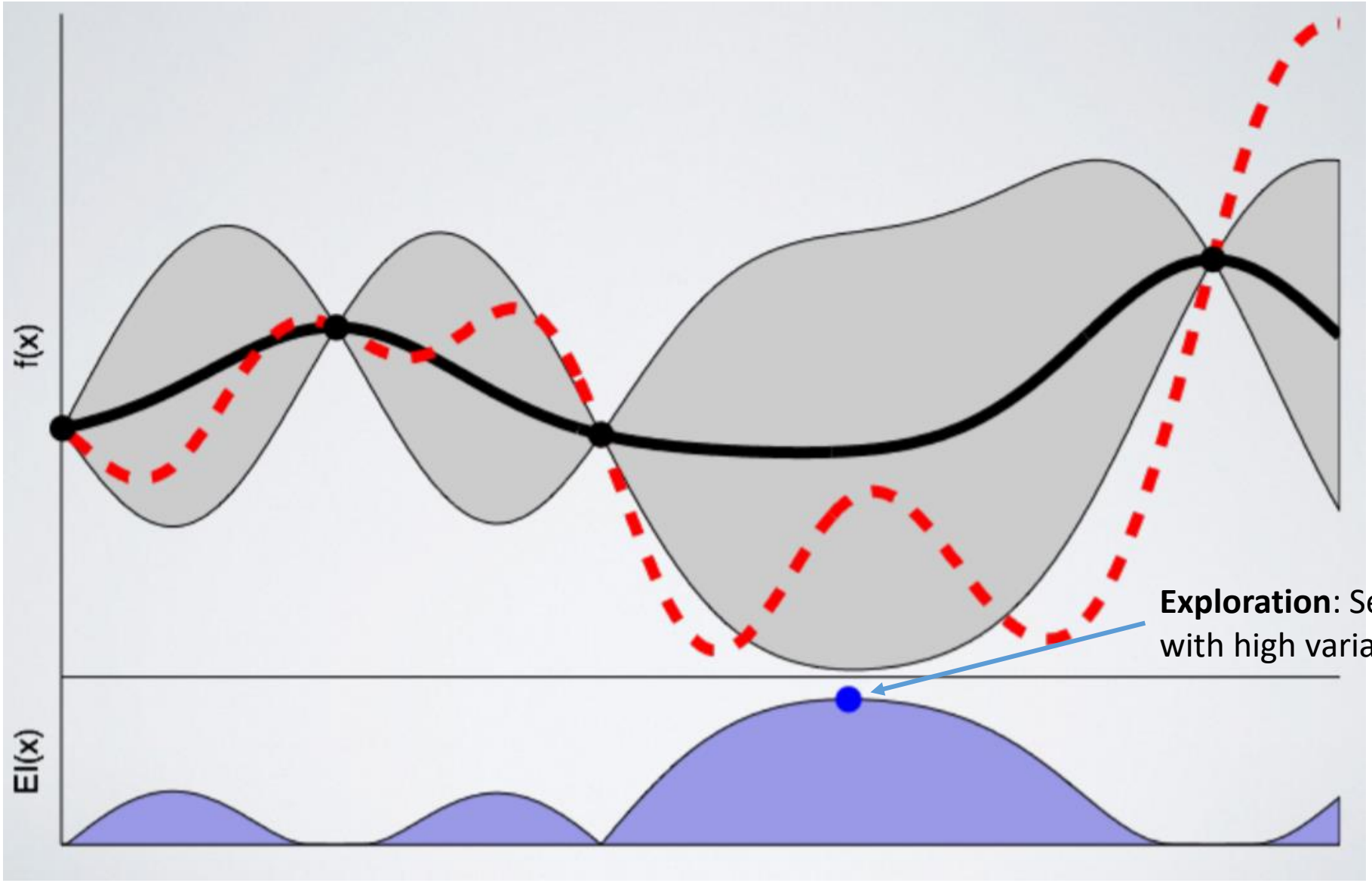

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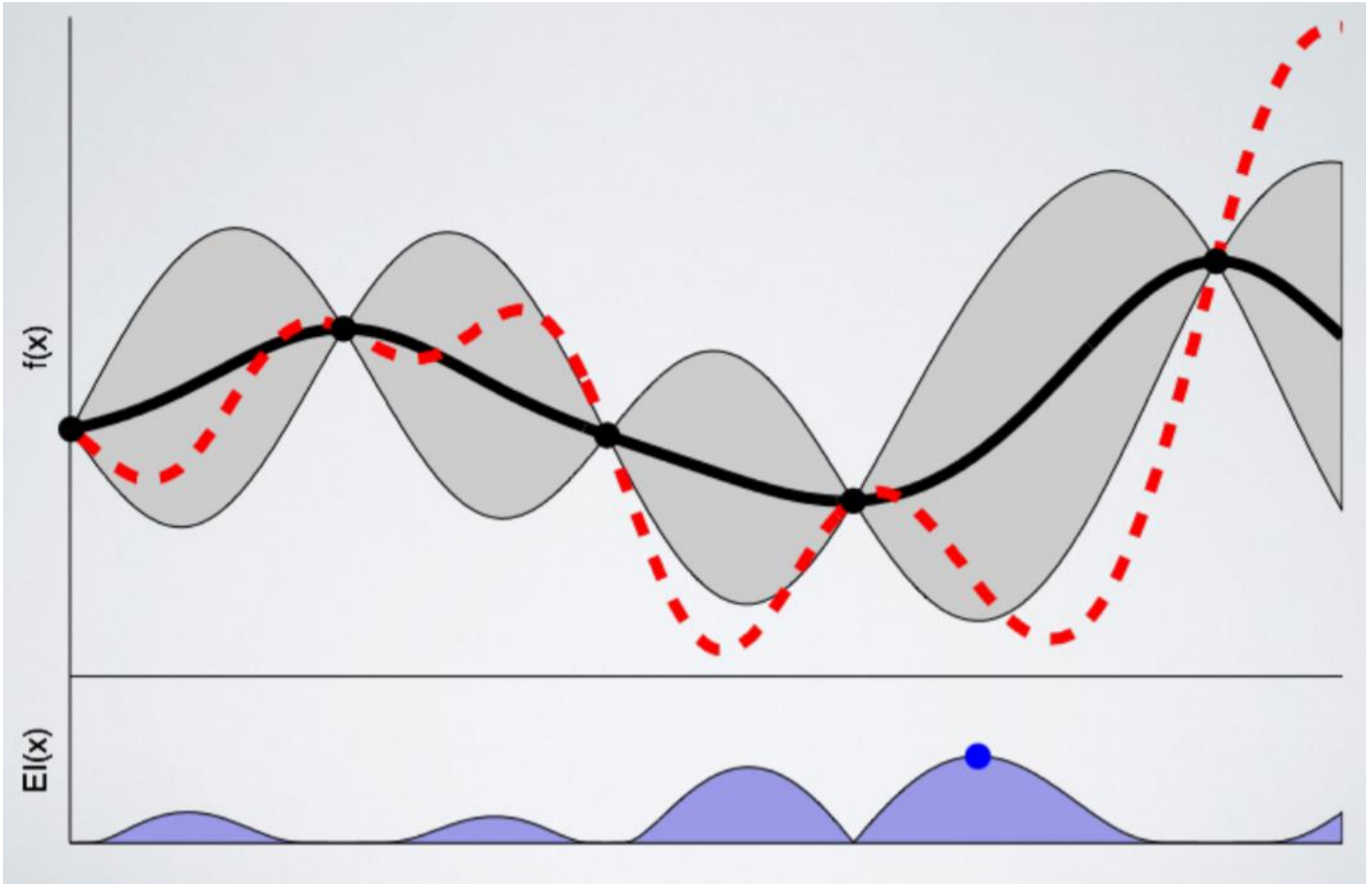

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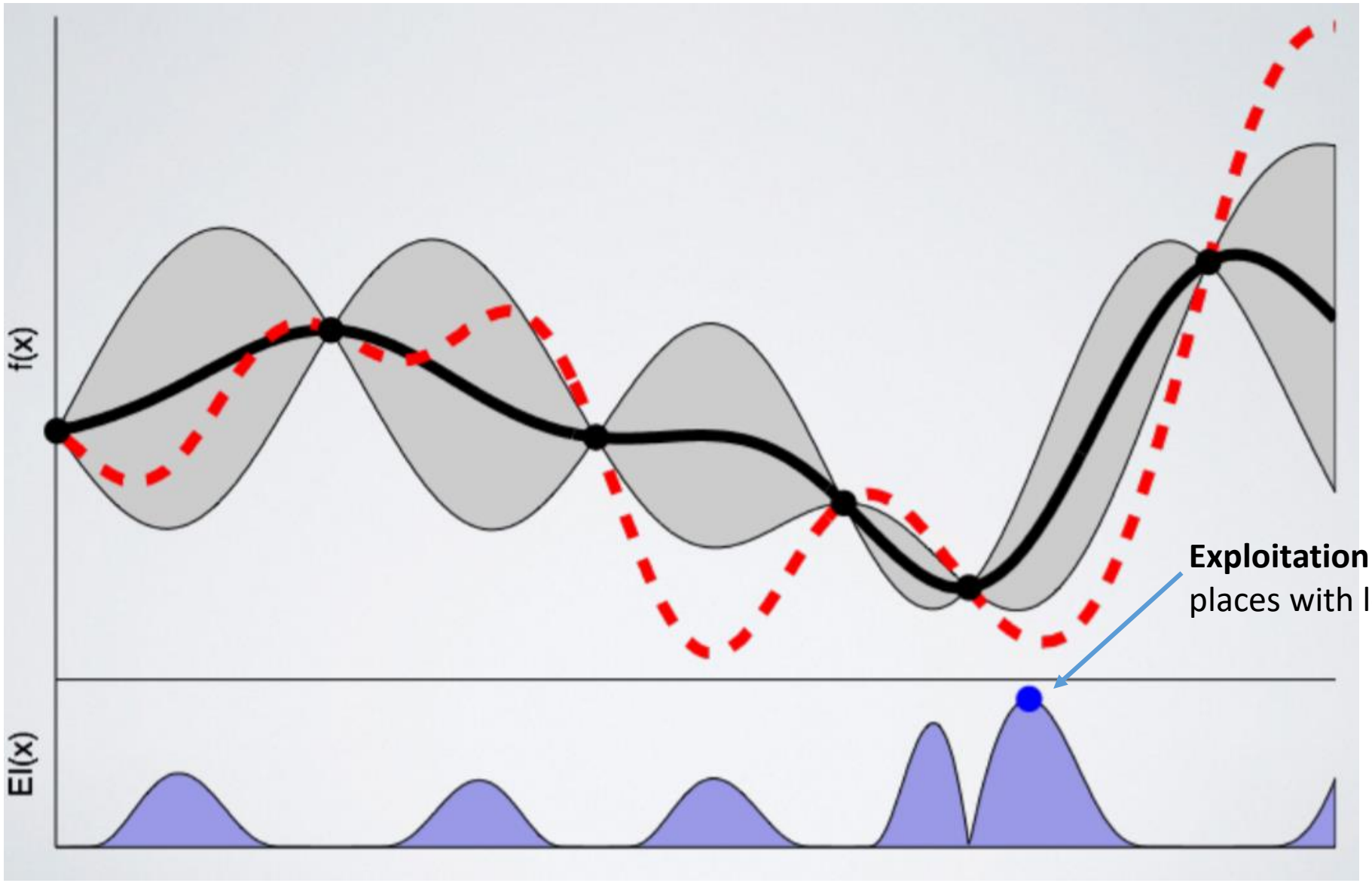

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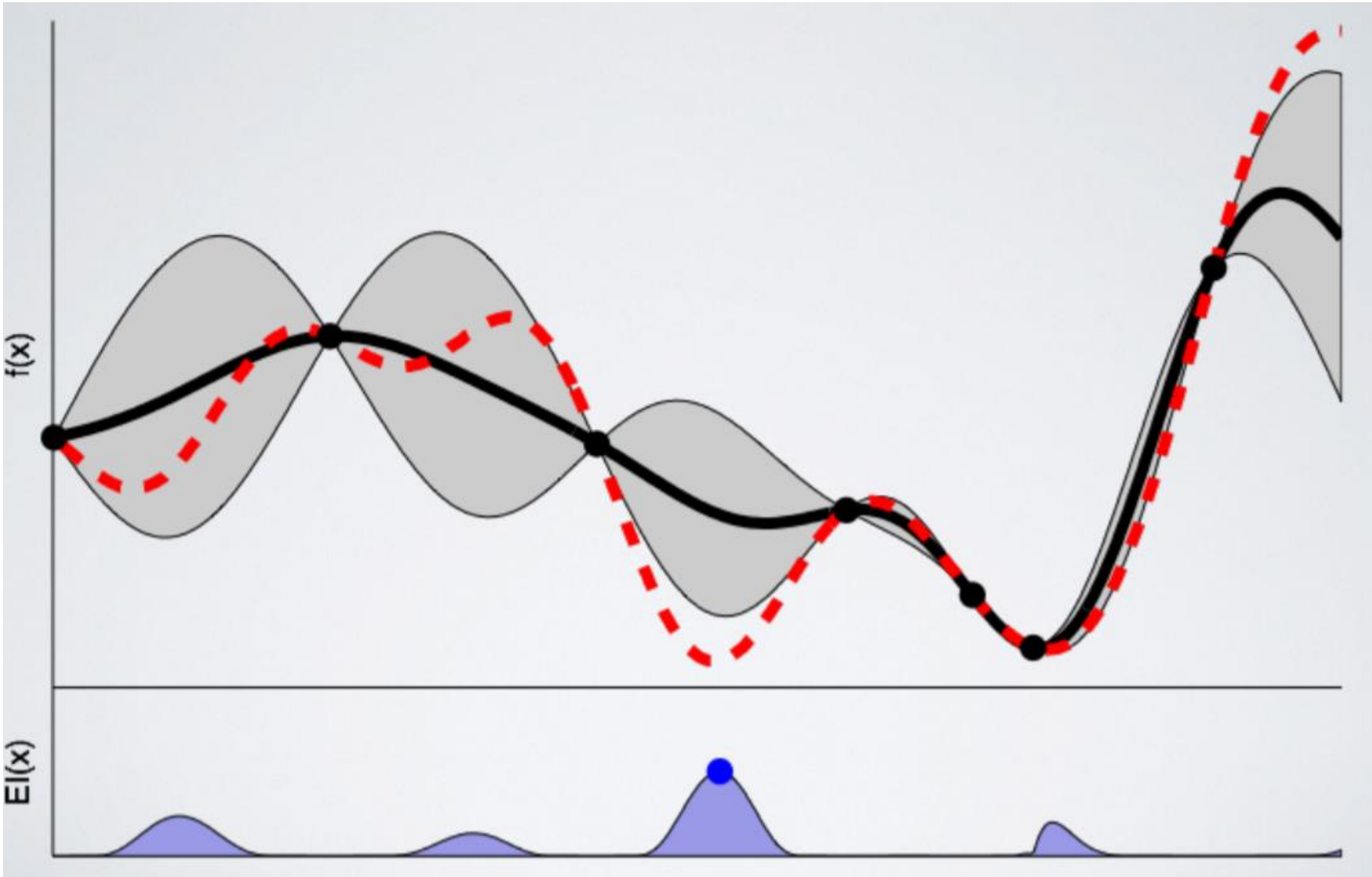

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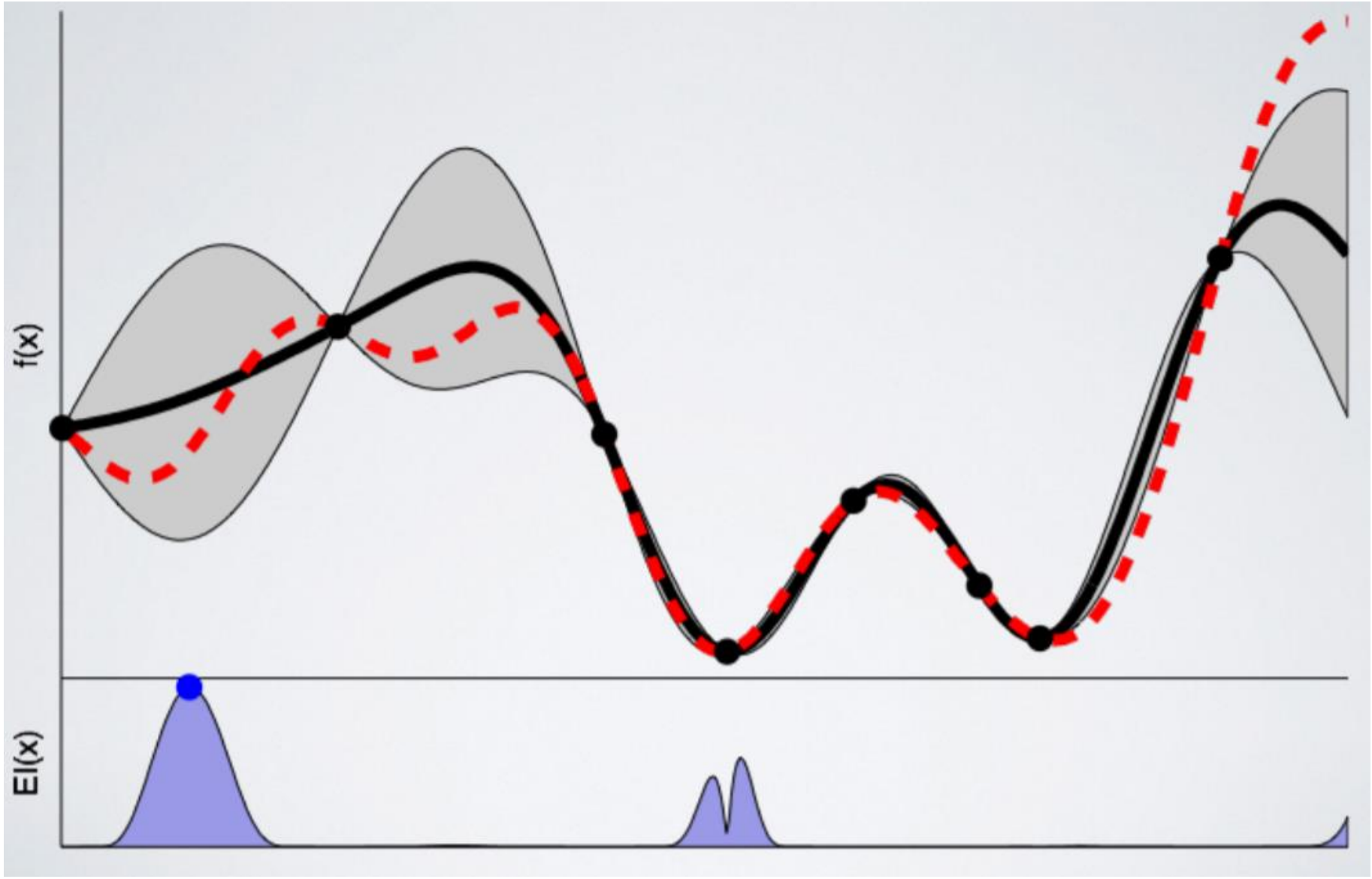

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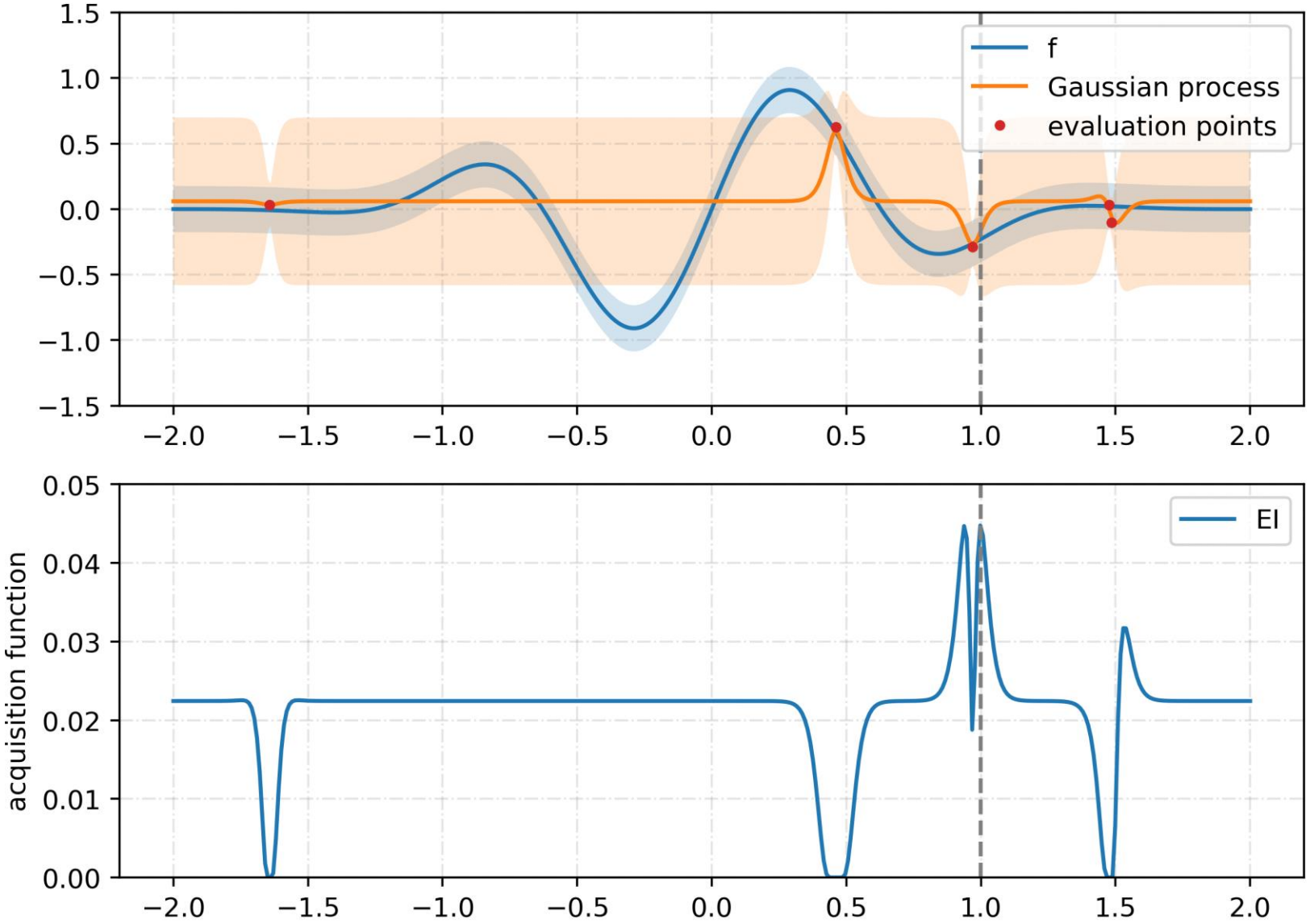

https://medium.com/criteo-labs/hyper-parameter-optimization-algorithms-2fe447525903

Recommendations

- Development phase: baby sitting.
- Optimization phase:
  - Random search: If you have the computing resources train many models at the same time and look for the best (on your validation set). This will give you a good baseline of hyperparameters tuning.
  - Use Bayesian optimization or such *Sequential Model Based Optimization.*

Take home

- Hyperparameters versus parameters.
- Hyperparameters tuning
  - Lots of hyperparameters in NN
  - Different methods to search the hyperparameters space:
    - Babysitting,
    - Grid-search,
    - Random search,
    - Bayesian optimization.
- These exists other optimization approaches (e.g. Evolutionary optimization).

References

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