Knowledge-Gradient Methods for Bayesian Optimization

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Jialei Wang

Wu, Poloczek, Wilson & F., NIPS'17
Bayesian Optimization with Gradients

Poloczek, Wang & F., NIPS'17
Multi Information-Source Optimization

Wu & F., NIPS'16
The Parallel KG Method for Batch Bayesian Optimization

Bayesian Optimization algorithms use acquisition functions

Generic BO algorithm:

Elicit a prior distribution on the function f (typically a GP).

while (budget is not exhausted) {

Find x that maximizes Acquisition(x,posterior)

Sample at x

Update the posterior distribution

}

There are a few commonly used acquisition functions

Most people use this one

- **Expected Improvement (EI)**

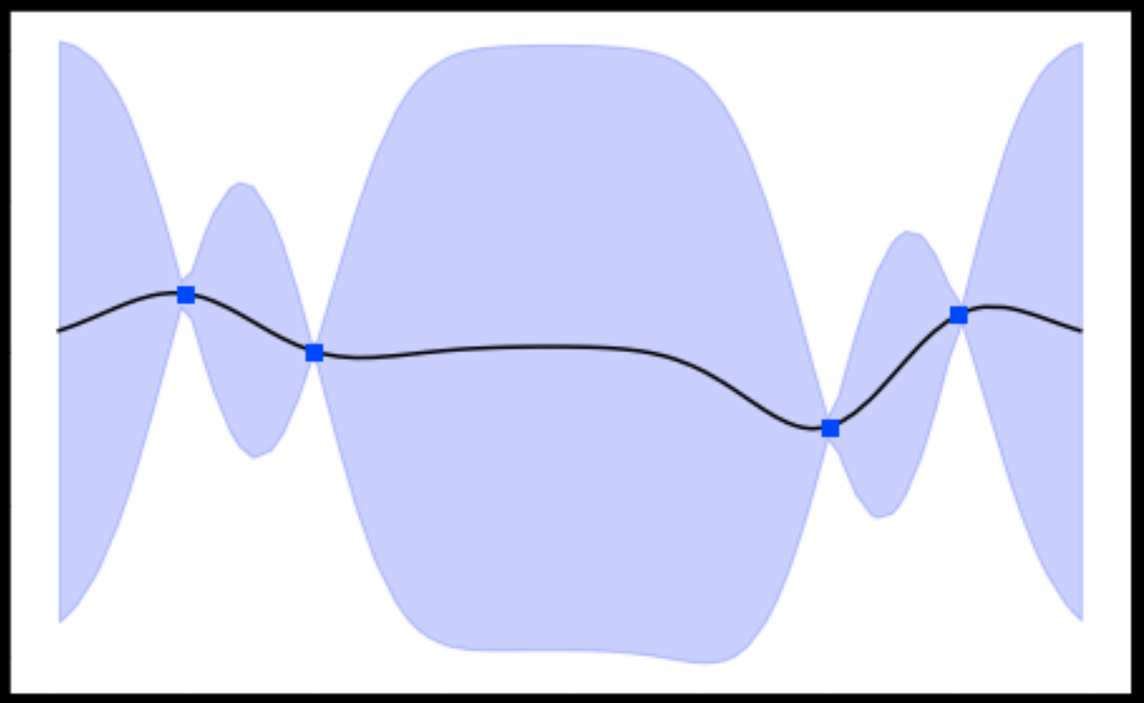
Some people use one of these

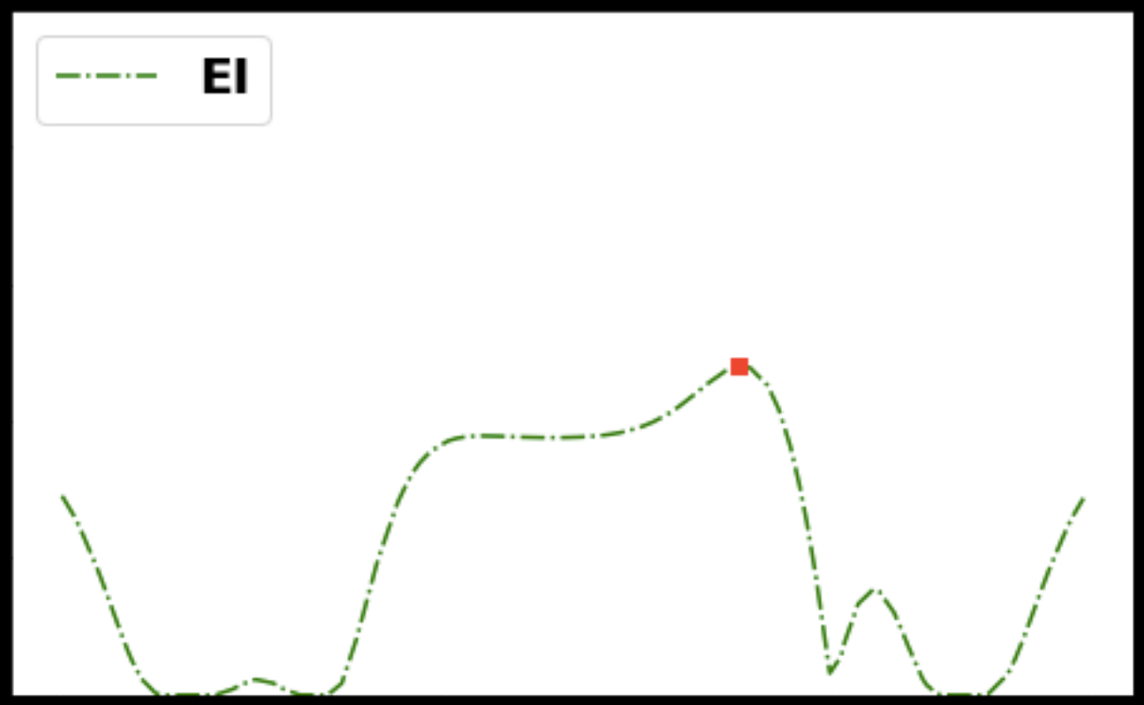
- Expected Improvement (EI)
- **Predictive Entropy Search (PES)**
- **Upper Confidence Bound (UCB)**
- **Probability of Improvement (P*)**

I'll tell you why you might want to try this one, & give you a link to code

- Expected Improvement (EI)
- Upper Confidence Bound (UCB)
- Predictive Entropy Search (PES)
- Probability of Improvement (P*)
- **Knowledge Gradient (KG)**

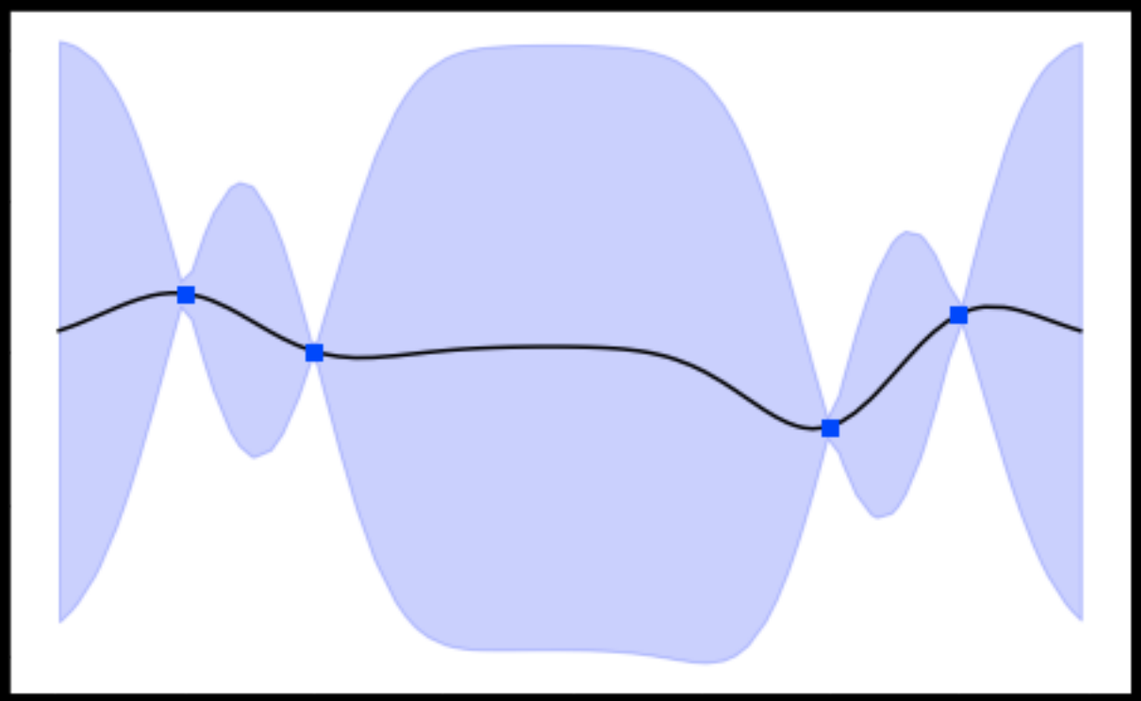
Let me remind you about EI

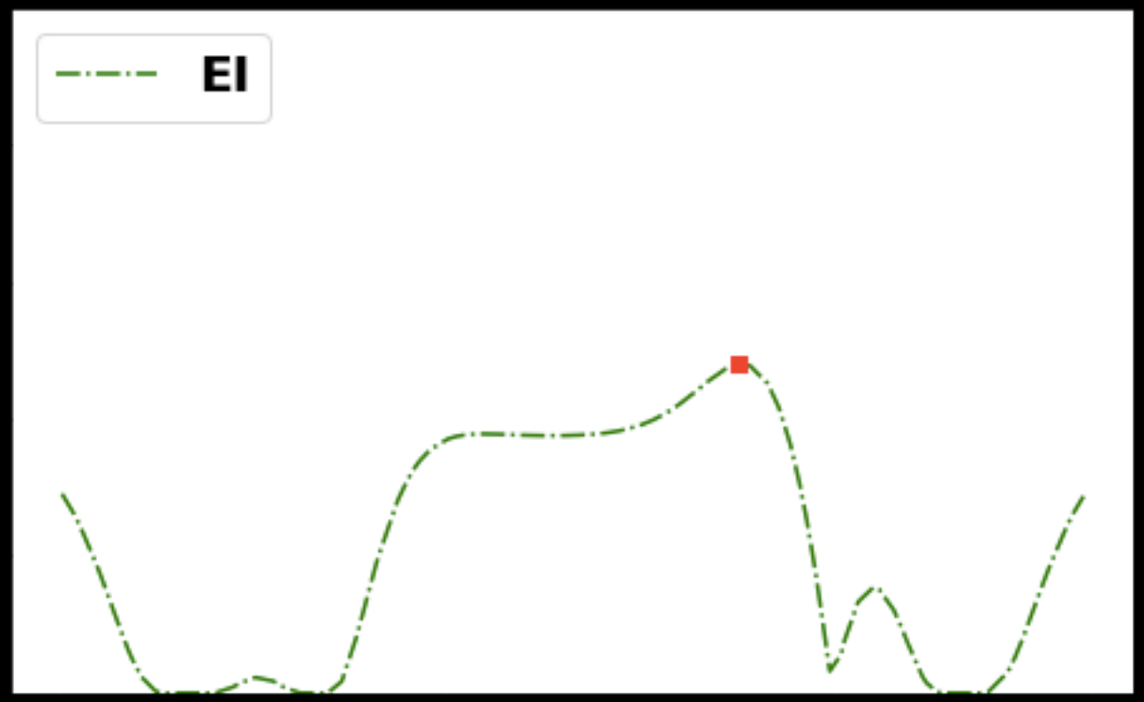




- We've evaluated $x^{(1)},\ldots x^{(n)}$, & observed $f(x^{(1)}),\ldots,f(x^{(n)})$ without noise.
- The best value observed is $f^*=\min(f(x^{(1)}),\ldots,f(x^{(n)}))$.
- If we evaluate at x, we observe f(x).
- The *improvement* is $(f^*-f(x))^+$
- The *expected improvement* is $EI(x)=E_n[(f^*-f(x))^+]$

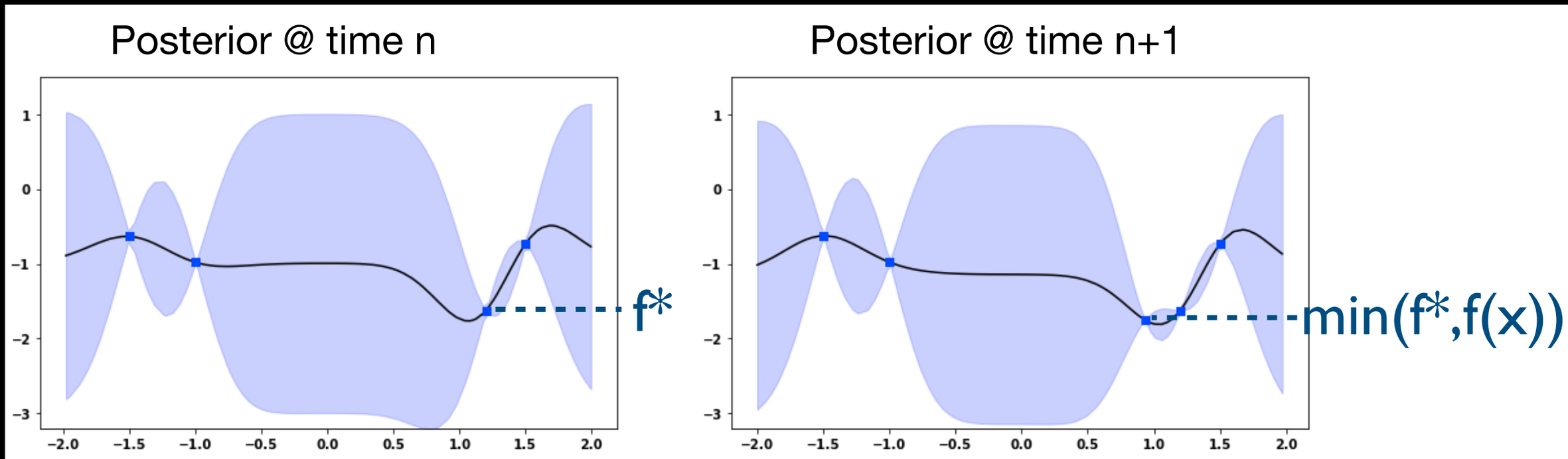
EI is one-step Bayes-optimal under assumptions





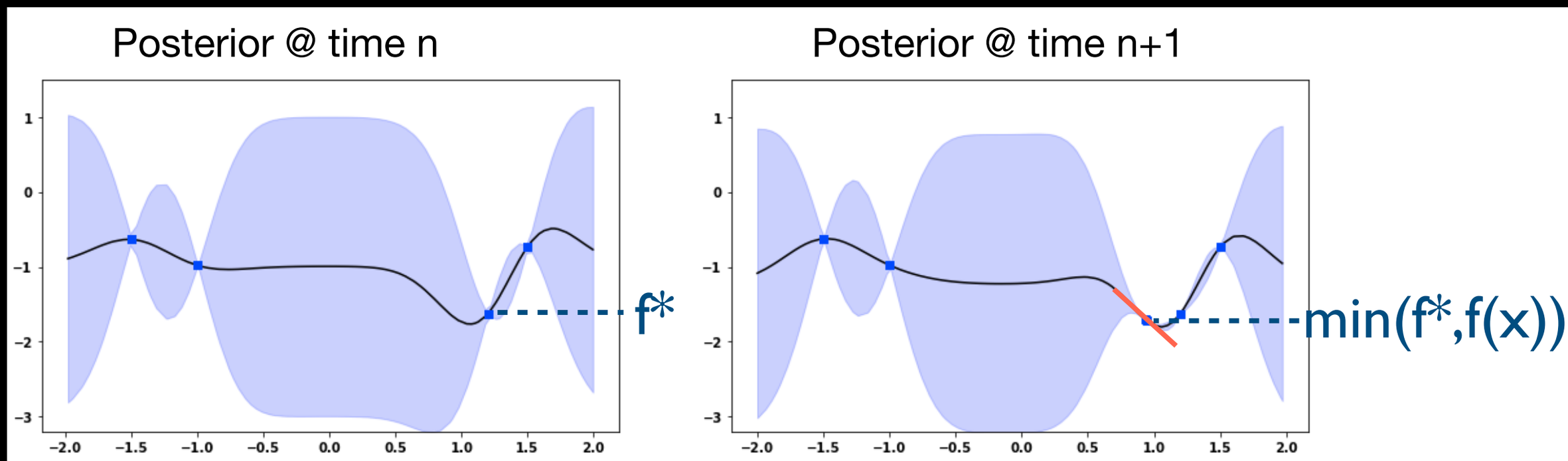
- One-step: We may evaluate f only one more time. After, we must report a solution.
- We are risk-neutral, and suffer loss equal to the value of the reported solution
- Evaluations are noise-free
- The solution we report must have known value

EI is one-step Bayes-optimal under assumptions

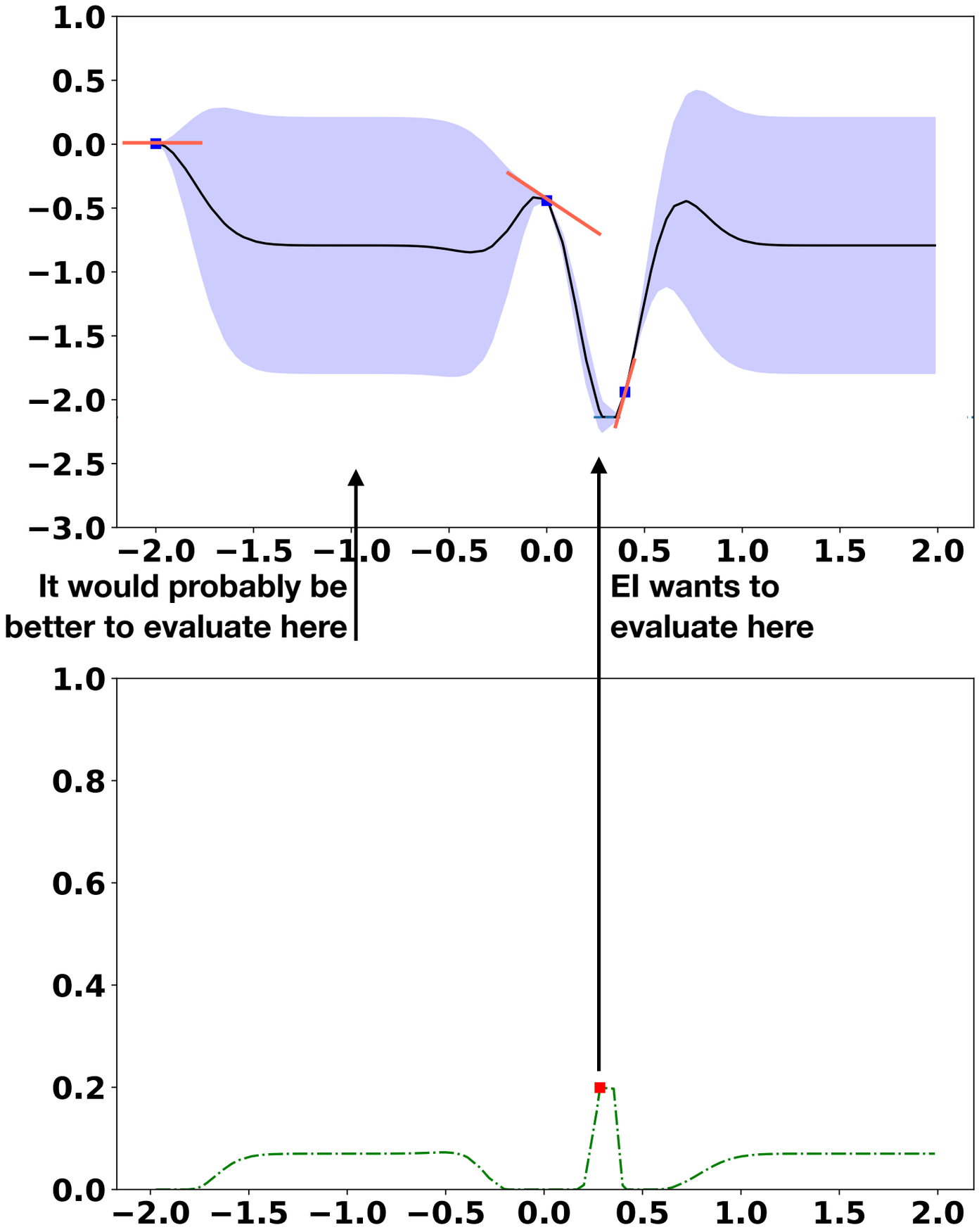


- Loss if we stop now:
  f*
- Loss if we stop after sampling f(x):
  min(f*,f(x))
- Reduction in loss due to sampling:
  $E_n[f^* - \min(f^*, f(x))] = E_n[(f^* - f(x))^+] = EI(x)$

EI places no value on some kinds of information

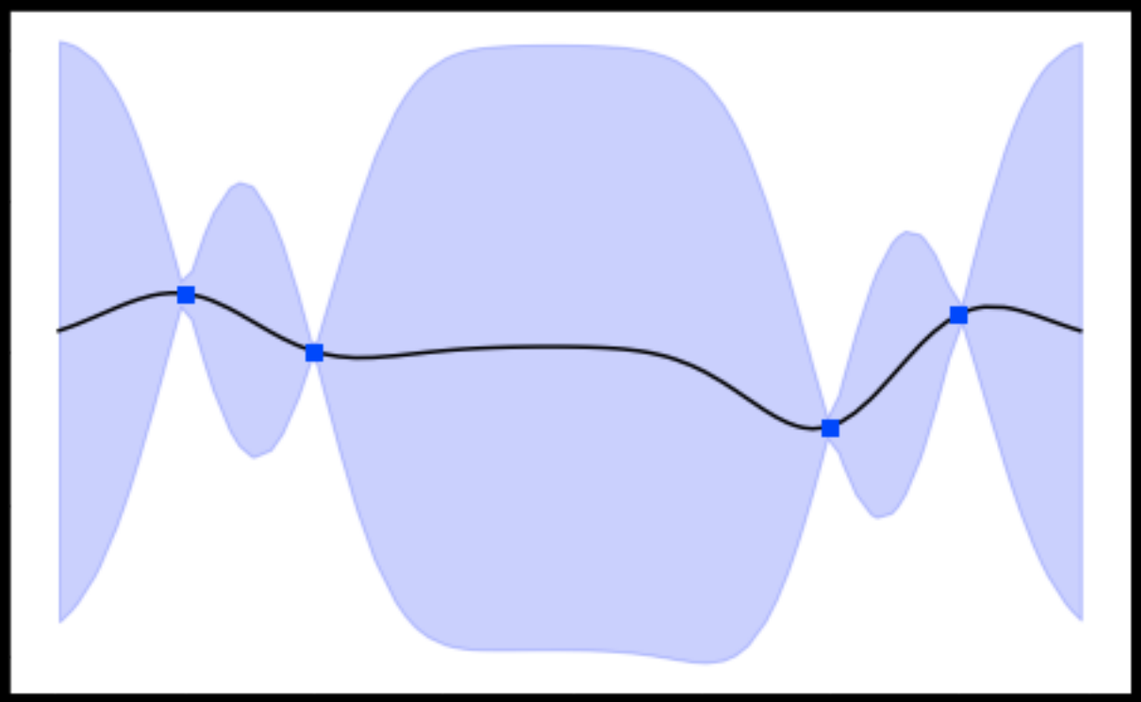


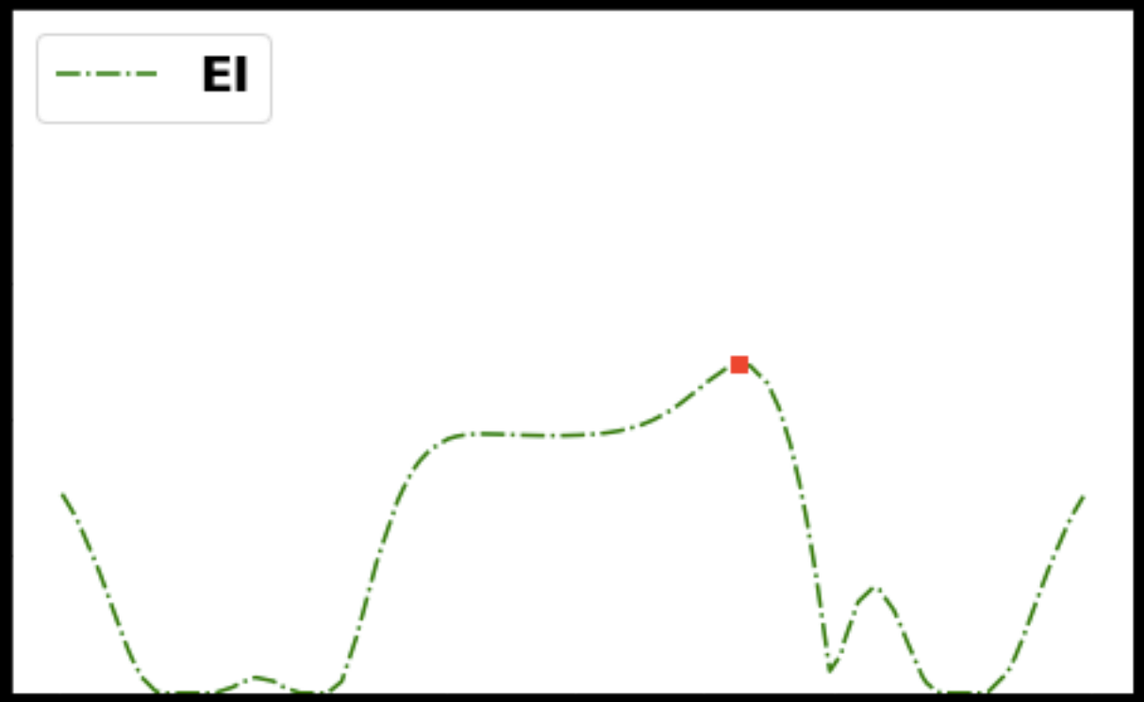
- Loss if we stop now:
  f*
- Loss if we stop after sampling f(x) & its gradient:
  min(f*,f(x))
- Reduction in loss due to sampling:
  $E_n[f^* - \min(f^*, f(x))] = E_n[(f^* - f(x))^+] = EI(x)$



As a consequence, EI can make poor decisions

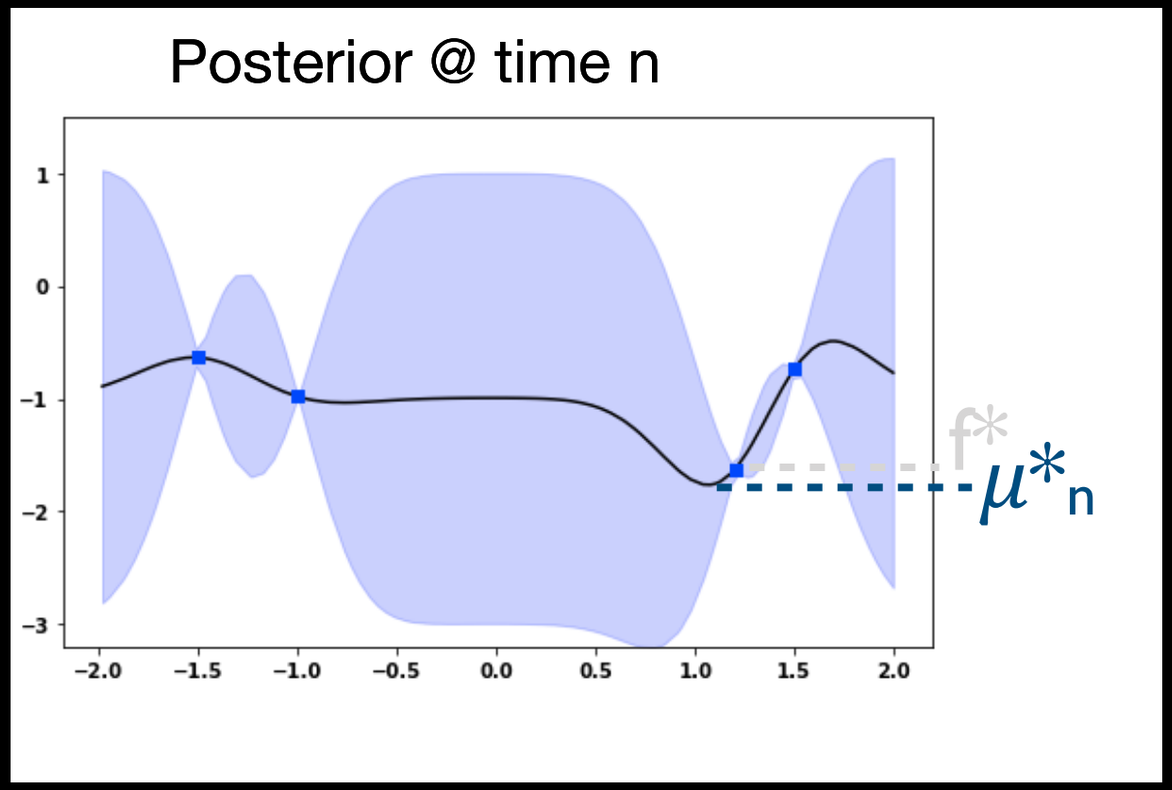
KG eliminates two of EI's assumptions





- One-step: We may evaluate f only one more time. After, we must report a solution.
- We are risk-neutral, and suffer loss equal to the value of the reported solution
- ~~Evaluations are noise-free~~
- ~~The solution we report must have known value~~

The KG acquisition function, KG(x) for an observation with gradients



- Loss if we stop now:
  $\mu^*_n = \min_x \mu_n(x)$

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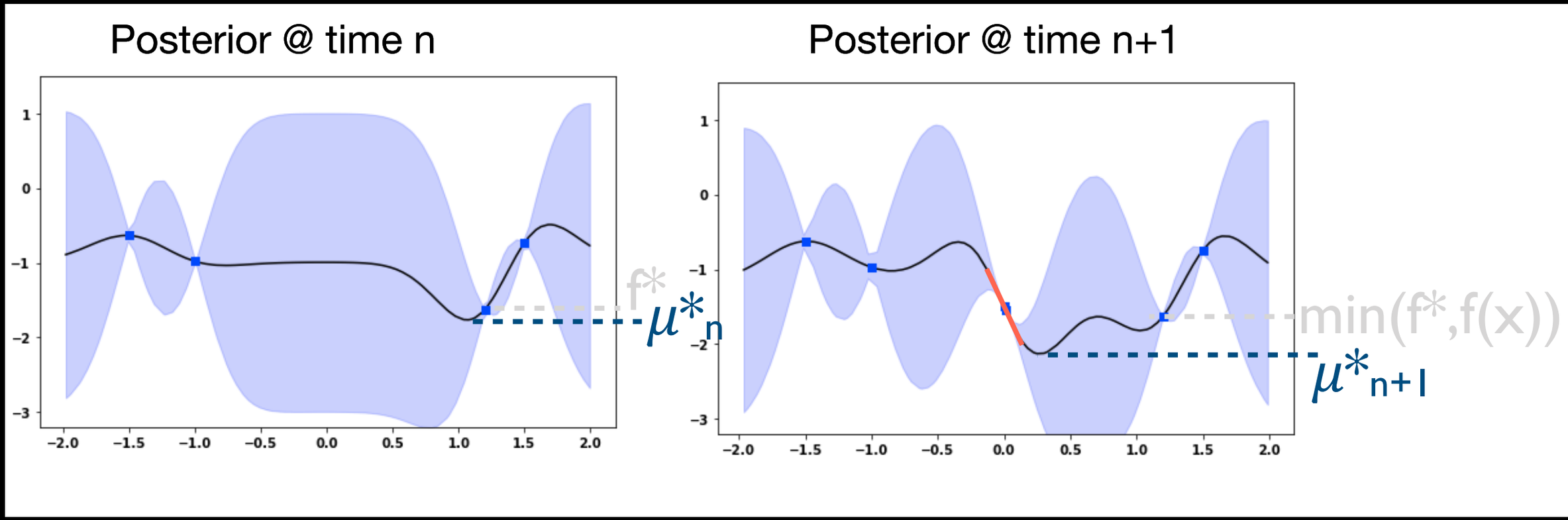
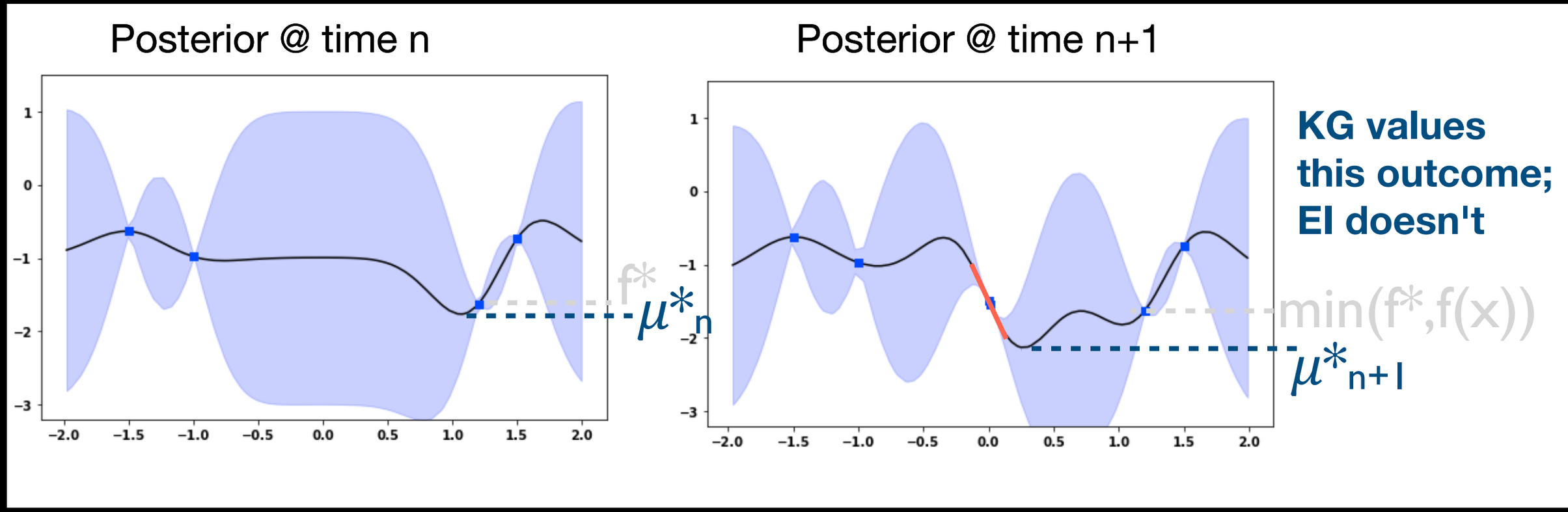


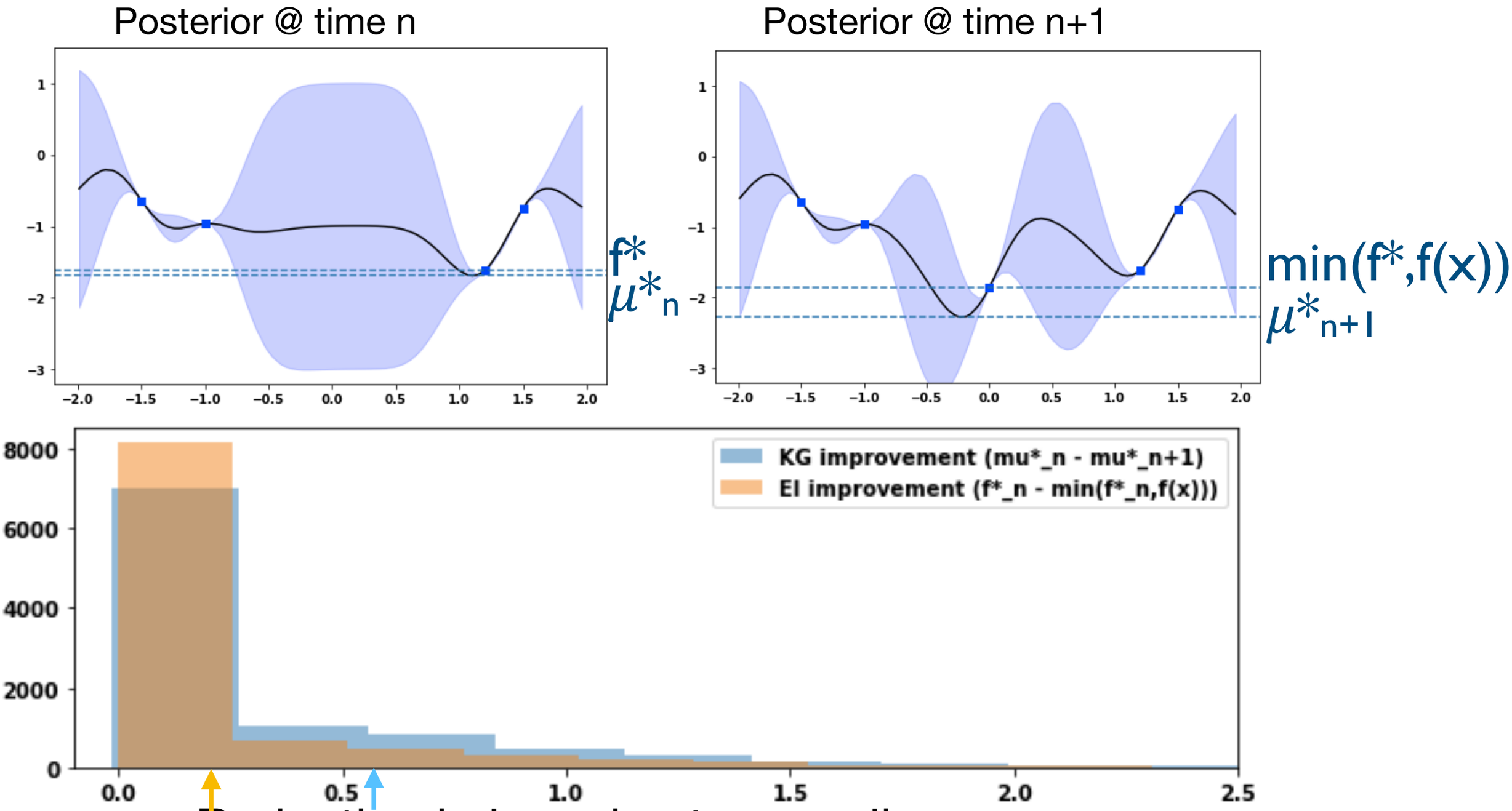
- Loss if we stop now:
  $\mu^*_n = \min_x \mu_n(x)$
- Loss if we stop after sampling f(x):
  $\mu^*_{n+1} = \min_x \mu_{n+1}(x)$

The KG acquisition function, KG(x) for an observation with gradients



- Loss if we stop now:
  $\mu^*_n = \min_x \mu_n(x)$
- Loss if we stop after sampling f(x):
  $\mu^*_{n+1} = \min_x \mu_{n+1}(x)$
- Reduction in loss due to sampling:
  $KG(x) = E_n[\mu^*_n - \mu^*_{n+1} \mid \text{query } x]$

Here's how we can compute the KG acquisition function for BO with gradients



- Reduction in loss due to sampling: $E_n[\mu^*_n - \mu^*_{n+1}]$

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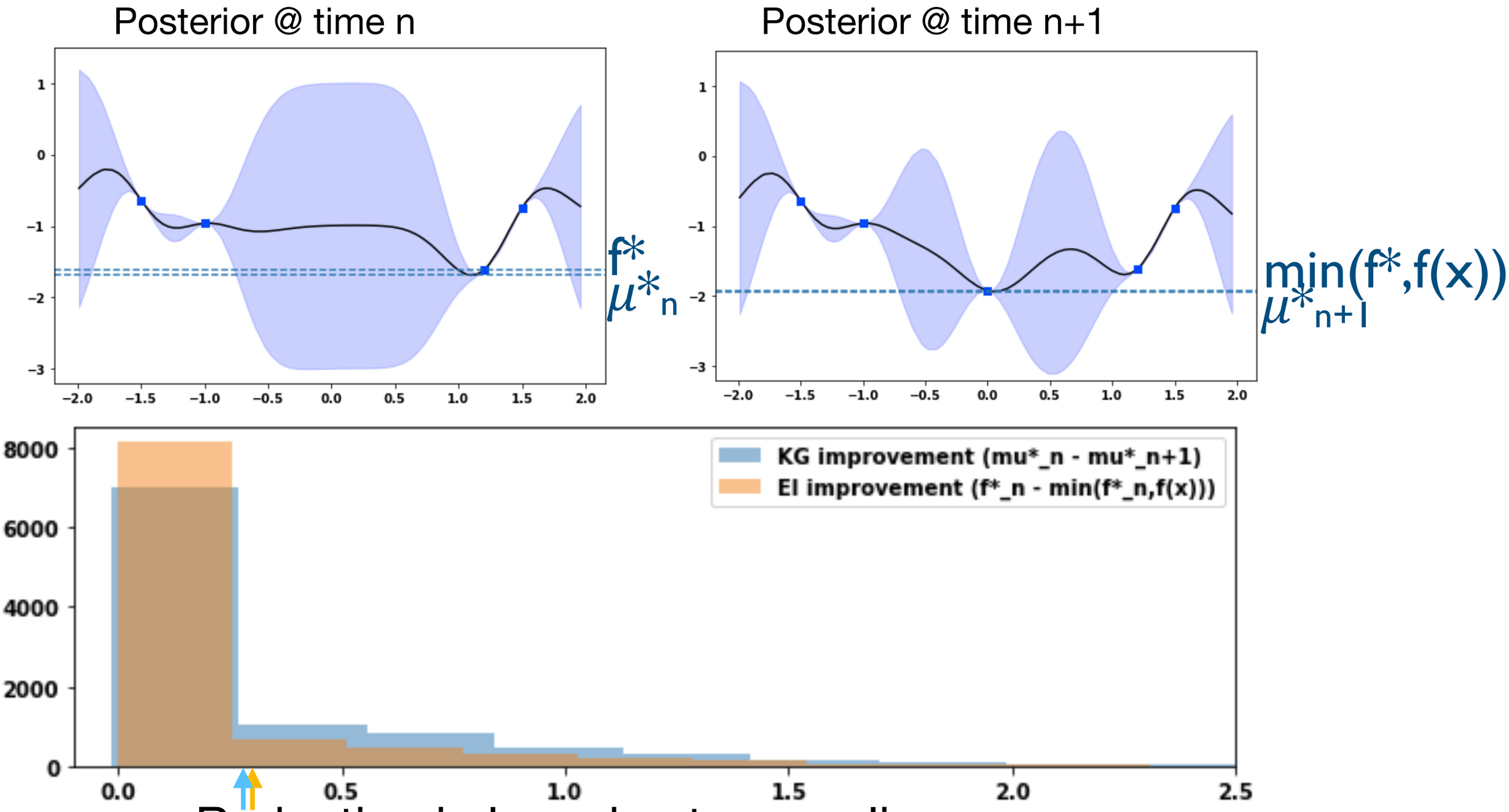

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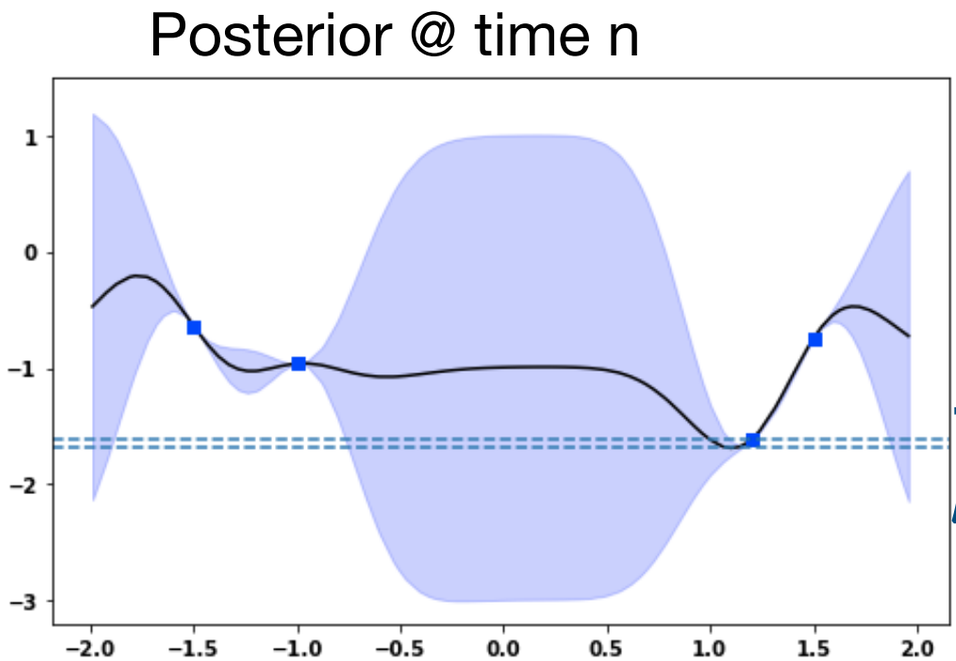
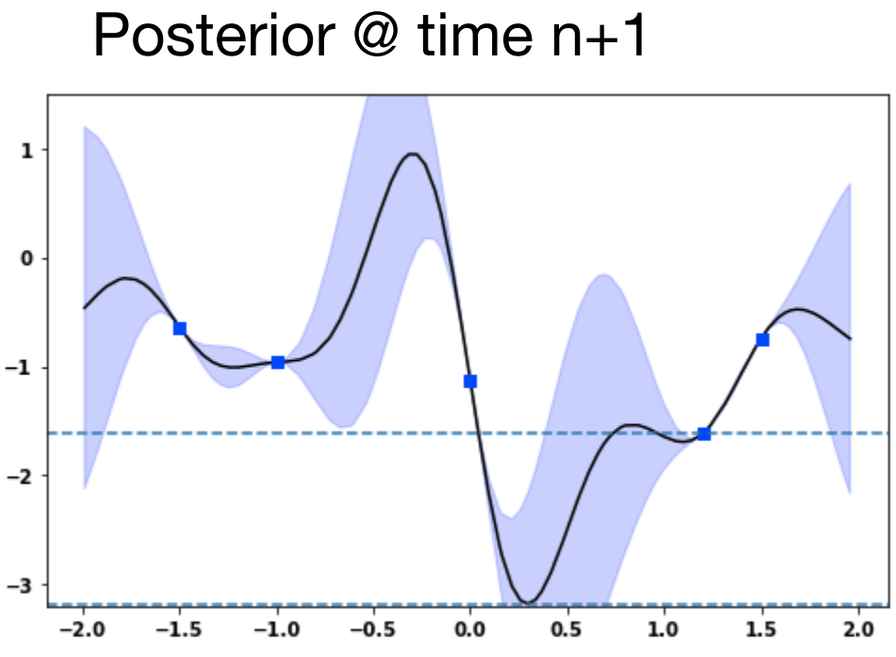
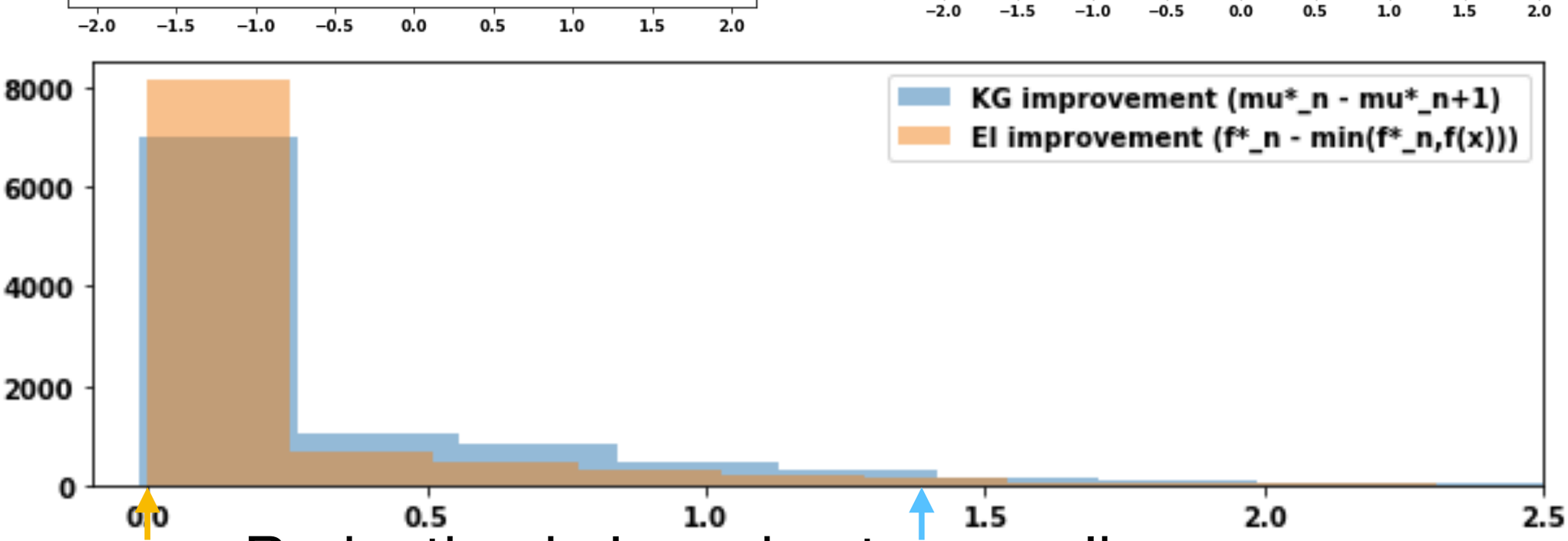




f*
μ^*_n

min(f*,f(x))

μ^*_{n+1}



- Reduction in loss due to sampling:
  $E_n[\mu^*_n - \mu^*_{n+1}]$

Here's basic pseudocode for computing the KG acquisition function

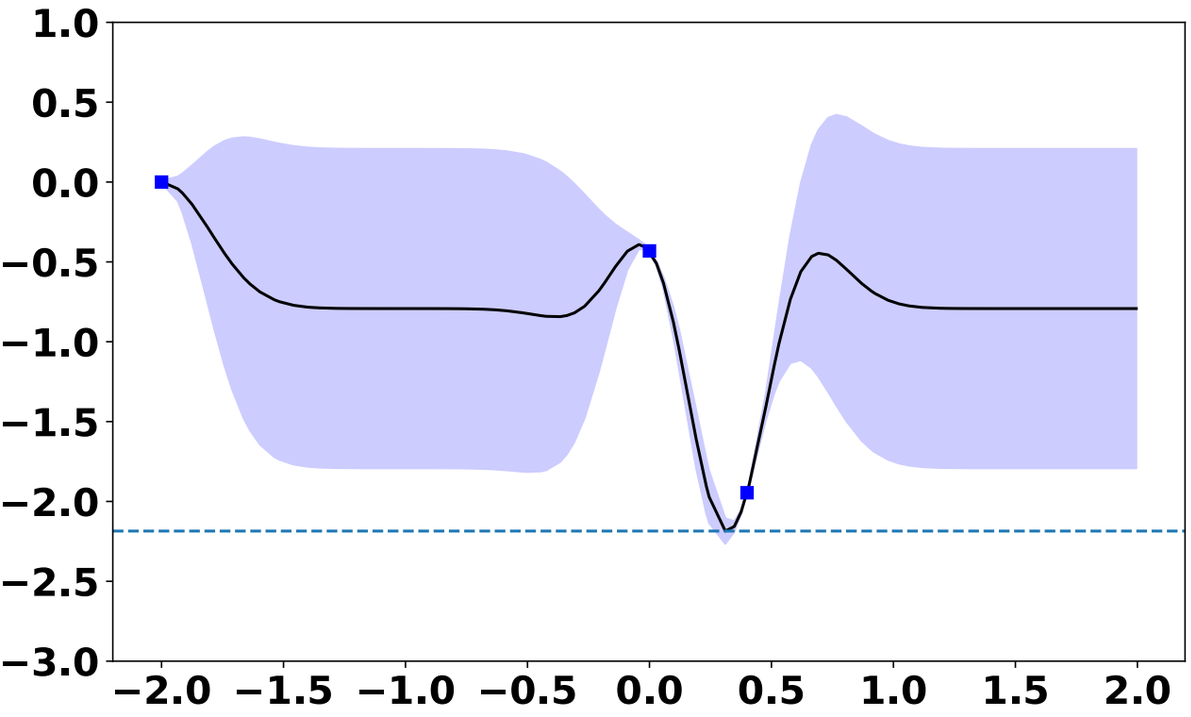
For i in 1:replications

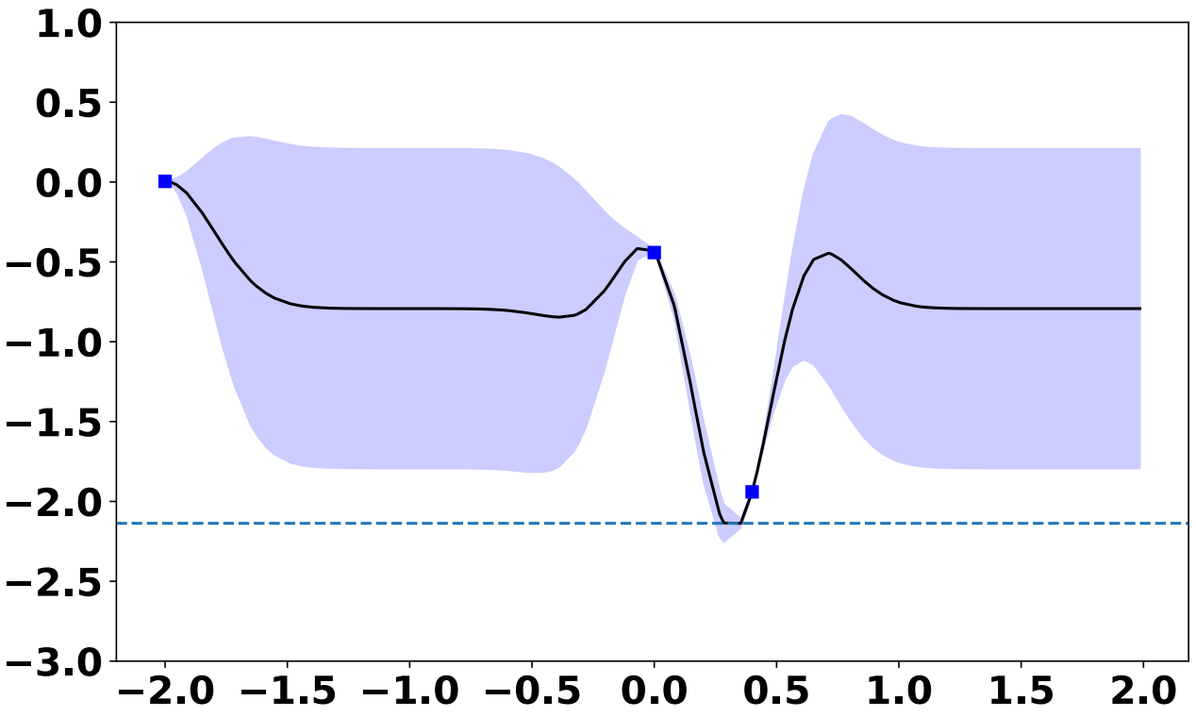
- Simulate f(x), ∇f(x) from the posterior
- Calculate $\mu^*_{n+1} = \min_{x'} \mu_{n+1}(x')$ from sim'd f(x), ∇f(x)
- Calculate $\mu^*_n - \mu^*_{n+1}$

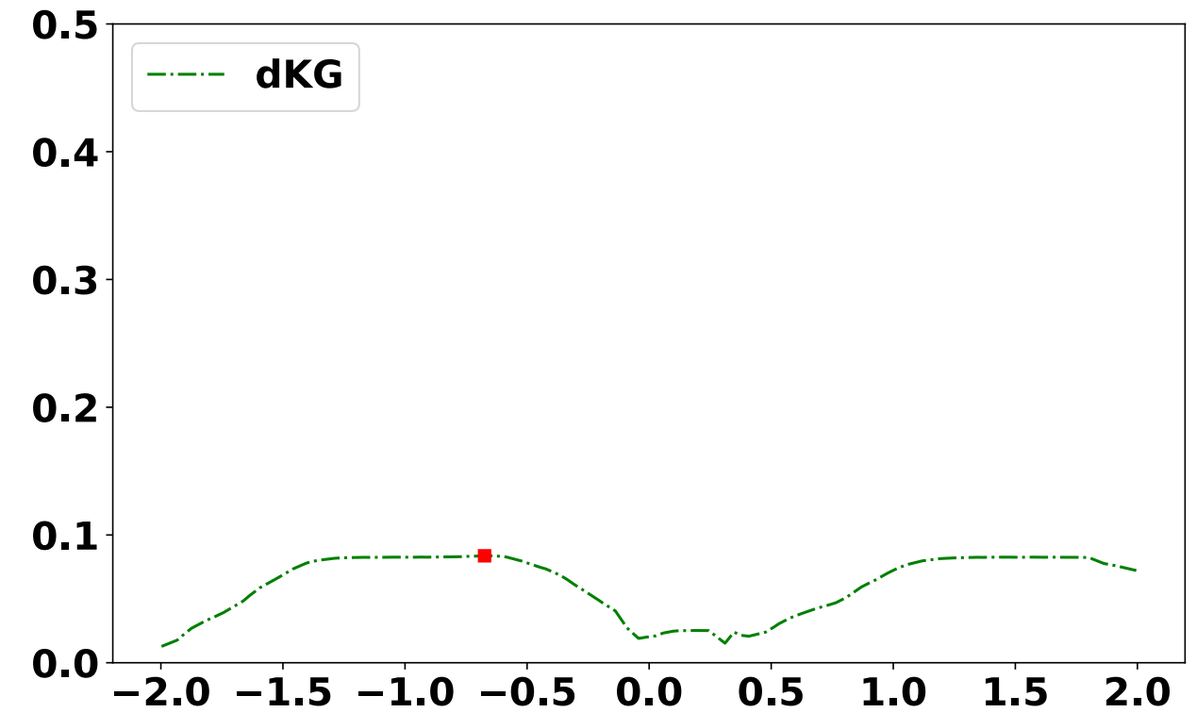
KG(x) is the average of the simulated $\mu^*_n - \mu^*_{n+1}$

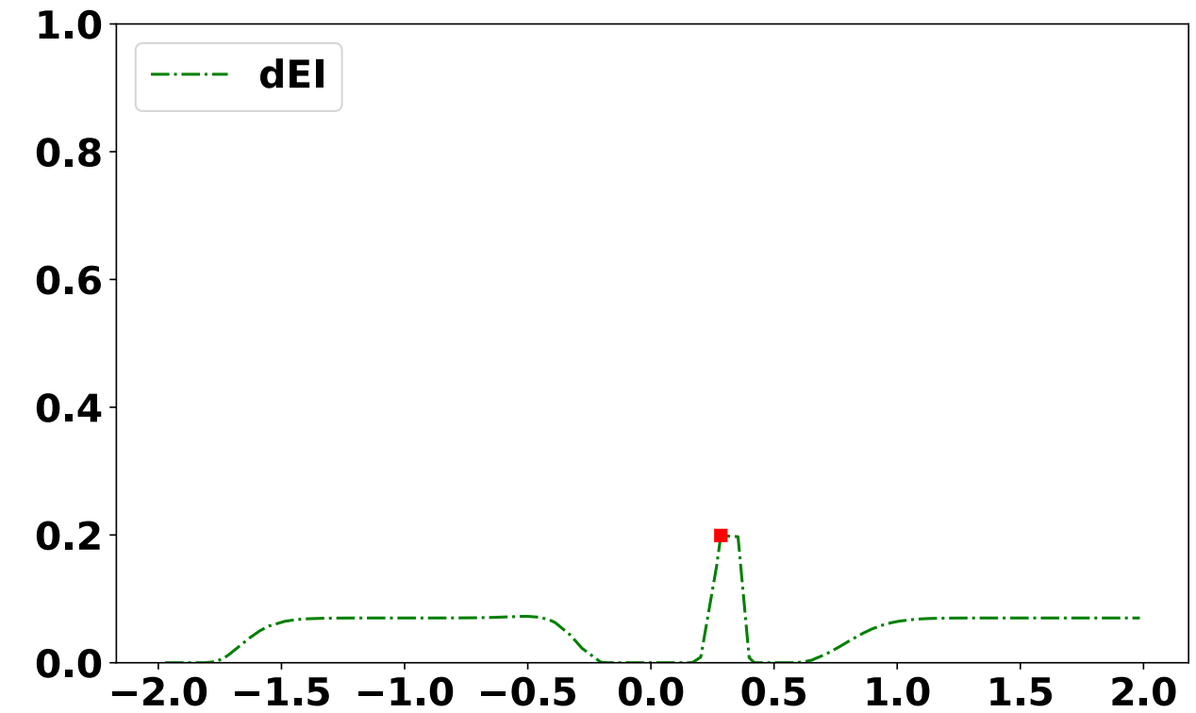
* I'll discuss a faster computational method in a few minutes

KG explores more effectively than EI when we have gradients









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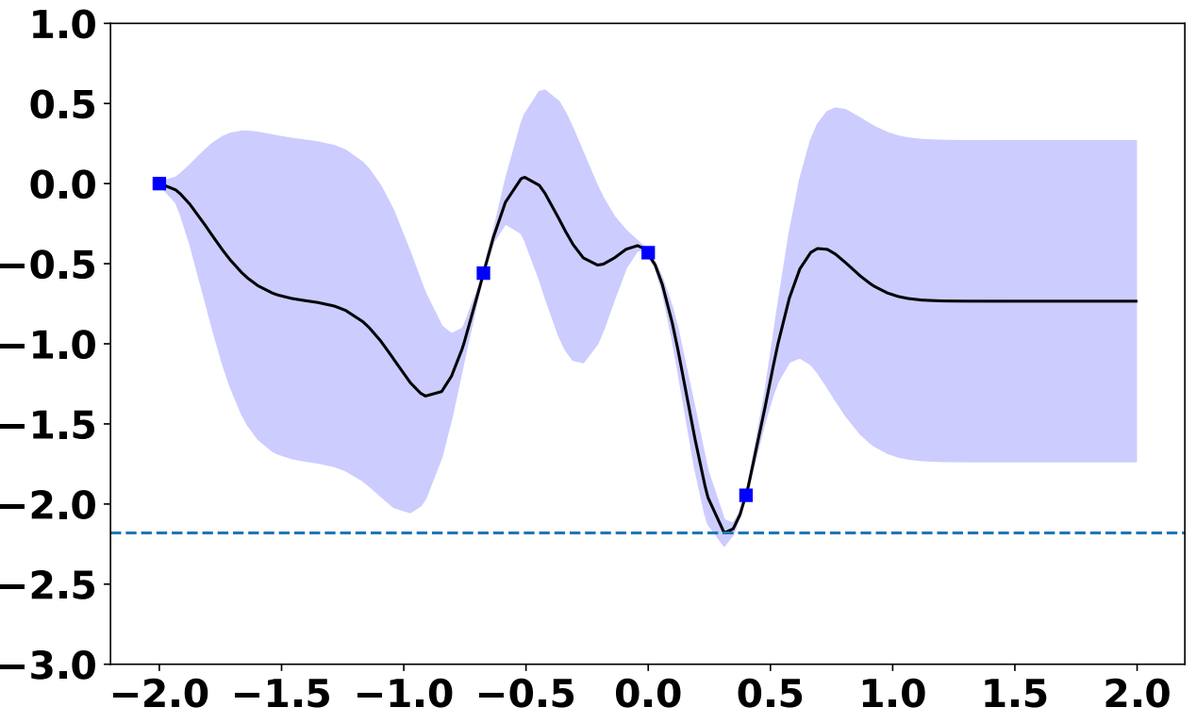

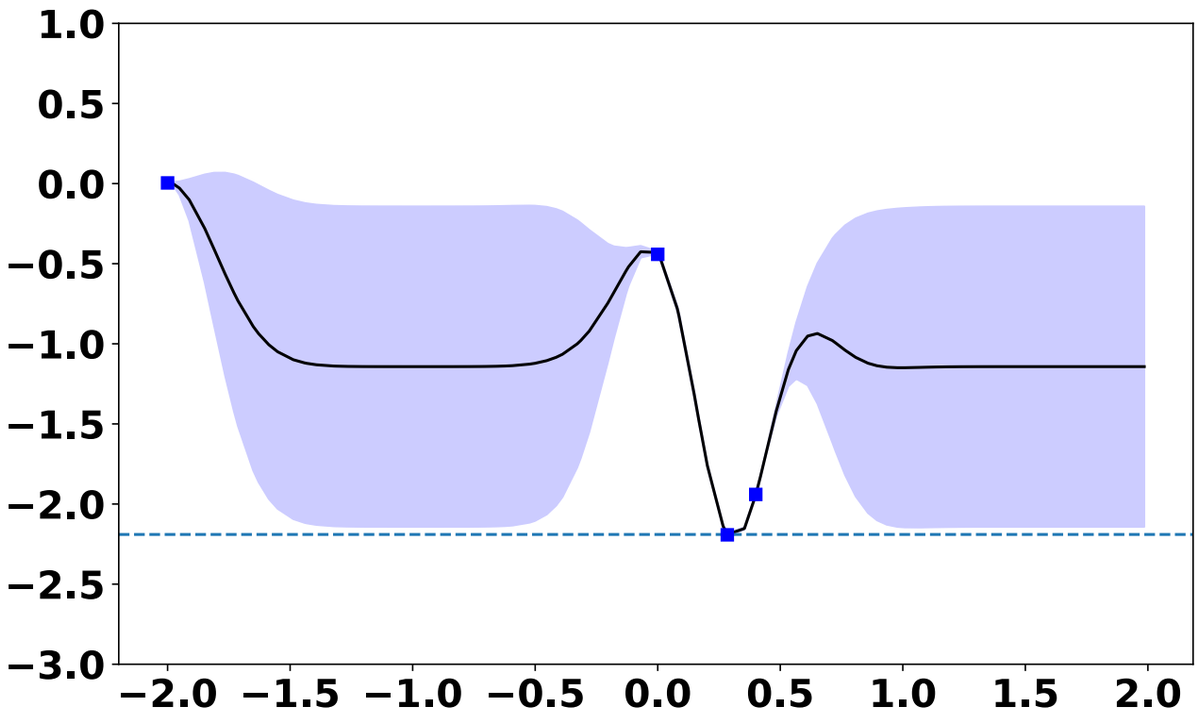

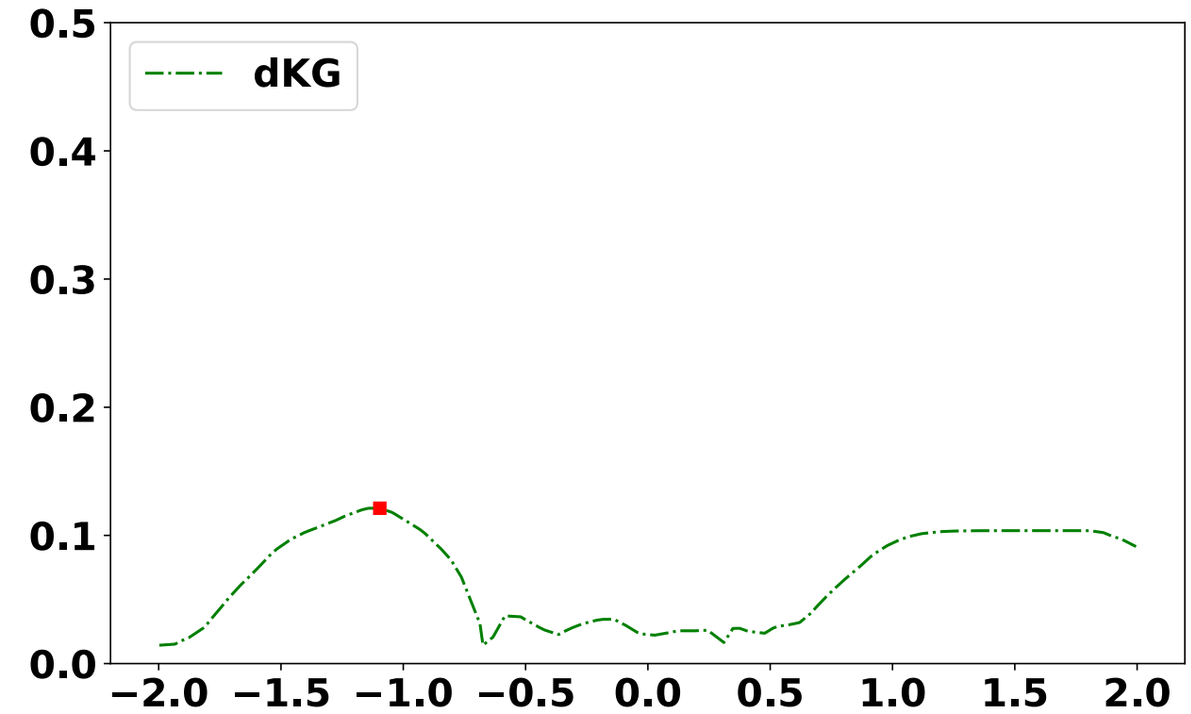

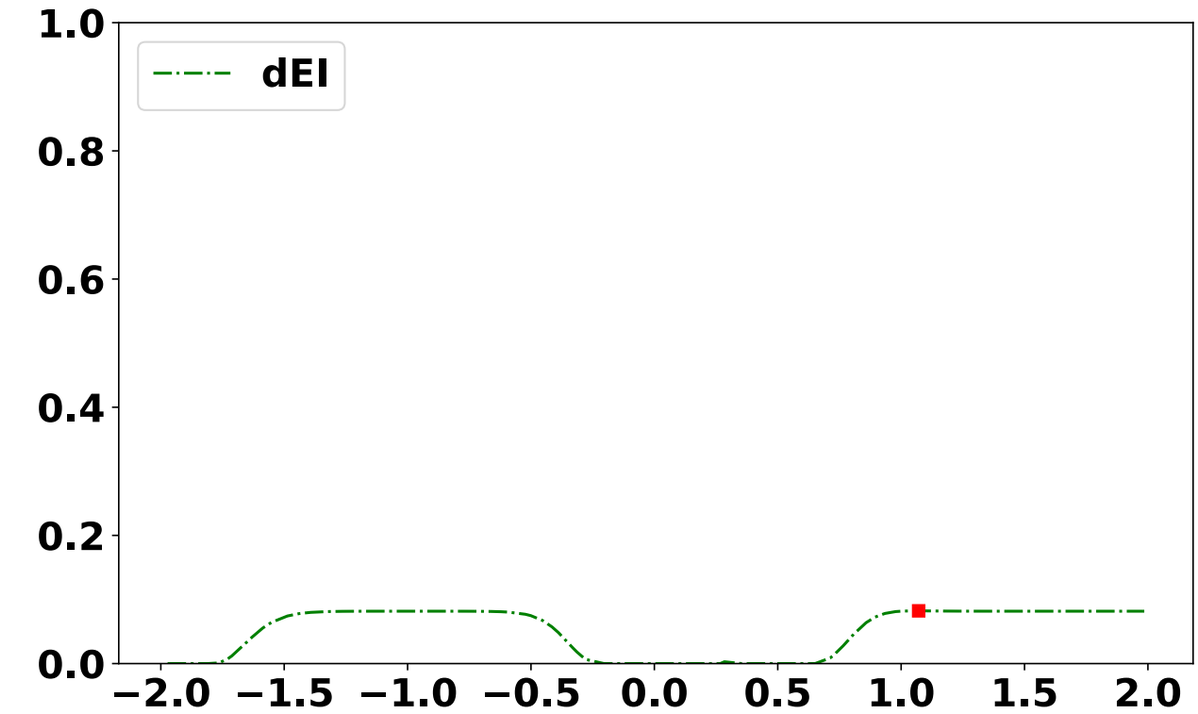

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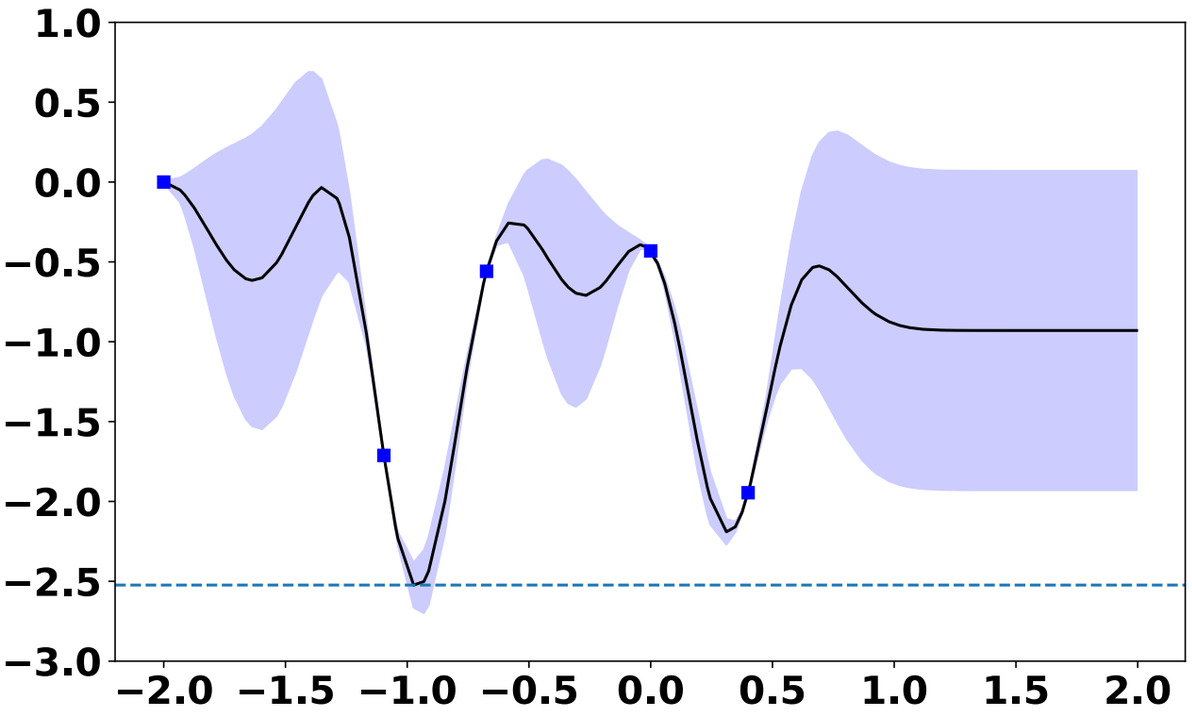

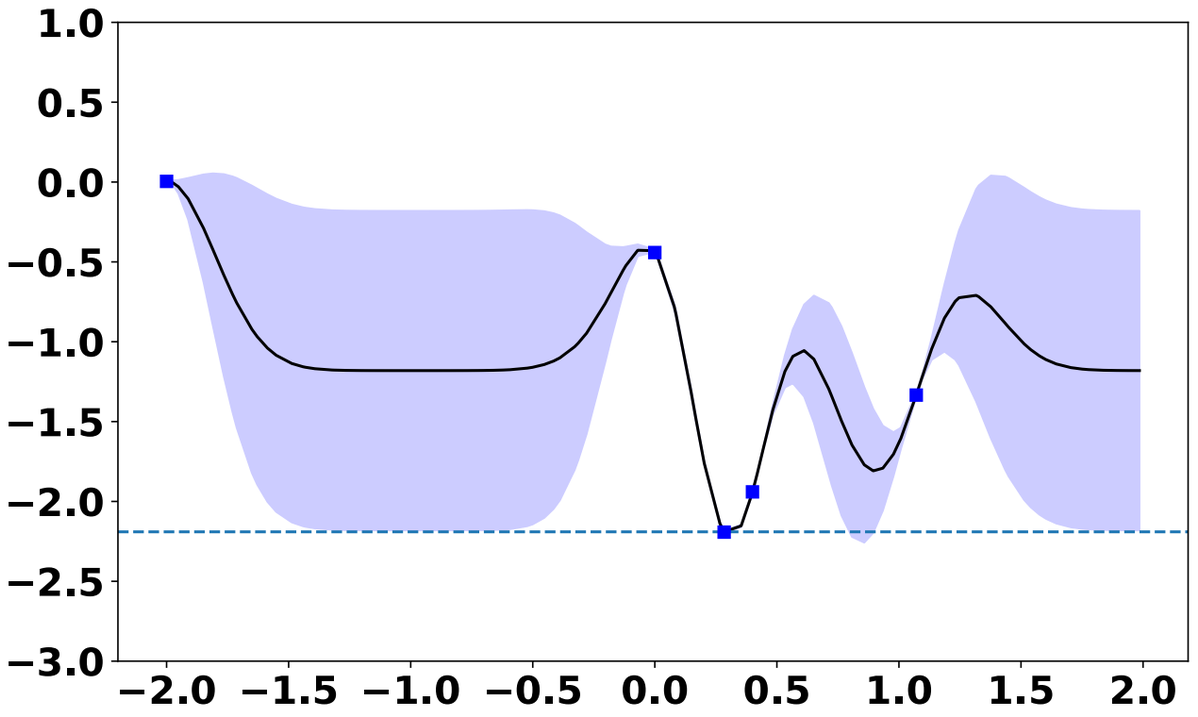

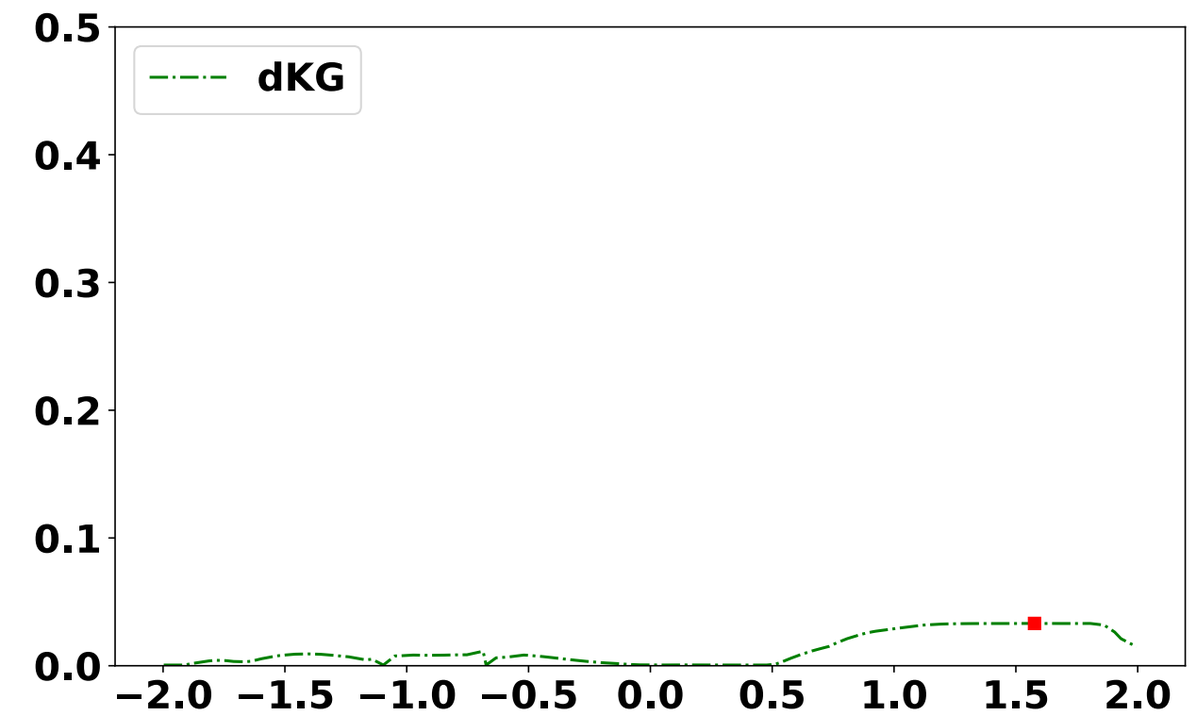

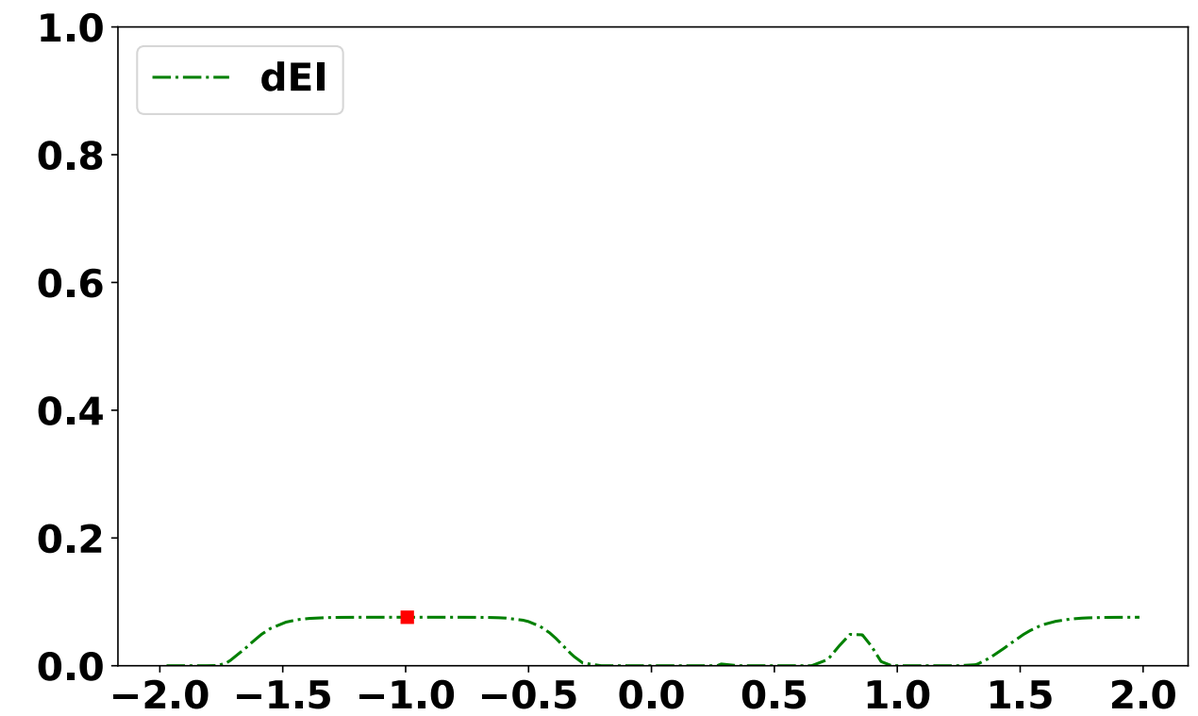

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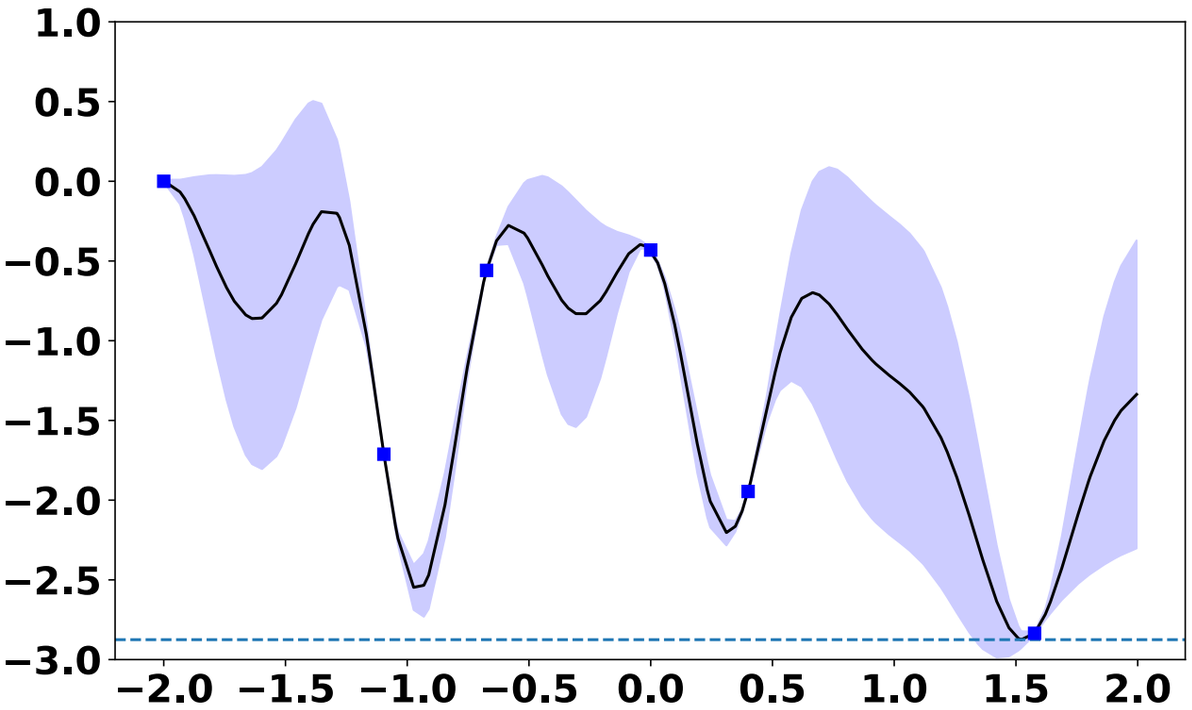

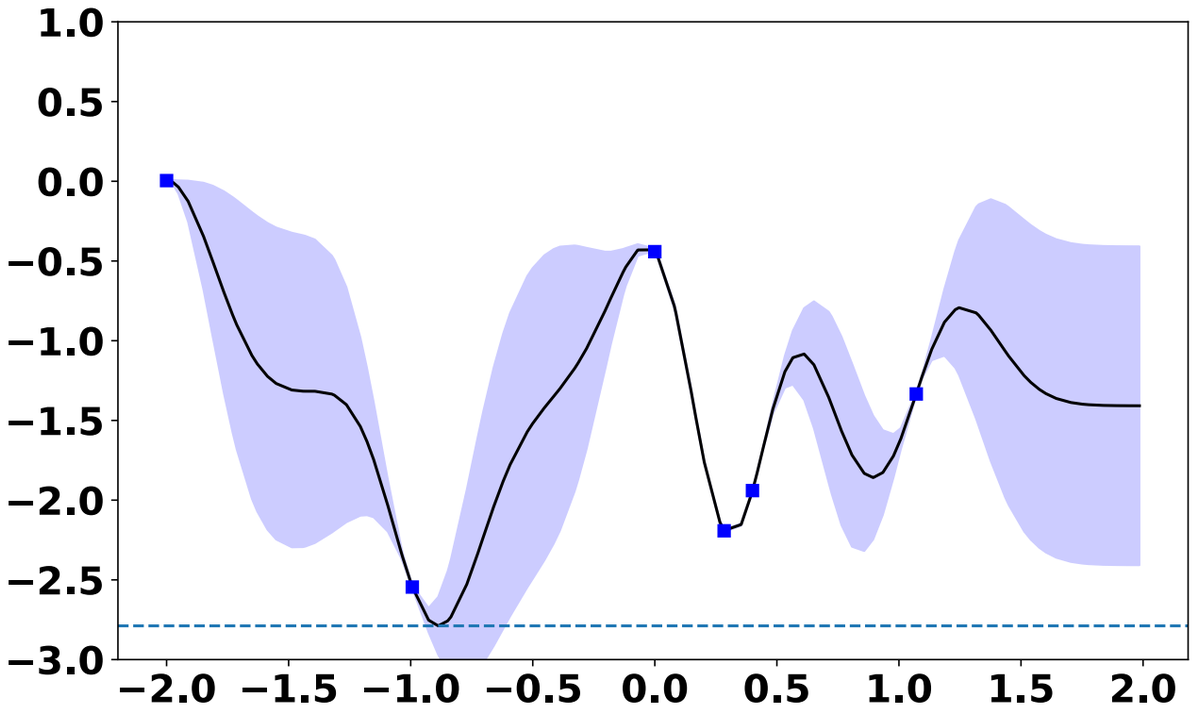

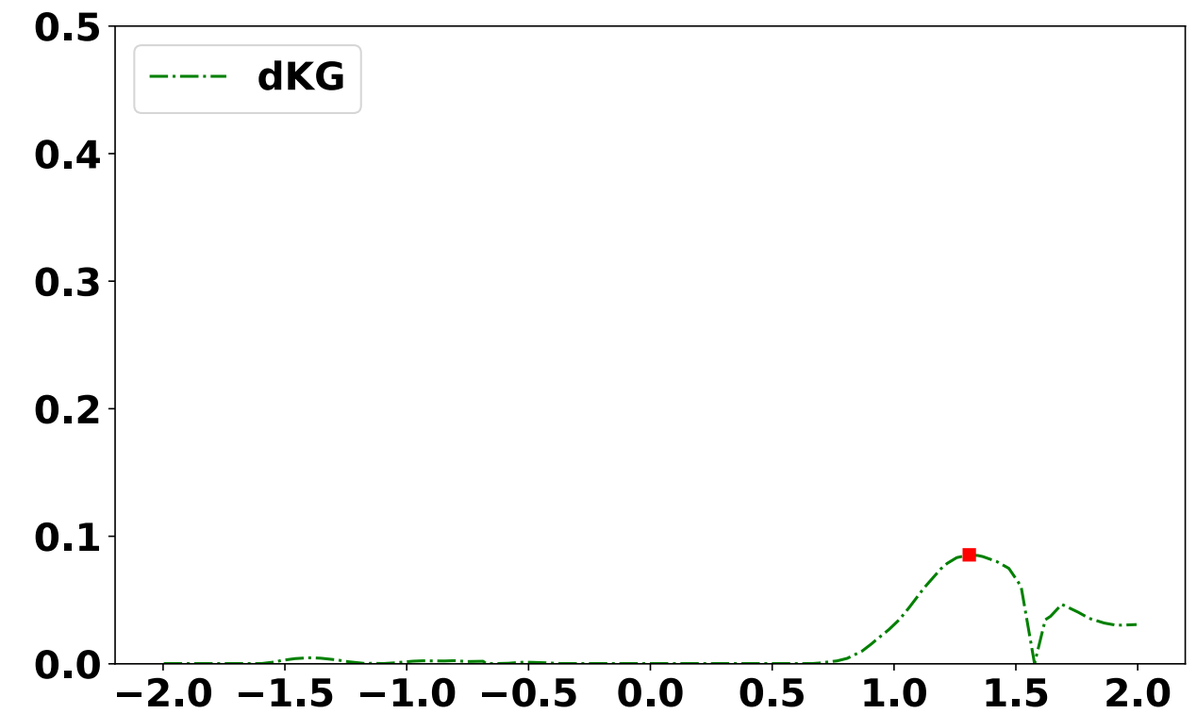

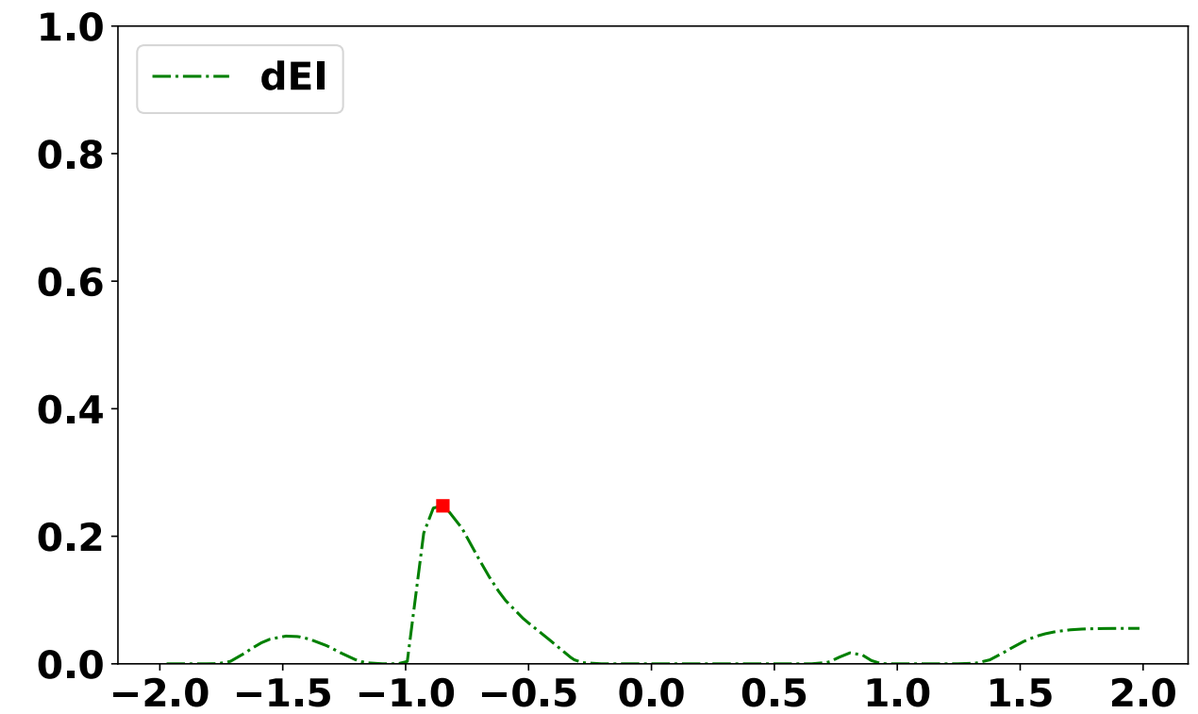

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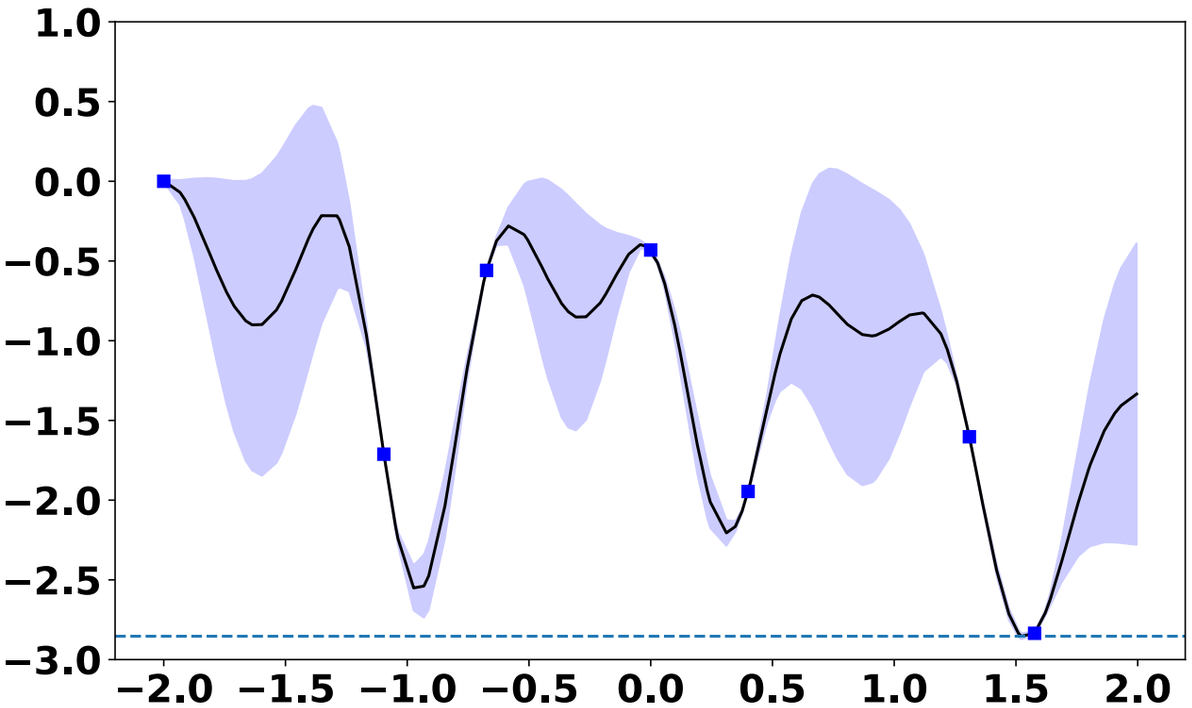
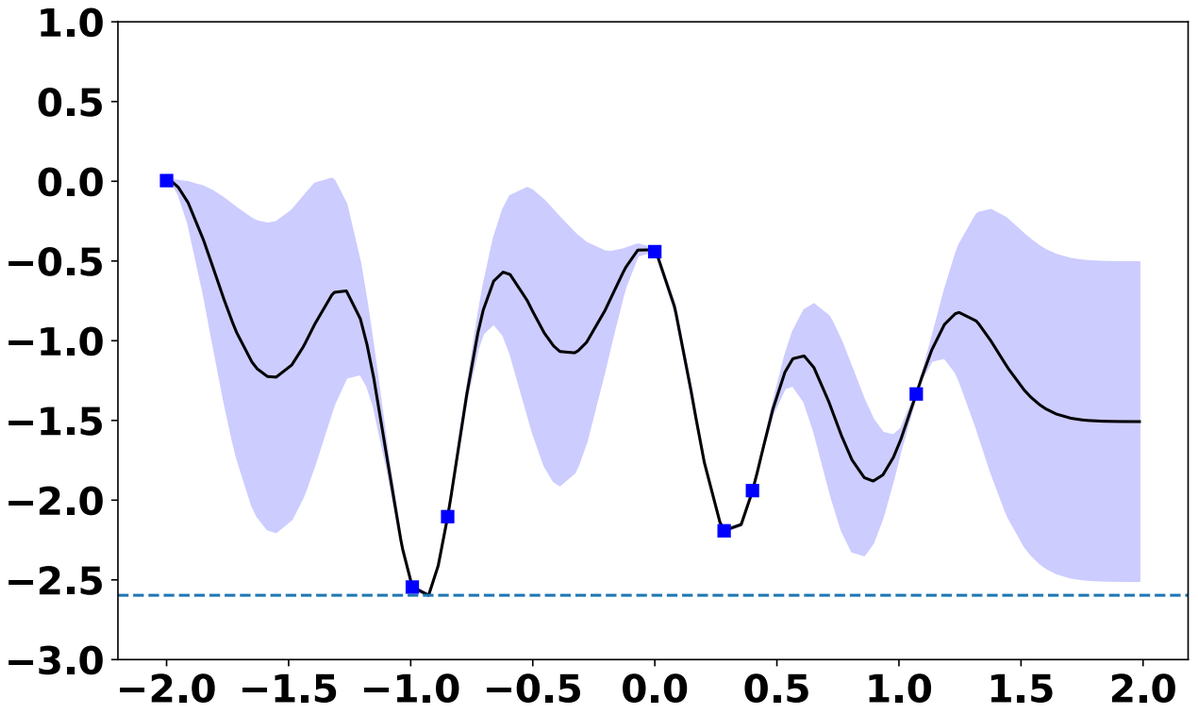
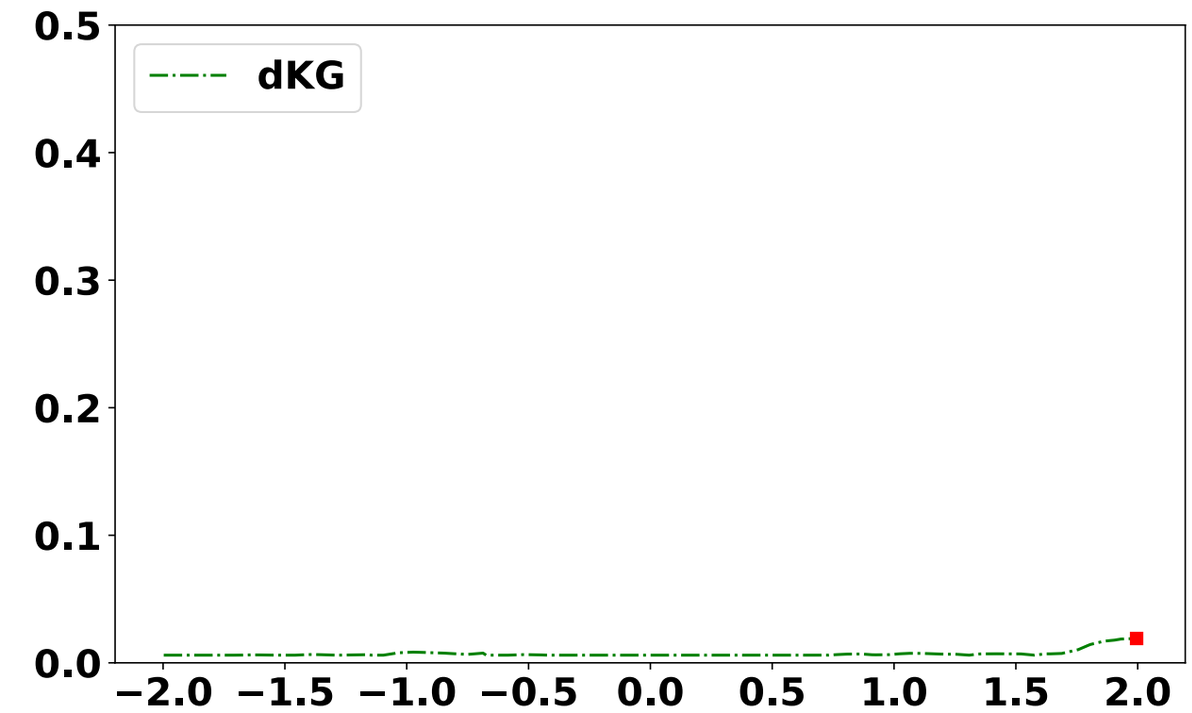
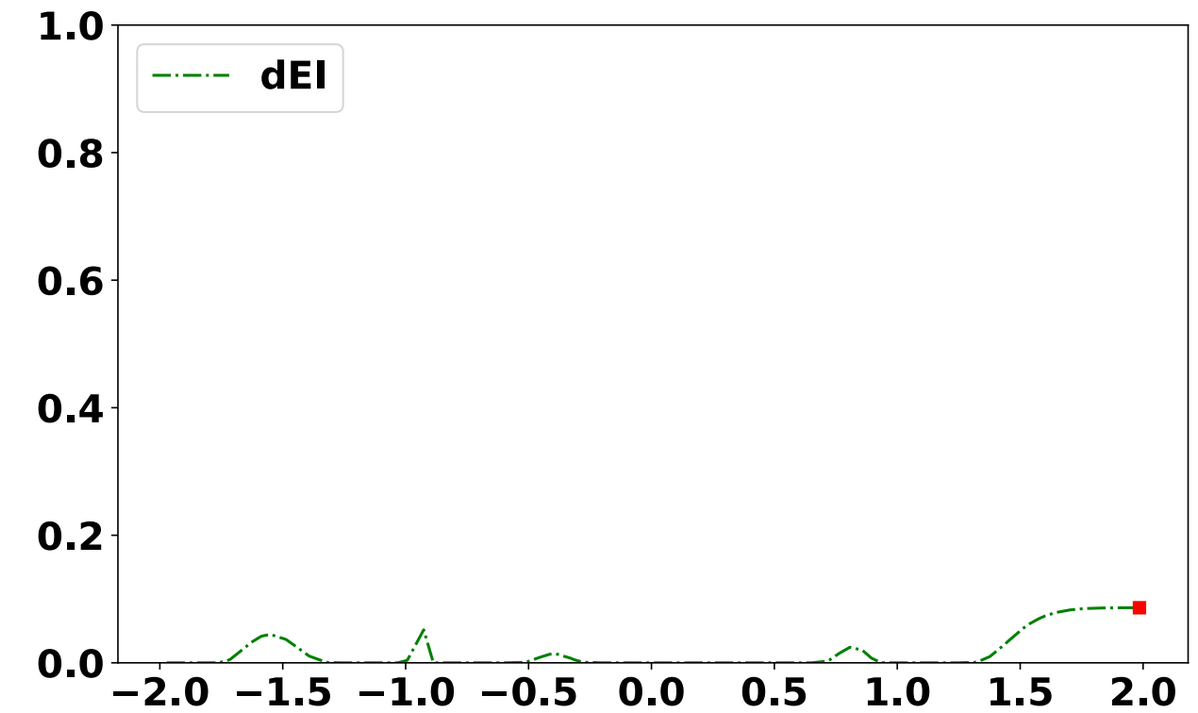
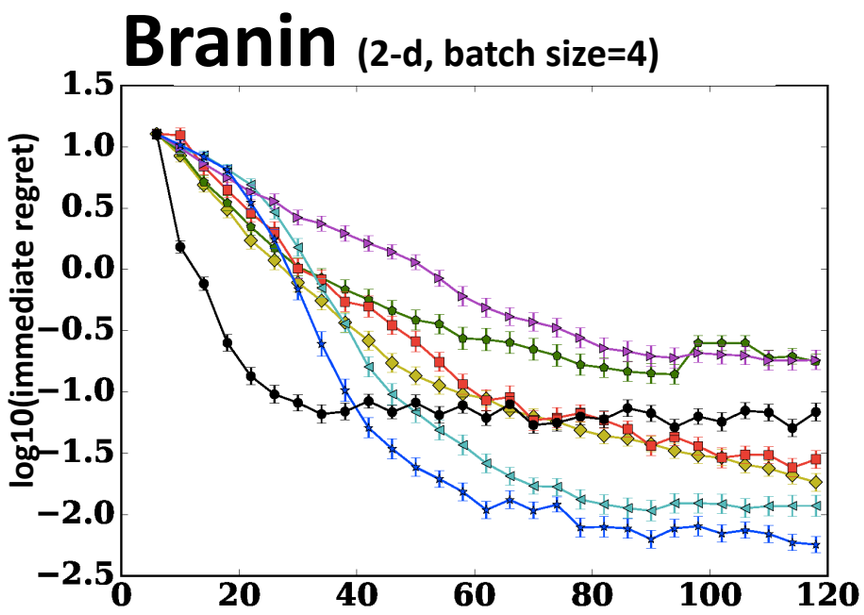


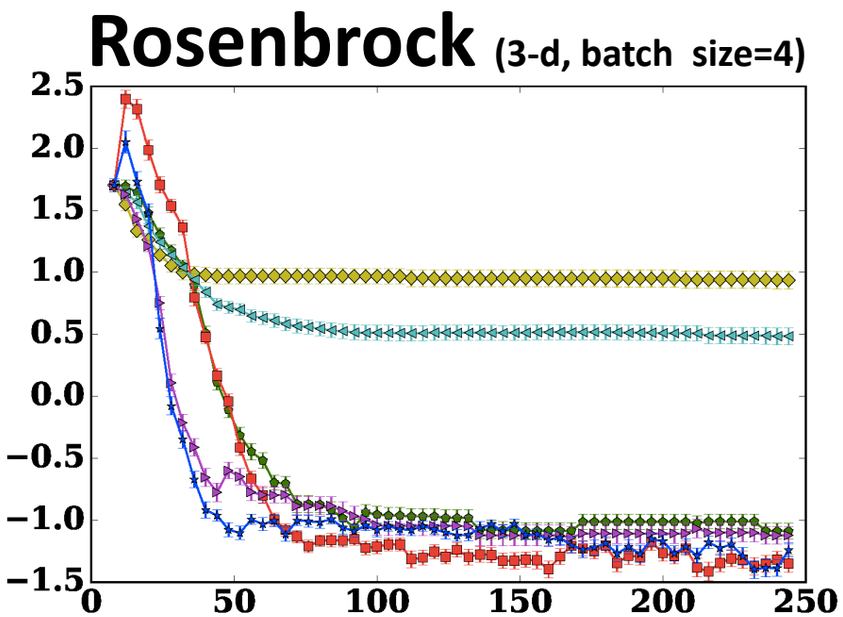


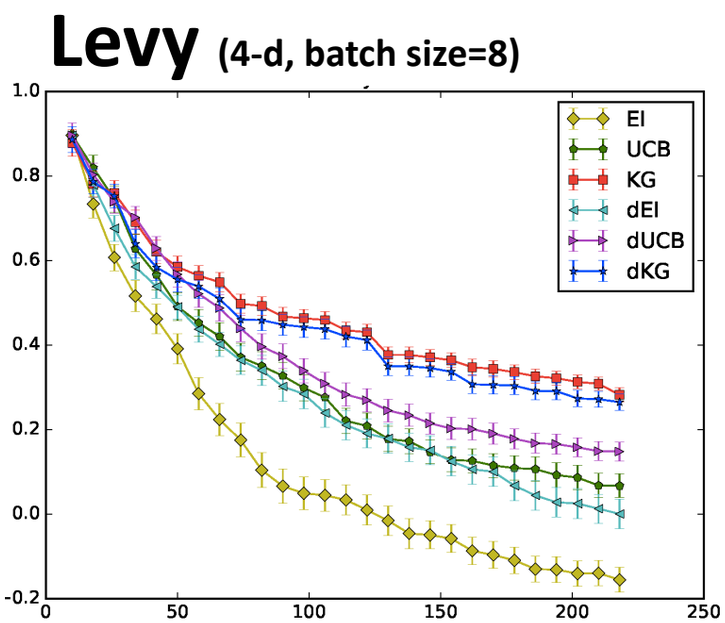


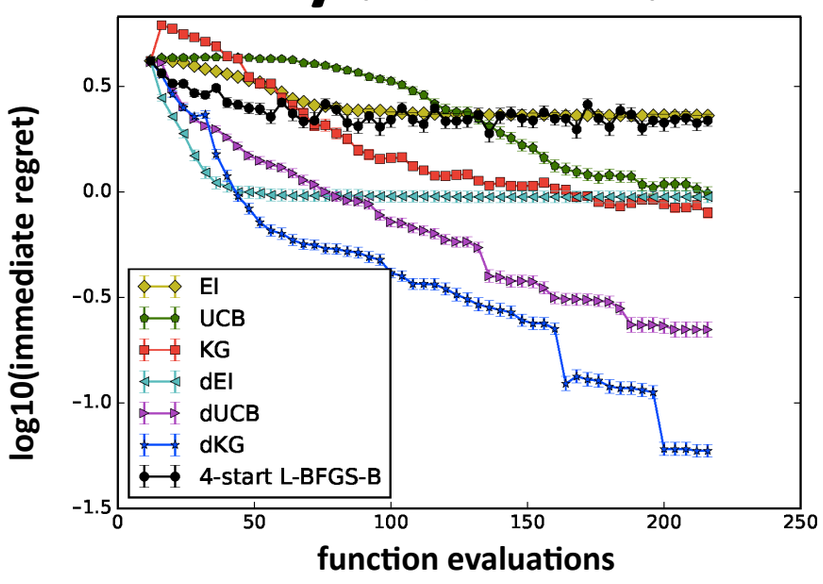


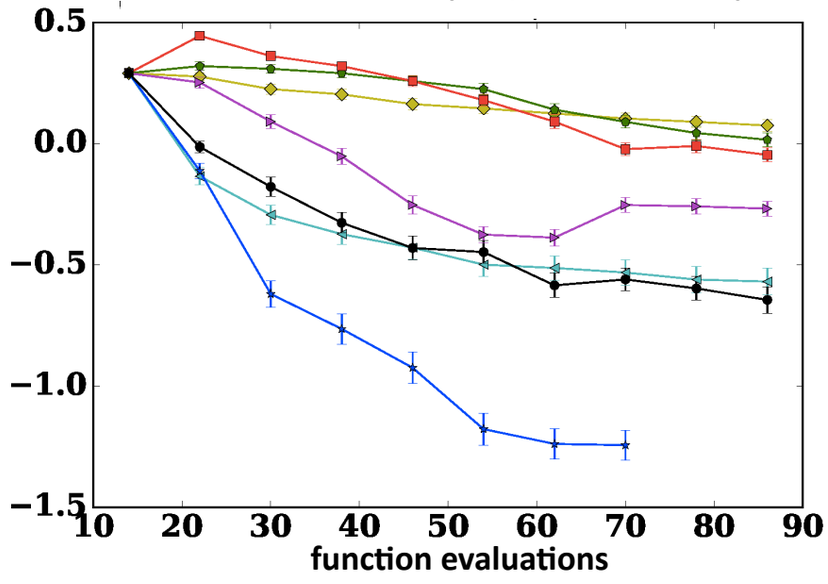
KG provides substantial value over EI when we have gradients

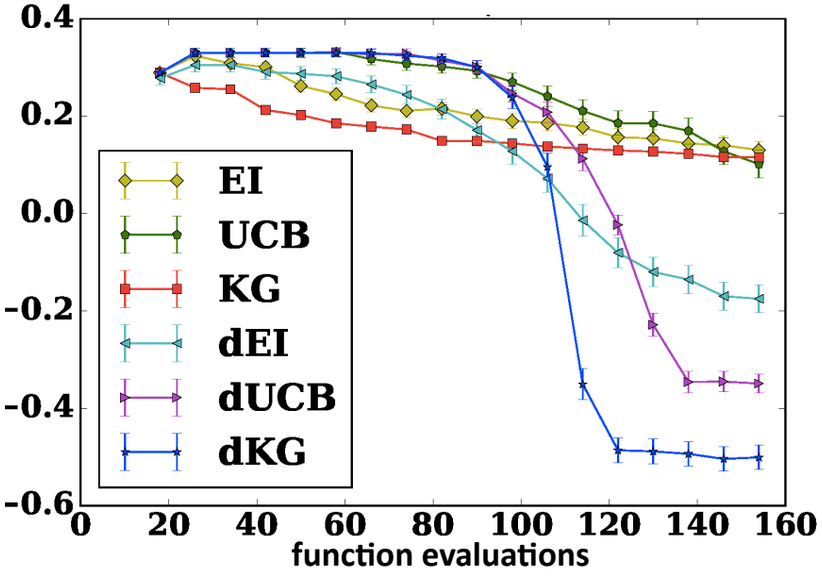












Wu, Poloczek, Wilson & F., Bayesian Optimization with Gradients, NIPS'17

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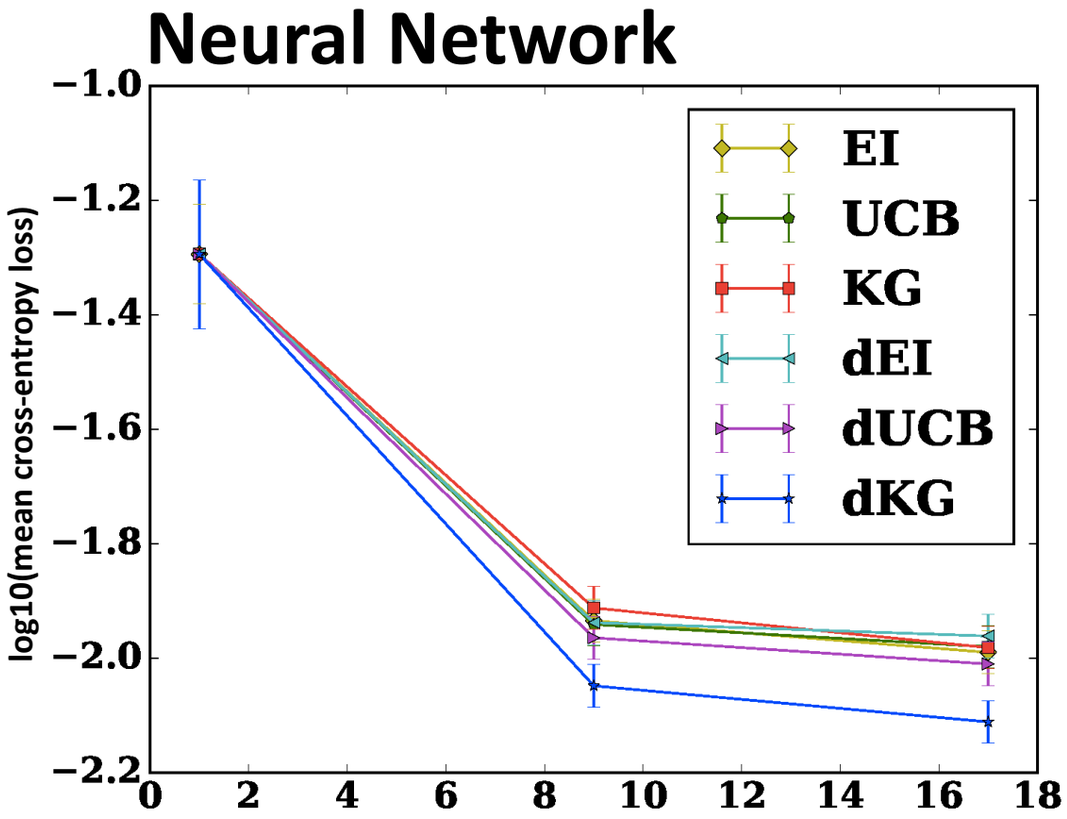
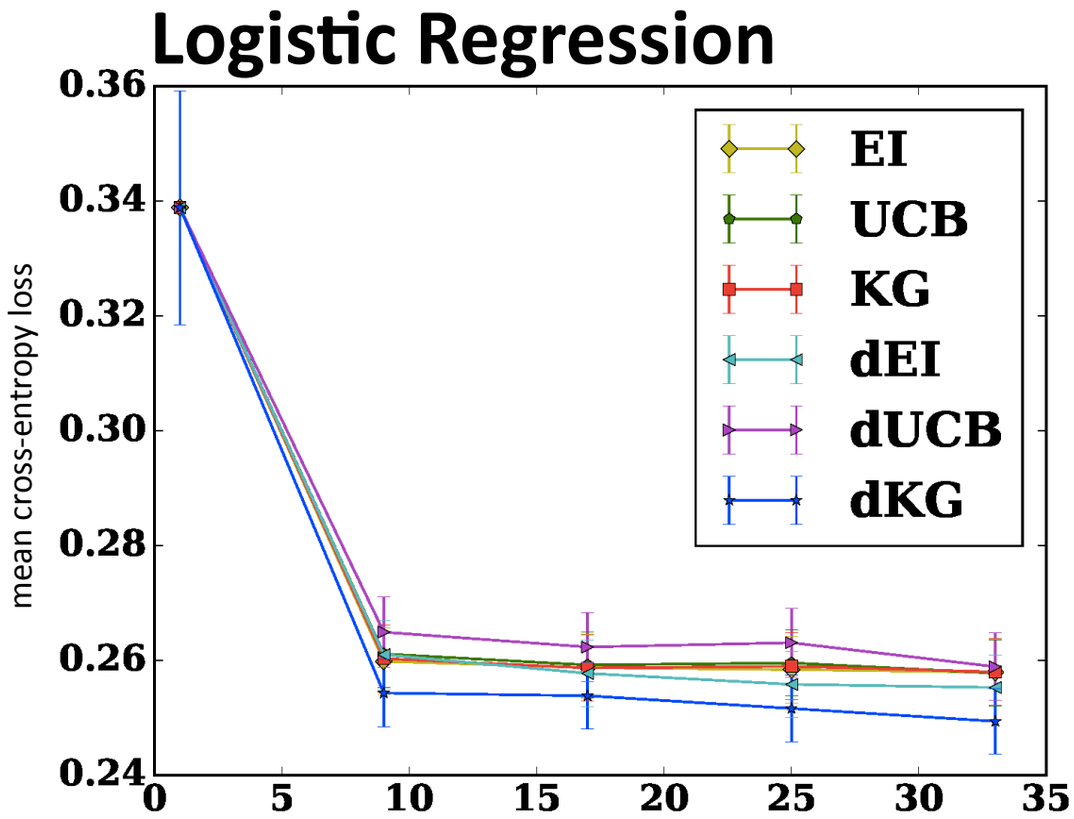
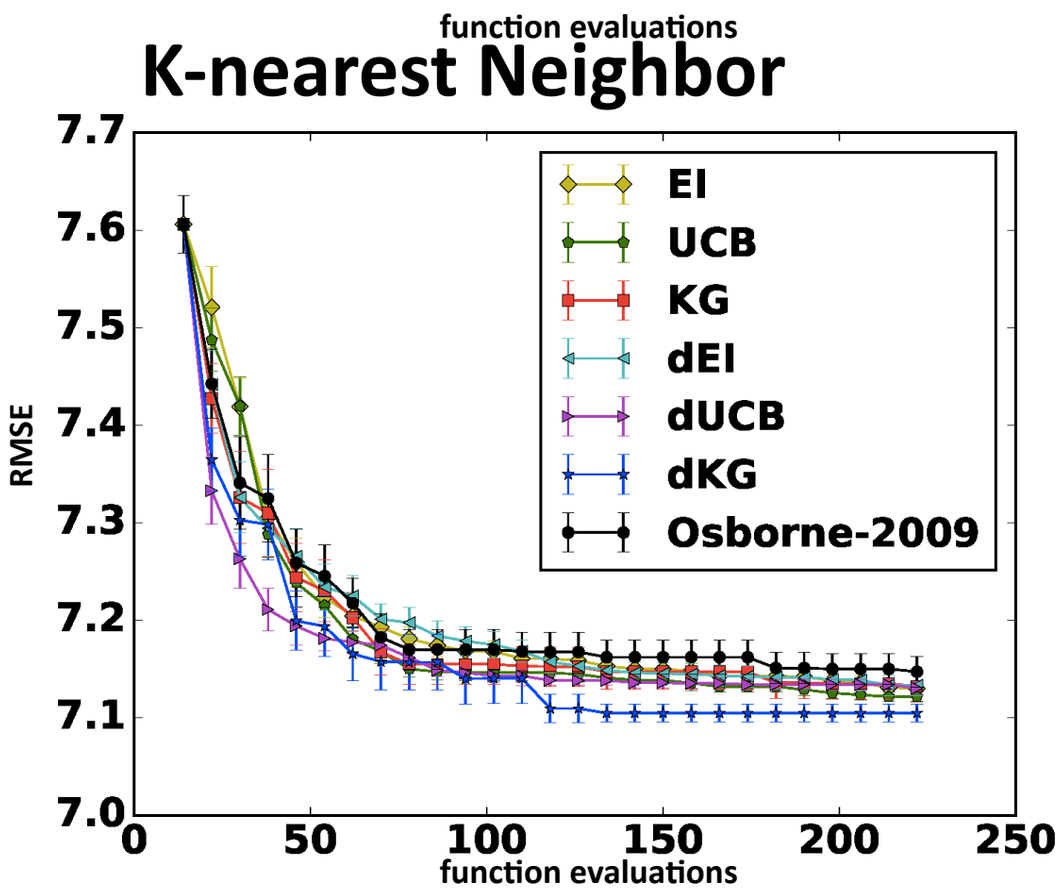
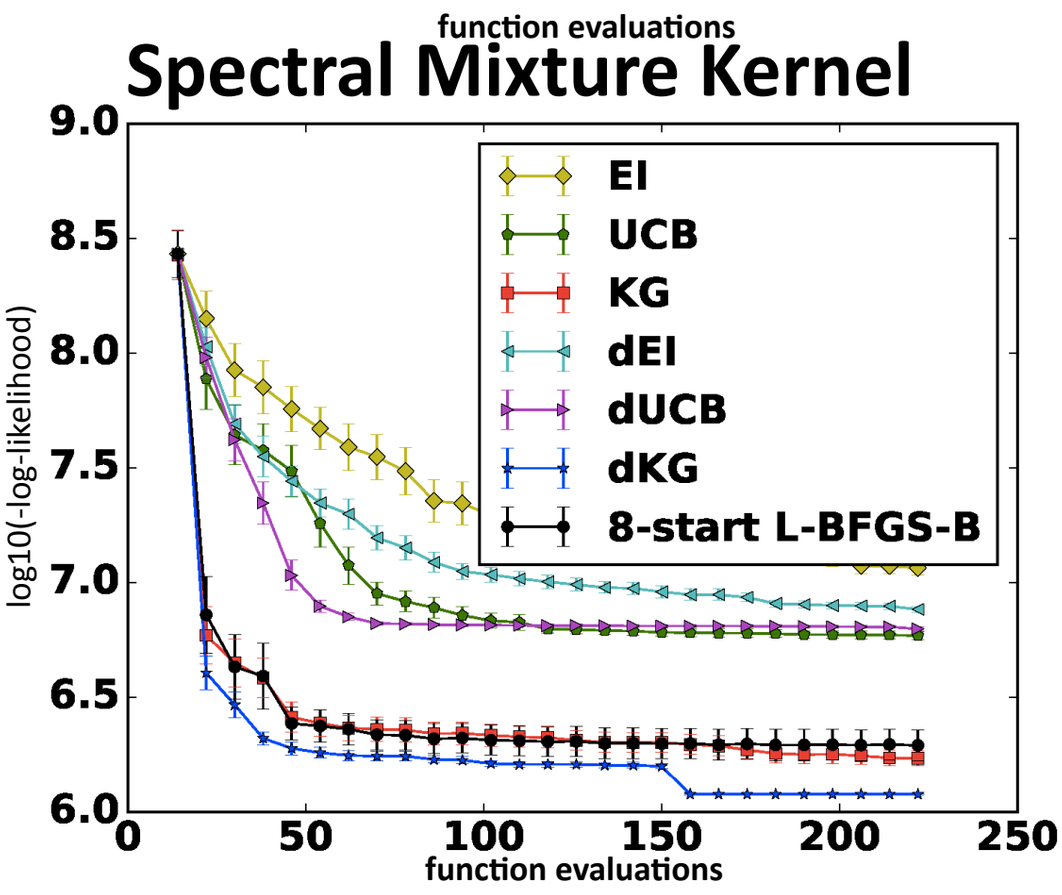




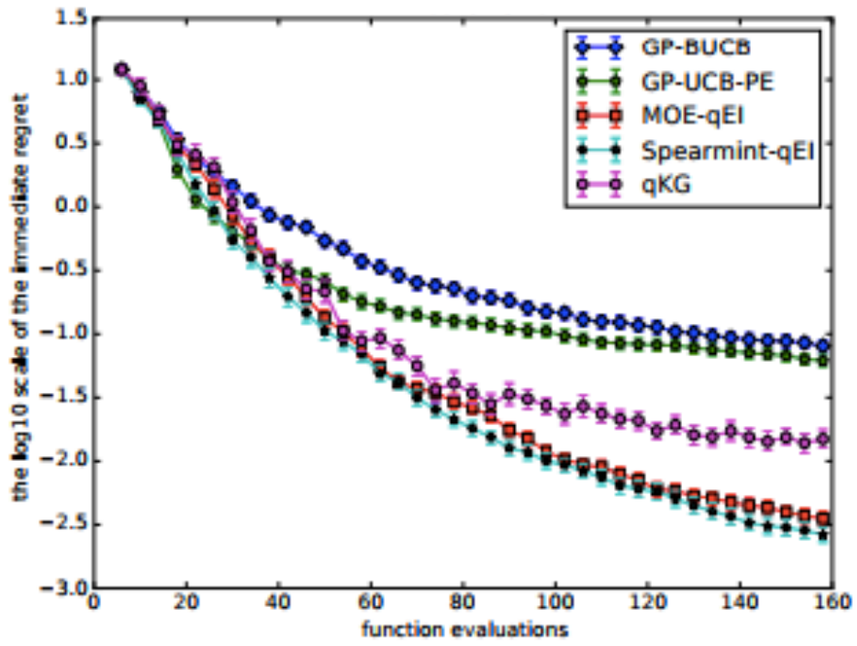




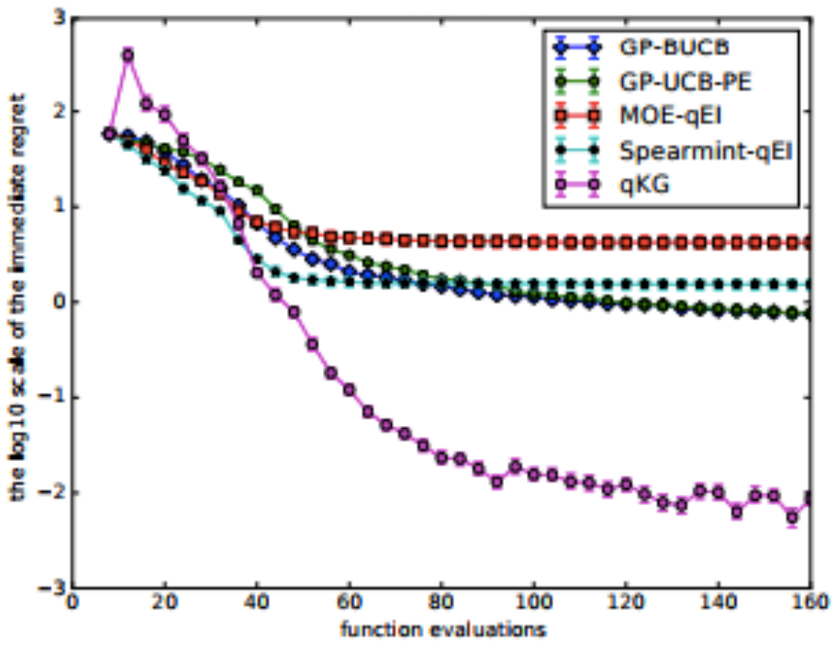
Wu, Poloczek, Wilson & F., Bayesian Optimization with Gradients, NIPS'17

KG provides substantial value over EI when we **don't have gradients** when there is noise, or we are in > 1 dim.

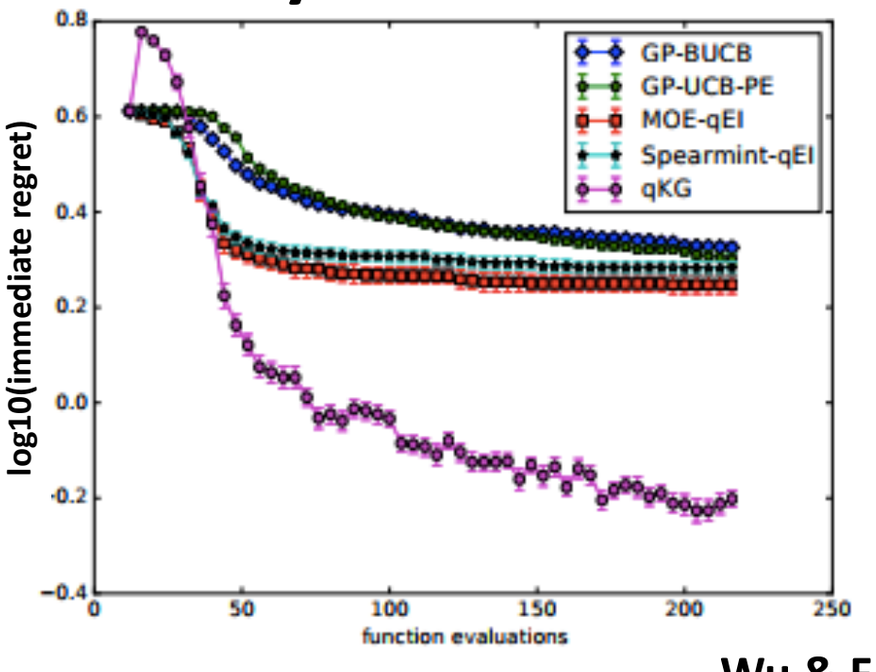
Branin (2-d, batch size=4, no noise)



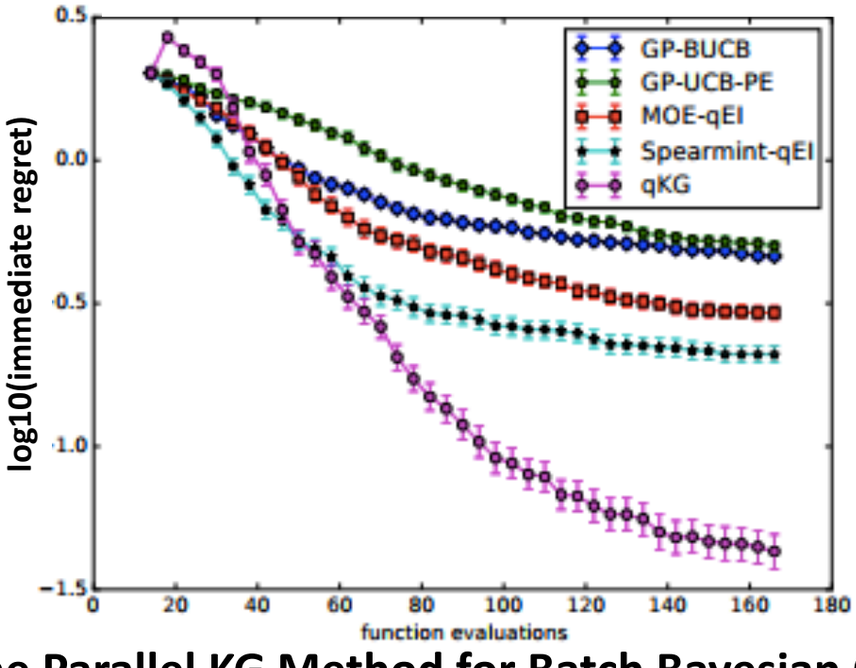
Rosenbrock (3-d, batch size=4, no noise)



Ackley (5-d, batch size=4, no noise)



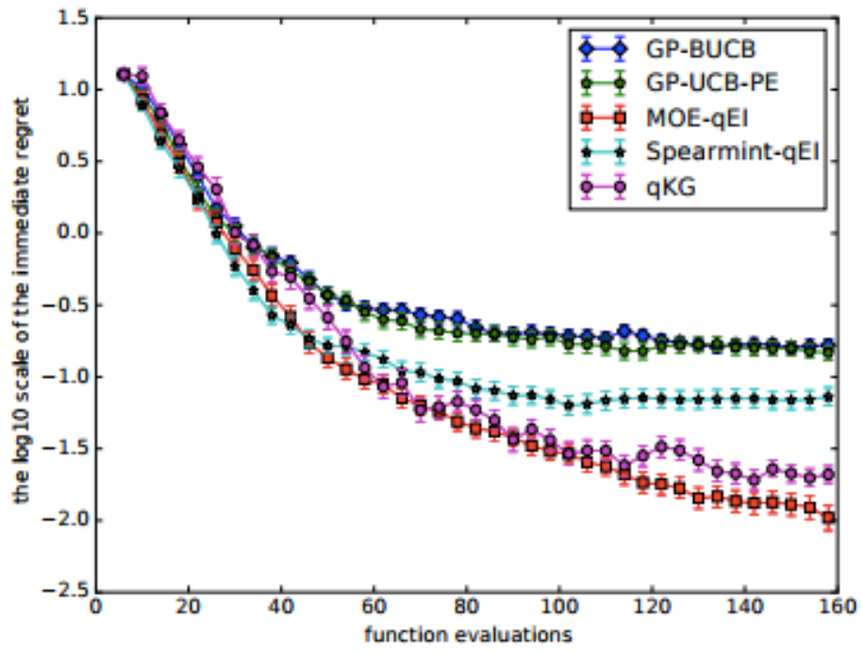
Hartmann (6-d, batch size=4, no noise)



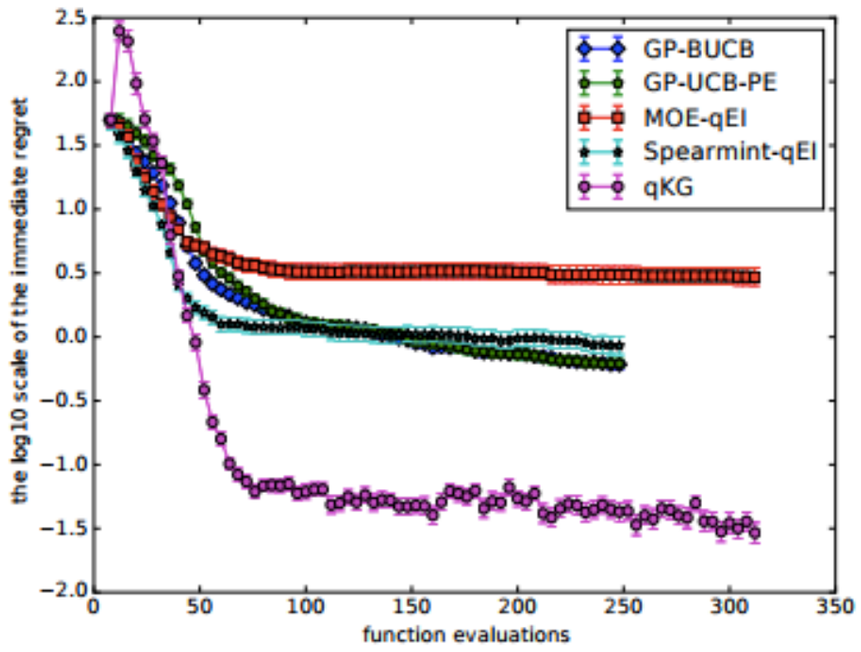
Wu & F., The Parallel KG Method for Batch Bayesian Optimization, NIPS'16

KG provides substantial value over EI when we **don't have gradients** when there is noise, or we are in > 1 dim.

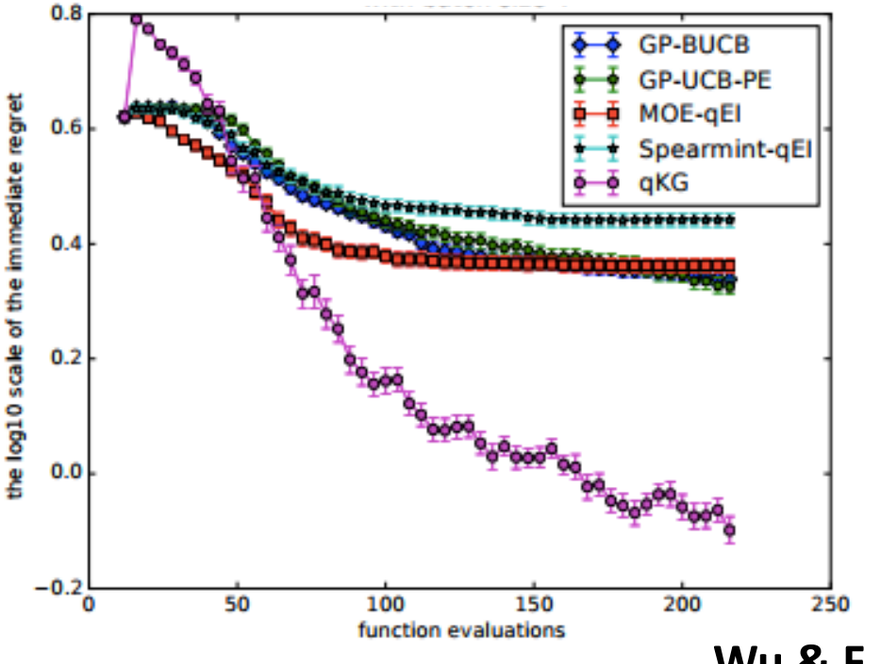
Branin (2-d, batch size=4, noisy)



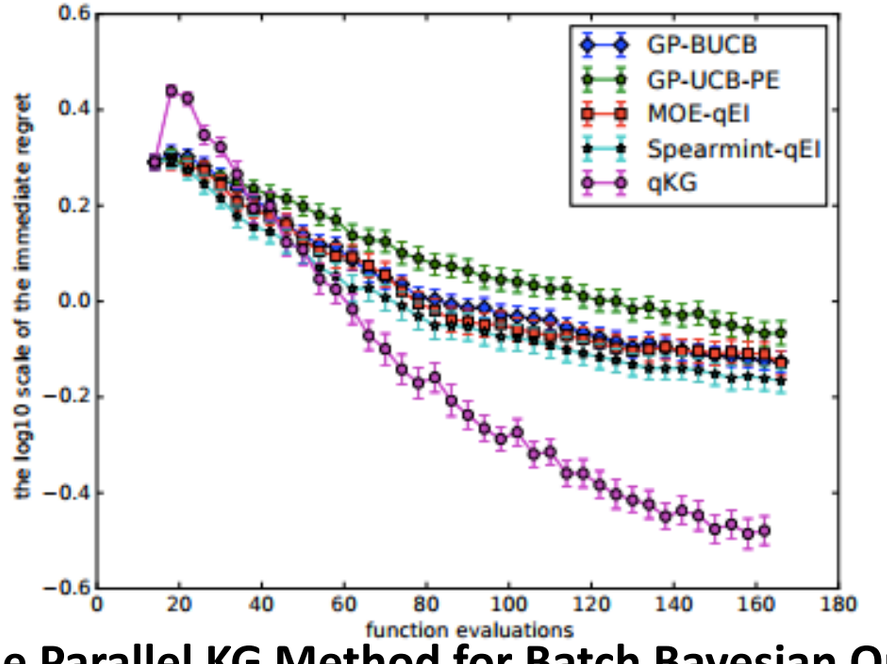
Rosenbrock (3-d, batch size=4, noisy)



Ackley (5-d, batch size=4, noisy)

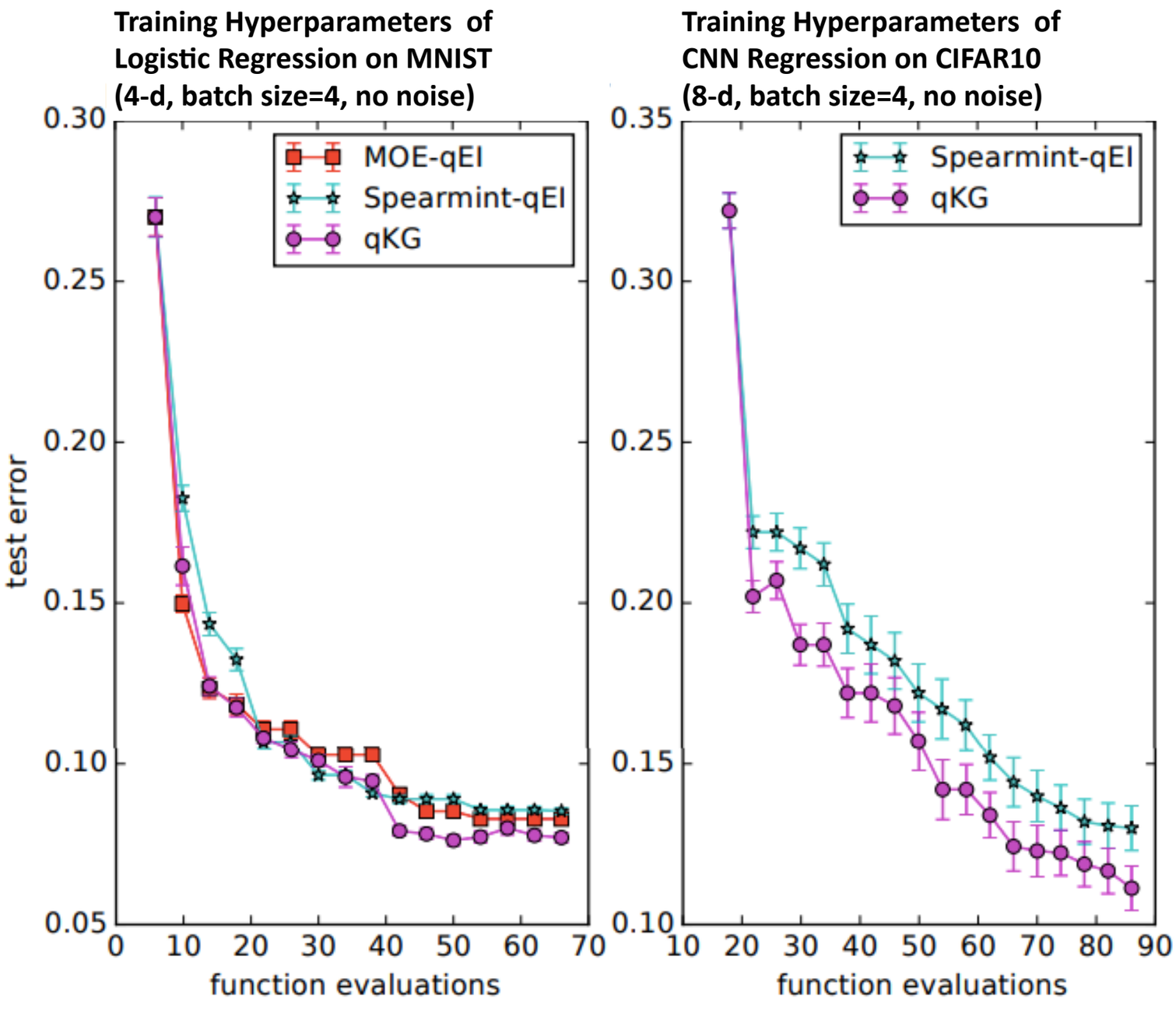


Hartmann (5-d, batch size=4, noisy)



Wu & F., The Parallel KG Method for Batch Bayesian Optimization, NIPS'16

KG provides substantial value over EI when we **don't have gradients** when there is noise, or we are in > 1 dim.



Wu & F., The Parallel KG Method for Batch Bayesian Optimization, NIPS'16

How can we optimize KG(x) efficiently?

Recall this method for computing the KG acquisition function, KG(x)

For i in 1:replications

- Simulate f(x), ∇f(x) from the posterior
- Calculate $\mu^*_{n+1} = \min_{x'} \mu_{n+1}(x')$ from sim'd f(x), ∇f(x)
- Calculate $\mu^*_{n+1} - \mu^*_n$

KG(x) is the average of the simulated $\mu^*_{n+1} - \mu^*_n$ values

Our approach to maximizing $\mathrm{dKG}(\mathrm{x}_{1:q})$

1. Estimate $\nabla \mathrm{dKG}(\mathrm{x}_{1:q})$
   using infinitesimal perturbation analysis (IPA).

2. Use multistart stochastic gradient ascent to find an approximate solution to solve argmax $\mathrm{dKG}(\mathrm{x}_{1:q})$.

Here's how we estimate ∇dKG

- $Y=[f(x_i), \nabla f(x_i) : i=1:q\ ]'$ is multivariate normal with dim. $q(d+1)$
- $Y=m(x_{1:q}) + C(x_{1:q})Z$, where Z is a standard normal random vector
- Write the dependence of $\mu_{n+q}(x)$ on $x_{1:q}$ and Y explicitly as $\mu_{n+q}(x; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)$
- $\nabla dKG(x_{1:q}) = \nabla E[\min_{x \text{ in } A}\ \mu_{n+q}(x; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)]$
  $= E[\nabla \min_{x \text{ in } A}\ \mu_{n+q}(x; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)]$
  $= E[\nabla \mu_{n+q}(x^*; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)],$

  where $x^* = \text{argmin}_{x \text{ in } A}\, \mu_{n+q}(x; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)$
  and its dependence on $x_{1:q}$ is ignored when taking the gradient.

Here's how we estimate ∇dKG

1. Calculate the mean $m(x_{1:q})$ and the Cholesky decomposition $C(x_{1:q})$ of the covariance matrix of $Y=[f(x_i), \nabla f(x_i) : i=1:q\ ]'$ under the time n posterior distribution.
2. Simulate a standard normal random vector Z. Let $Y = m(x_{1:q}) + C(x_{1:q})Z$
3. Use a nonlinear solver to calculate x^* in $\operatorname{argmin}_x\ \mu_{n+q}(x; x_{1:q}, Y)$
4. Our estimator of $\nabla KG(x_{1:q})$ is $G=\nabla\mu_{n+q}(x^*; x_{1:q}, m(x_{1:q}) + C(x_{1:q})Z)$, holding x^* fixed

Our estimator of the gradient is unbiased

Theorem: When the posterior mean μ_n and covariance kernel Σ_n are continuously differentiable and the domain A is compact,
G is an unbiased estimator of $\nabla dKG(x_{1:q})$

Proof:

- Use conditions in L'Ecuyer 1990 to interchange ∇ and expectation.
- Use the envelope theorem (Milgrom and Segal 2002) to hold x^* fixed

KG converges to a globally optimal solution over a discrete domain

Theorem: When the domain A is discrete & finite, the KG algorithm is consistent, i.e.,

$$\lim_{N\to\infty} f(x^*(\mathrm{dKG}, N)) = \max_{x\in A} f(x)$$

almost surely under the prior, where *x*(KG,N)* is the solution computed by KG after N batches of samples.

Wu, Poloczek, Wilson & F., Bayesian Optimization with Gradients, NIPS'17

KG is useful for other BO problems too: multi-task, multi-fidelity & multi-information source optimization

Poloczek, Wang & F., Multi Information-Source Optimization, NIPS'17

KG is useful for other BO problems too: multi-task, multi-fidelity & multi-information source optimization

- objective f(s,x) ~ GP(mu,Sigma)
- cost c(s,x) ~ GP(mu,Sigma)
- s indexes information sources (IS)
  s=0 is the target we wish to optimize
  x indexes designs
- Goal: solve $\min_x f(0,x)$ using (possibly noisy) queries to f(s,x) at cost c(s,x)

Poloczek, Wang & F., Multi Information-Source Optimization, NIPS'17

Expected Improvement isn't that helpful when used directly in this problem

When you sample $s \neq 0$ at x:
you change the posterior on f,
but you don't observe $f(0,x)$.
There is no improvement in the best solution seen

Using EI requires hacking [see, e.g., Lam et al. 2015]

KG works out of the box

KG(s,x) := $E_n[\mu^*_n - \mu^*_{n+1} \mid$ query x using IS s],

where, $\mu^*_n := \min_x \mu_n(x)$

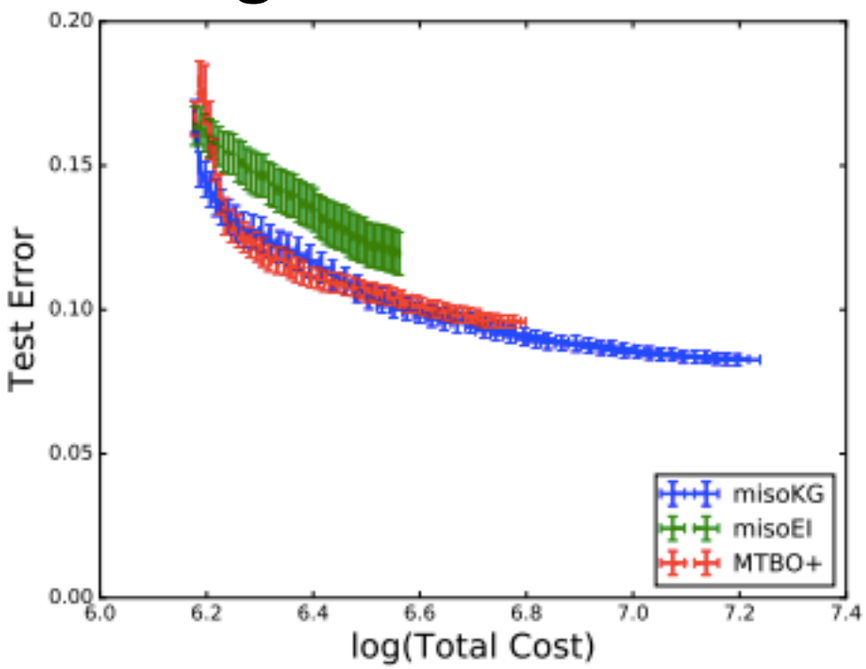
$\mu_n(s,x) := E_n[f(0,x)]$ is the posterior mean on the target at x

Since cost varies, we sample the s,x that maximizes KG(s,x)/cost(s,x)

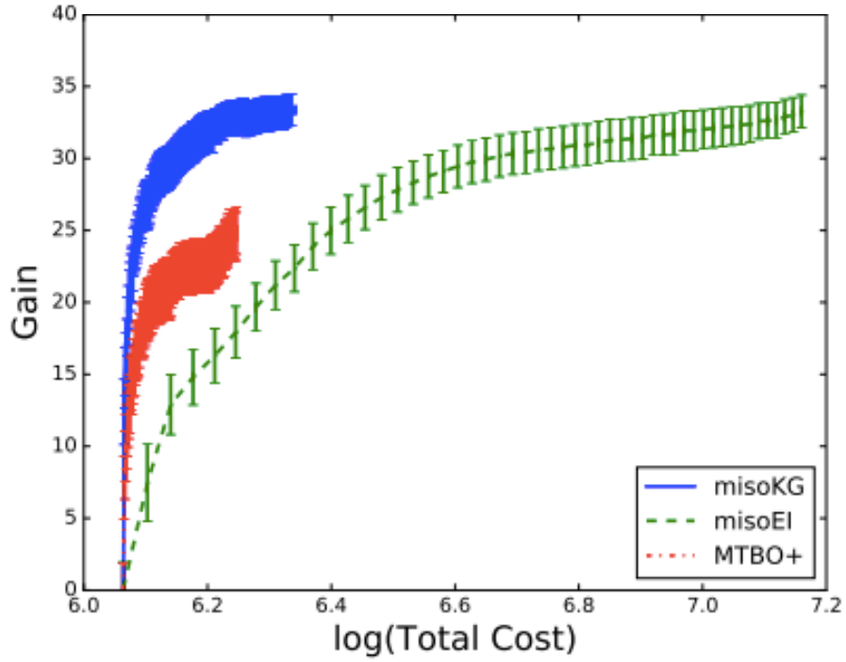
Poloczek, Wang & F., Multi Information-Source Optimization, NIPS'17

KG provides substantial value over EI (and predictive entropy search)

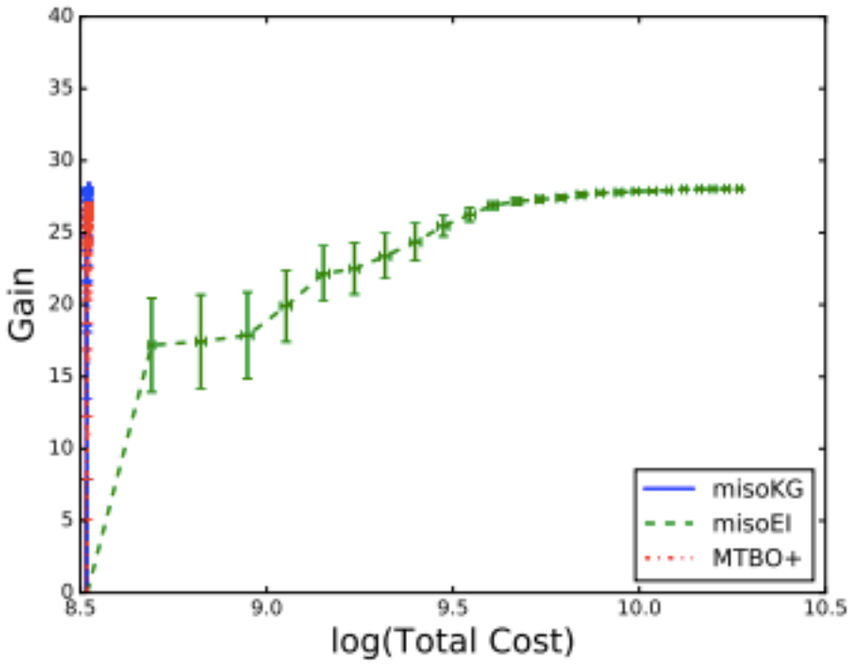
Image Classification [Swersky et al. 2013]



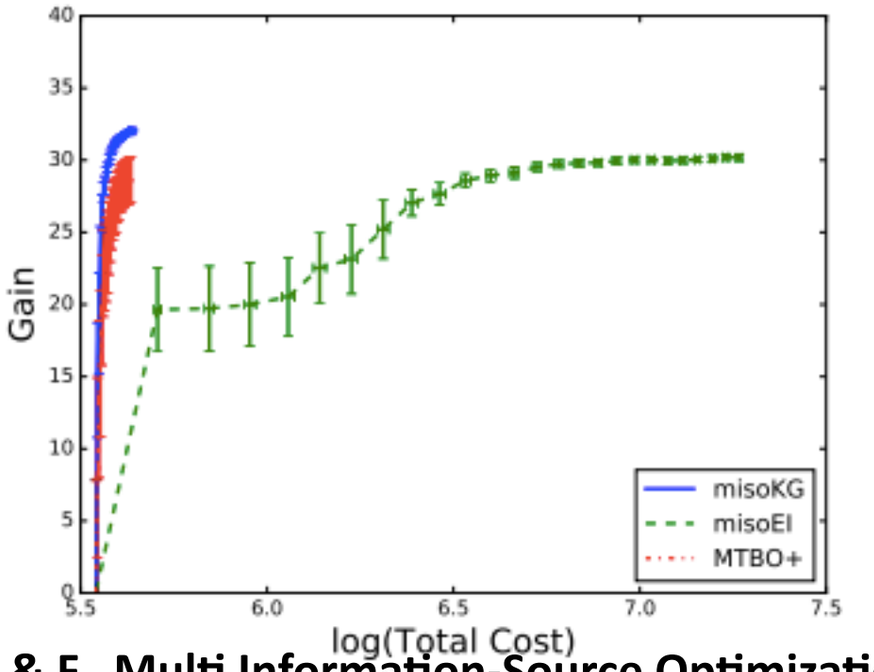
Assemble to Order



Rosenbrock [Lam et al. 2015]



Rosenbrock #2



Poloczek, Wang & F., Multi Information-Source Optimization, NIPS'17

Predictive Entropy Search (PES)

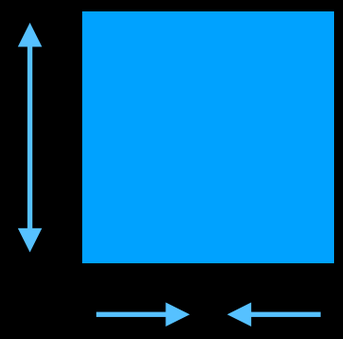
- PES [Hernandez-Lobato et al. 2014] selects the sample that maximizes the expected reduction in the entropy of x*

$$PES(x) = H[p_n(x^*)] - E[H(p_{n+1}(x^*)) \mid \text{query } x]$$

- Works well, if reducing the entropy of x* corresponds to reducing simple regret
- Much more expensive to compute than EI

Reducing the entropy of x* by a lot doesn't always mean you reduce simple regret by a lot

- Our goal: solve $\min_x f(x)$, where x in R^2
- Let $g(x_1,x_2) = f(x_1 / 10, x_2 * 10)$



- When we run PES on g instead of f, PES will work much harder to learn x_2* and will have very different simple regret

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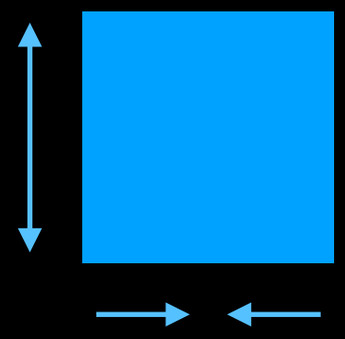

- When we run PES on g instead of f, PES will work much harder to learn x_2* and will have very different simple regret
- To make the problem worse, suppose f is additive across coordinates, and we observe directional derivatives

Reducing the entropy of x* by a lot doesn't always mean you reduce simple regret by a lot

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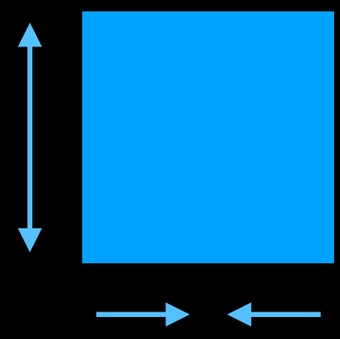
- Let $g(x_1,x_2) = f(x_1 / 10, x_2 * 10)$



- When we run PES on g instead of f, PES will work much harder to learn x_2* and will have very different simple regret
- In contrast, KG's simple regret is invariant to such transformations

Give KG a try

- KG tends to have better query efficiency than EI when the improvement in the posterior is not at the queried point.
- Both KG & PES value improvement in the posterior away from the queried point.
- KG directly values reduction in the simple regret, while PES values it indirectly.
- KG is slower to code & compute than EI. It is comparable to PES.

Code is available:
https://github.com/wujian16/Cornell-MOE (try this 1st)
https://github.com/misokg

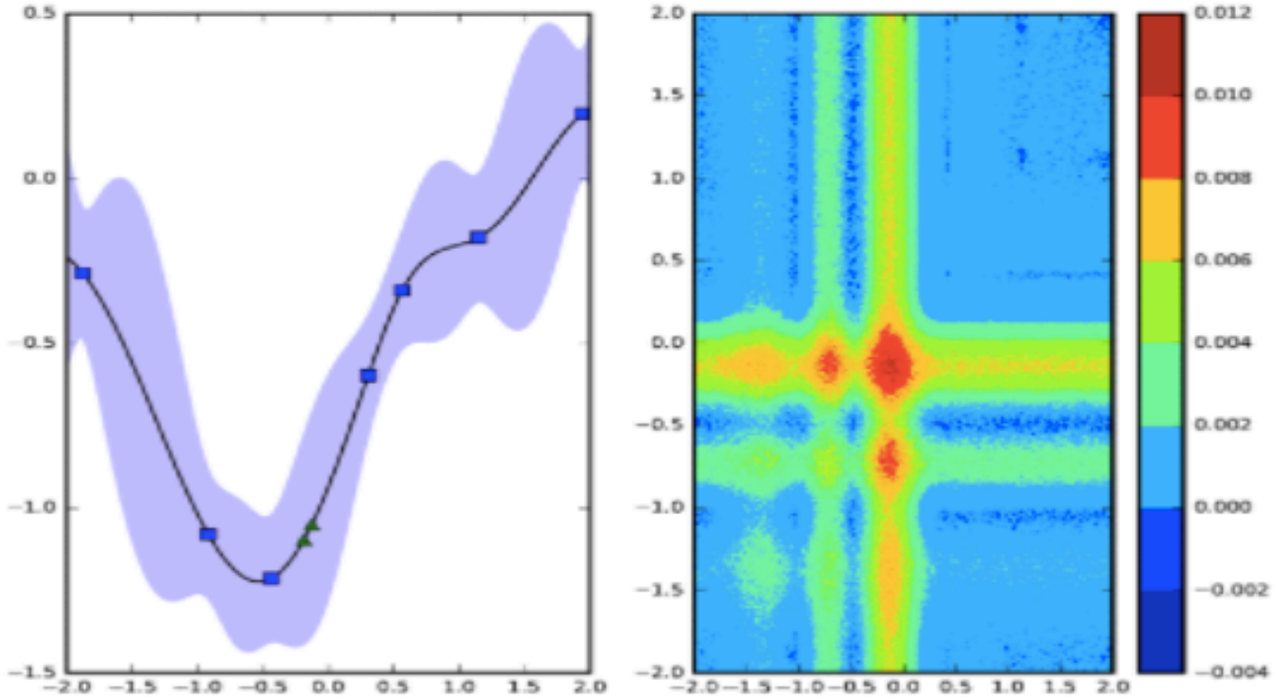
GitHub, Inc. [US] | https://github.com/wujian16/Cornell-MOE/blob/master/README.md

Introduction:

Below we show two demos:

a demo of q-KG on a 1-d derivative-free synthetic function with a batch size q=2.

The left-hand side shows the fitted statistical model and the points suggested by Cornell-MOE. Note that the function evaluation is subject to noise; the right-hand side visualizes the acquisition function according to q-KG criteria.



a demo of d-KG vs. d-EI on a 1-d synthetic function. d-KG explores much more efficiently.

Uber is hiring in BayesOpt:
Email pfrazier@uber.com
or zoubin@uber.com