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TECHNISCHE UNIVERSITÄT BERLIN

UNIVERSITÀ DEGLI STUDI DI PADOVA

BIFOLD

Bayesian methods for Variational Quantum Eigensolvers



AQTIVATE CONFERENCE

29.09.2026

Samuele Pedrielli

BIFOLD · Technische Universität Berlin · Università di Padova

Context / Variational Quantum Eigensolver



Goal

Given a Hamiltonian, find its lowest-energy eigenstate.

$$H\,|\psi_0\rangle = E_0|\psi_0\rangle$$

E_0 : lowest possible energy. $|\psi_0\rangle$:corresponding ground state.

KNOWN: THE HAMILTONIAN H

It defines the problem & how energy is evaluated.

UNKNOWN: THE GROUND STATE

Its ground-state eigenvector is unknown.

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> **VQE addresses this problem using *both* a quantum and a classical computer.**

How

Prepare a parametrized state on a quantum computer:

$$|\psi(\theta)\rangle = U(\theta)|0\rangle$$

θ: adjustable parameters

Measure its energy on a on a quantum computer:

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0$$

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Minimize the energy on a classical computer:

$$\theta^* = \underset{\theta}{\operatorname{argmin}}\, E(\theta)$$

Prepare → measure → update θ

Finite shots give noisy,
costly energy estimates.

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We focus on the classical optimization part of the algorithm.

Context / Optimization Strategies



Two ways to optimize VQE

Sequential Minimal Optimization

$$\theta_d^* = \underset{\theta_d}{\operatorname{argmin}}\, E_d(\theta_d)$$

Look only at one parameter slice θ_d.
Minimize that slice.
Move to the next parameter θ_{d+1}.

Bias + regularization

Pedrielli et al. [2605.15813]

Gradient descent

$$\theta^* = \theta - \eta \hat{g}$$

Estimate the gradient $\hat{g}$.
Take a step set by the optimizer (ADAM).

GradCoRe

Pedrielli et al. [2502.02625]

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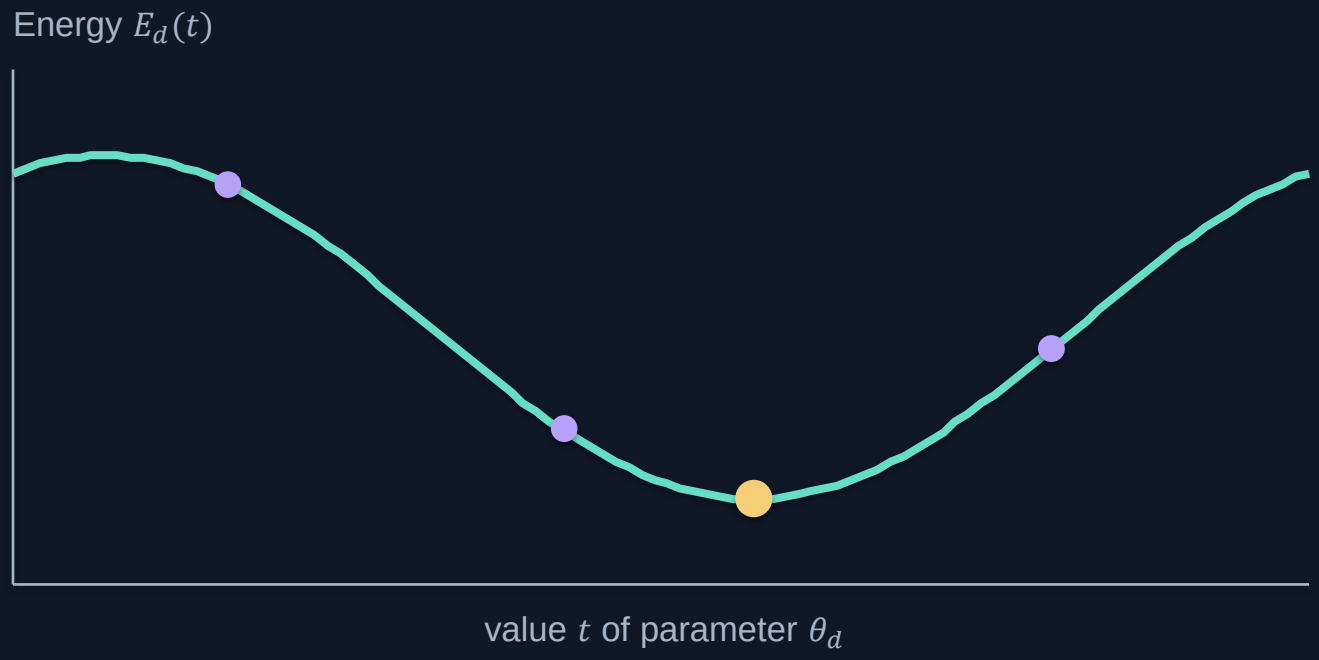
Context / Sequential Minimal Optimization



Fix all but one angle → the energy is a sinusoid

$$E_d(t) = a + b \cdot \cos(t) + c \cdot \sin(t)$$



Nakanishi et al. [1903.12166]
Ostaszewski et al. [1905.09692]

3 coefficients

3 distinct energy values

analytic parameter minimum

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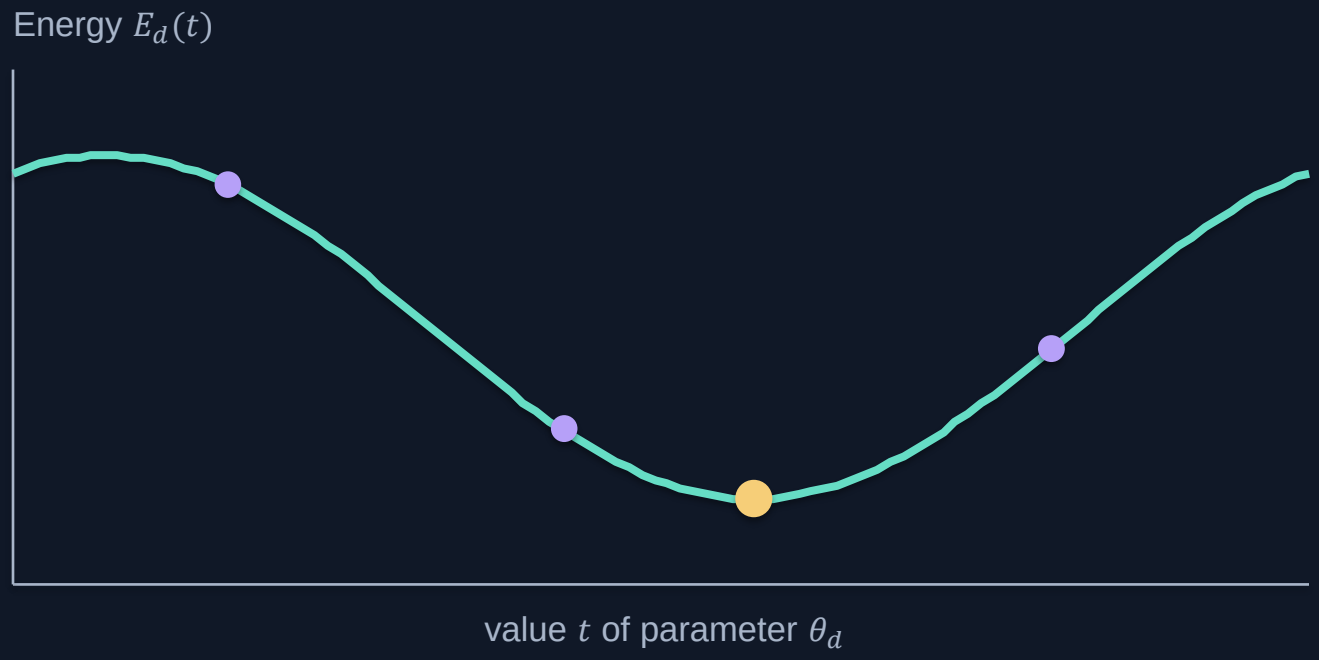

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This sinusoidal slice makes exact coordinate minimization possible in the noisless case.

SMO-NFT repeatedly solves this one-dimensional problem

SMO: minimize one coordinate at a time. NFT: use the exact sinusoidal form.

NFT = Nakanishi–Fujii–Todo

1

Select parameter θ_d

All other angles stay fixed.

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Using the energy evaluations.

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$\theta_d^* = \operatorname{atan2}(c, b) + \pi$

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Repeat; a sweep visits all D.

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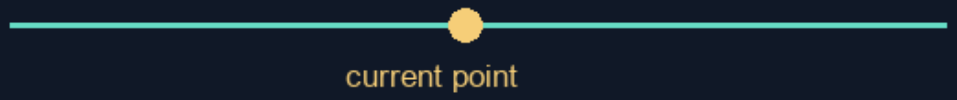
> **In this way you need *two* energy evaluations instead of three.**

One NFT update: choose, measure, fit, move, repeat

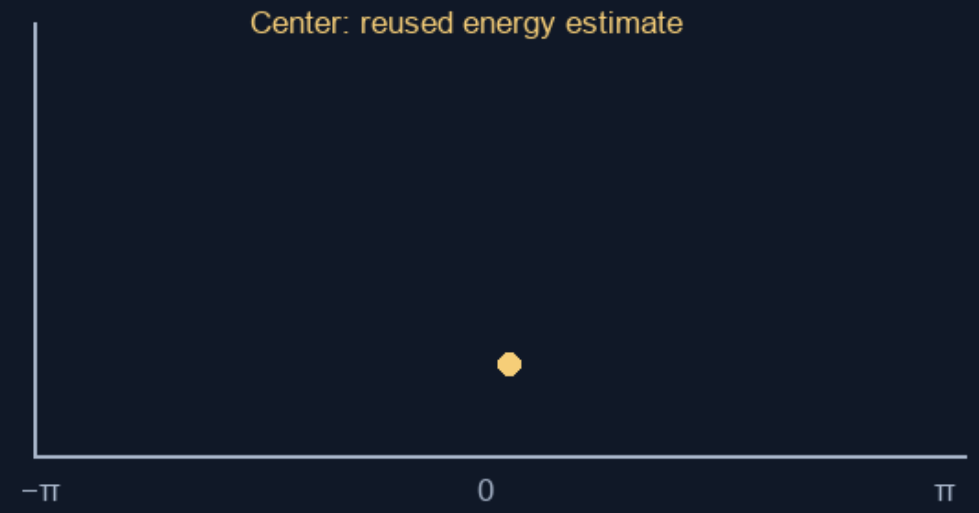
1 Start from the current point

Parameter space: one active coordinate



Only coordinate d is free

Energy along the active coordinate



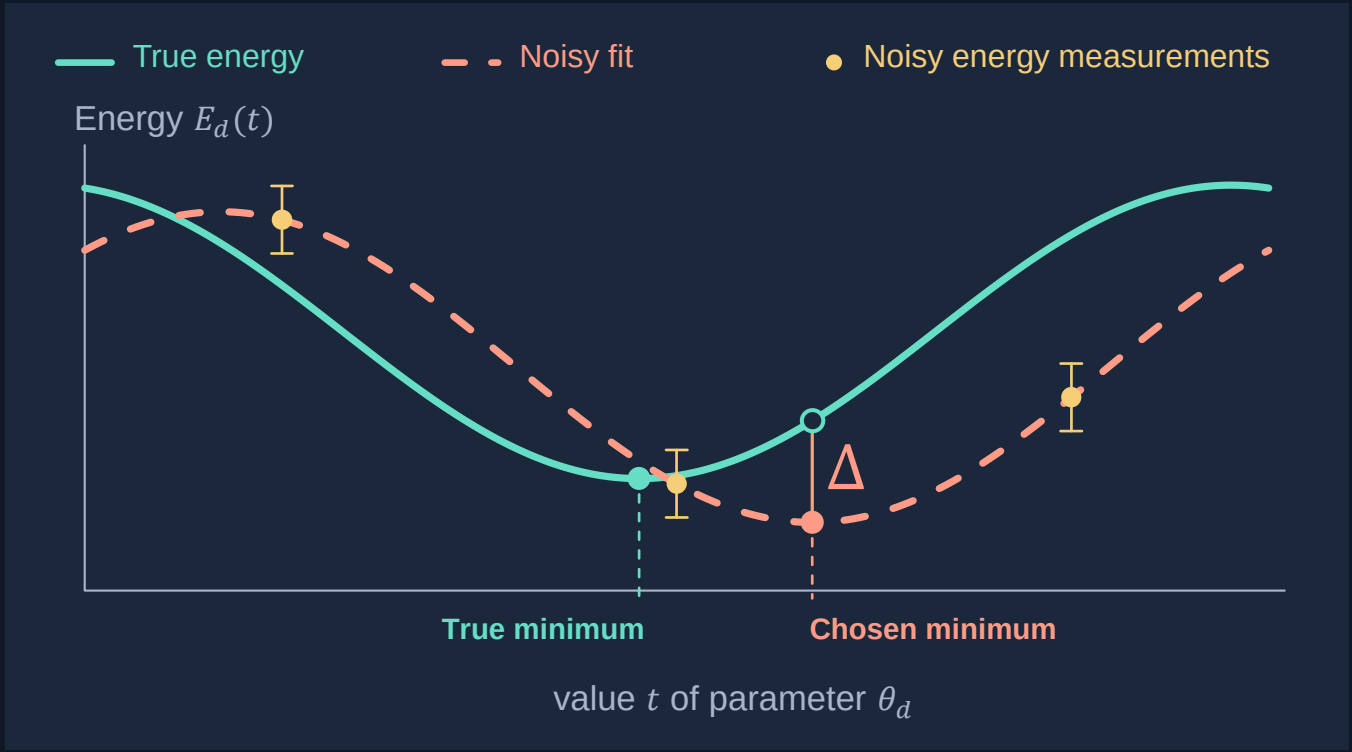
Illustrative NFT update · existing center estimate + two new energy evaluations · no benchmark data

Problem / SMO-NFT · Finite Measurements



Finite shots make the NFT update uncertain

Noisy energy samples perturb the sinusoid that SMO–NFT minimizes.



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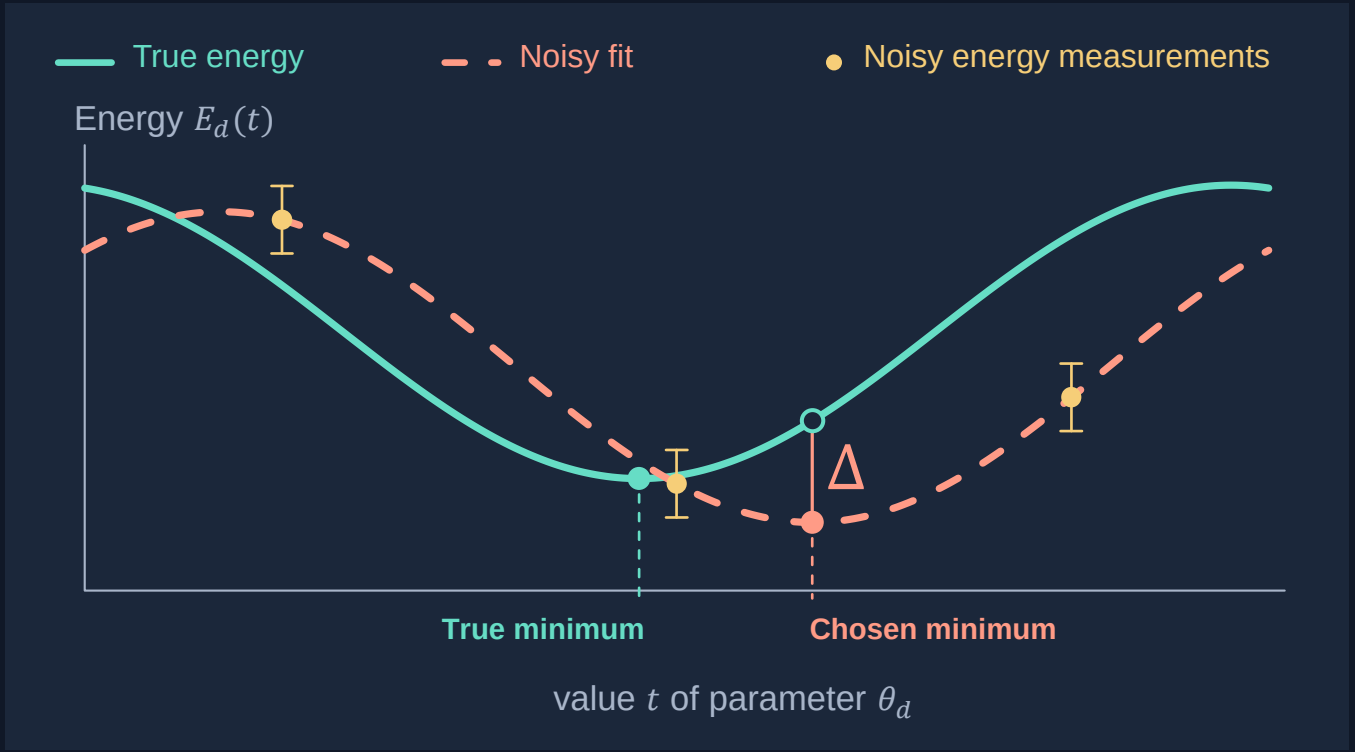

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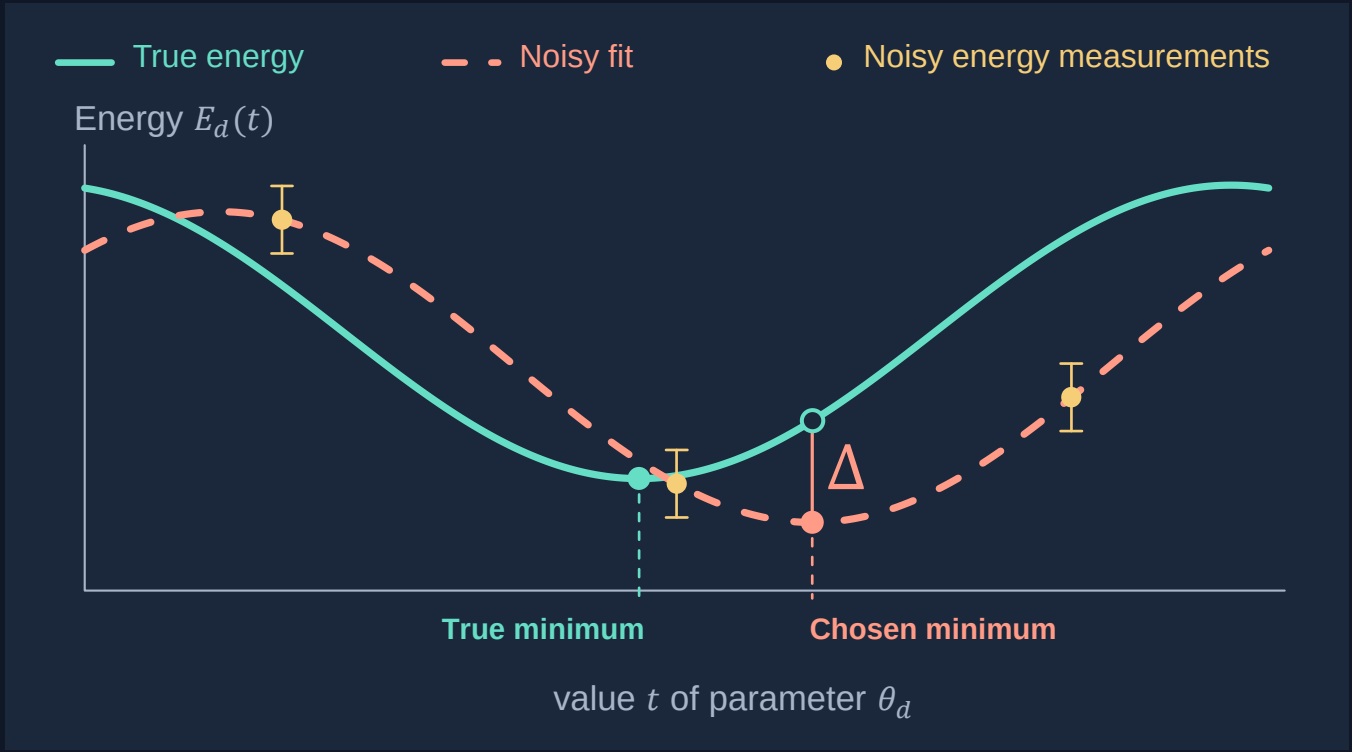

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The fitted minimum is too low on average. Reusing it propagates this bias.

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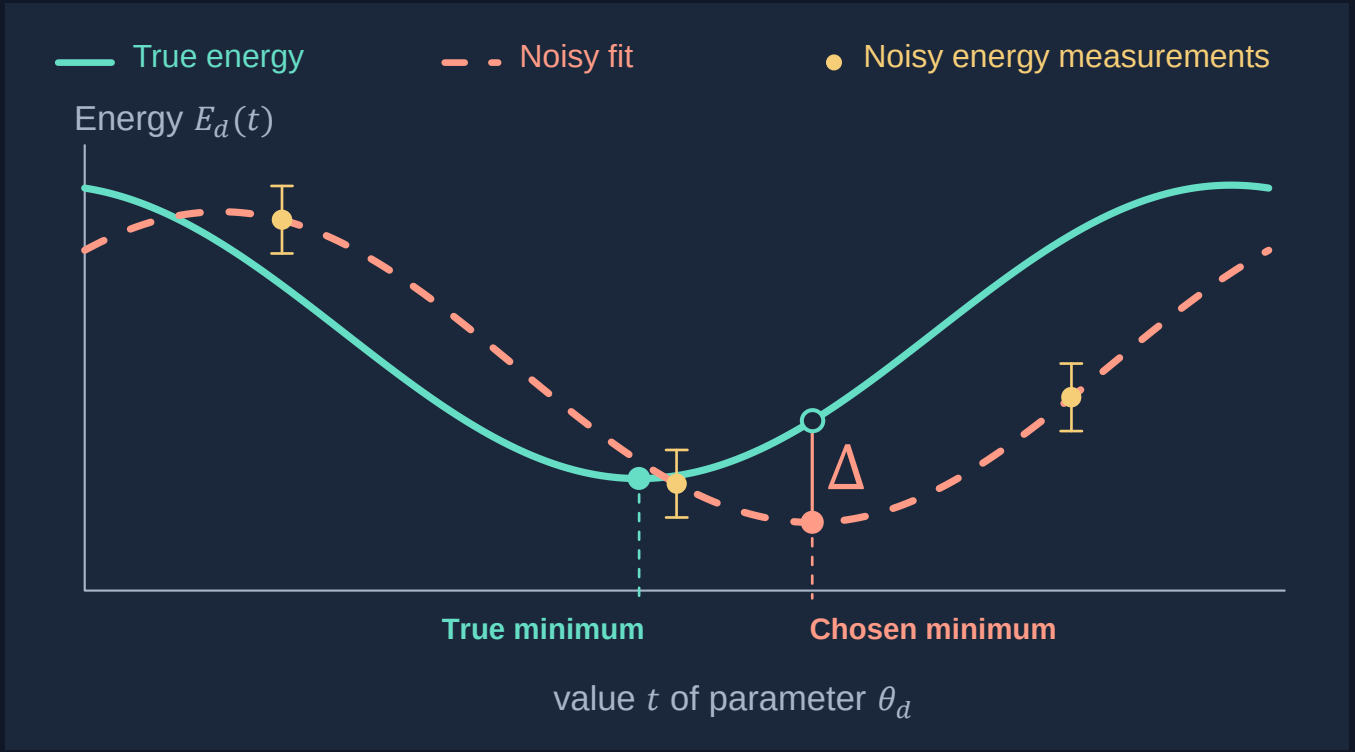

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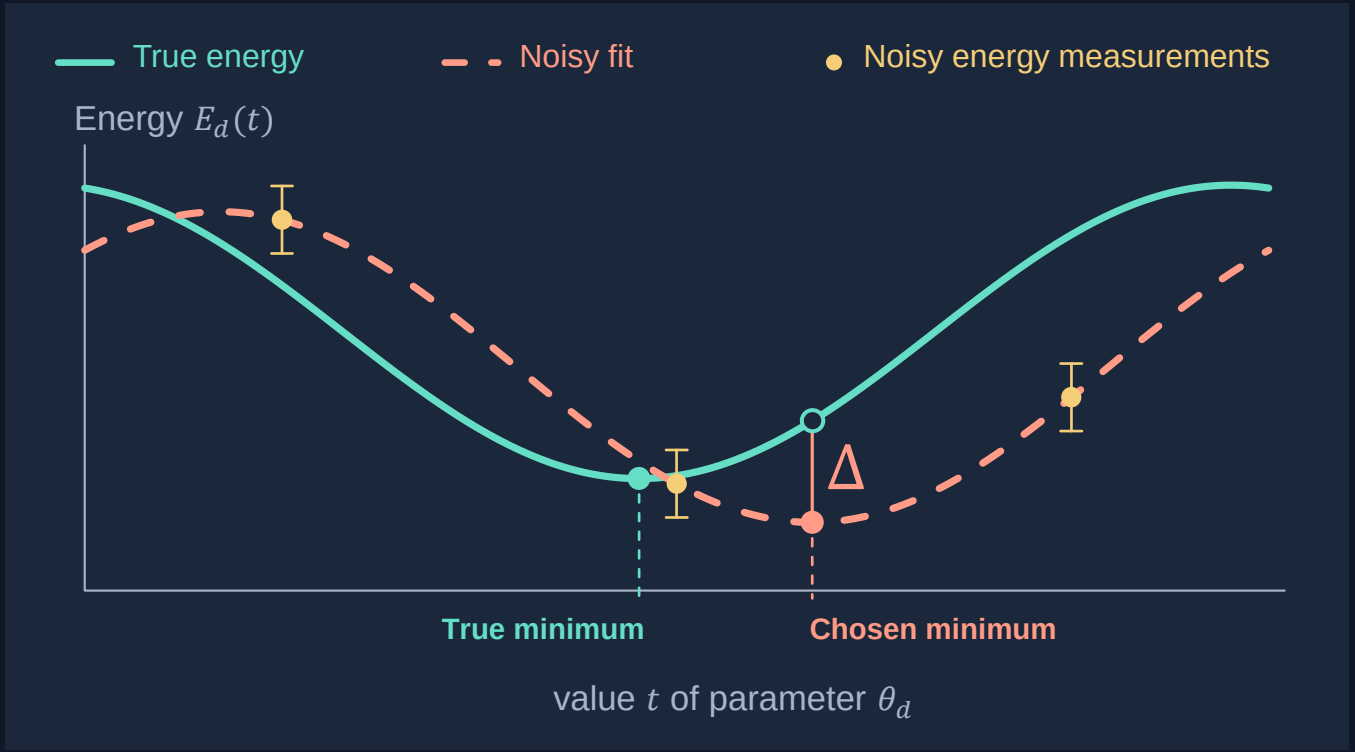

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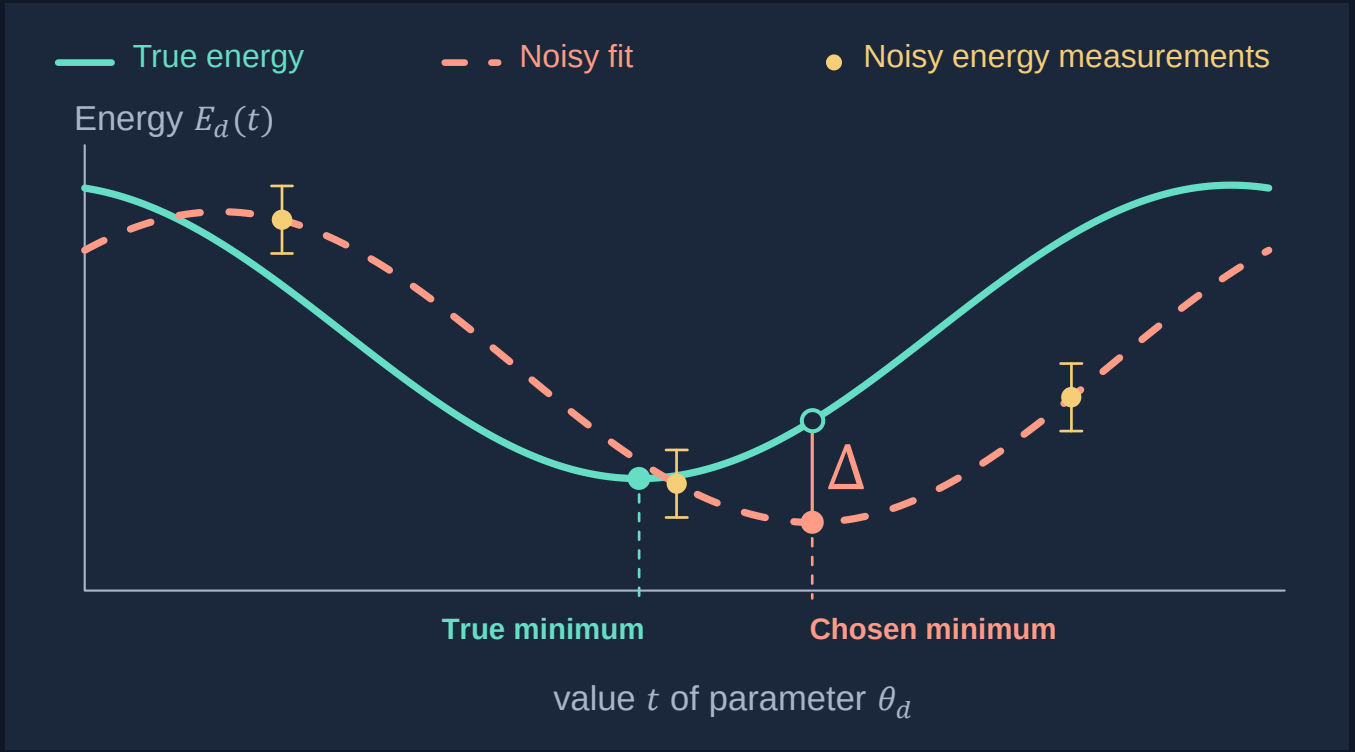

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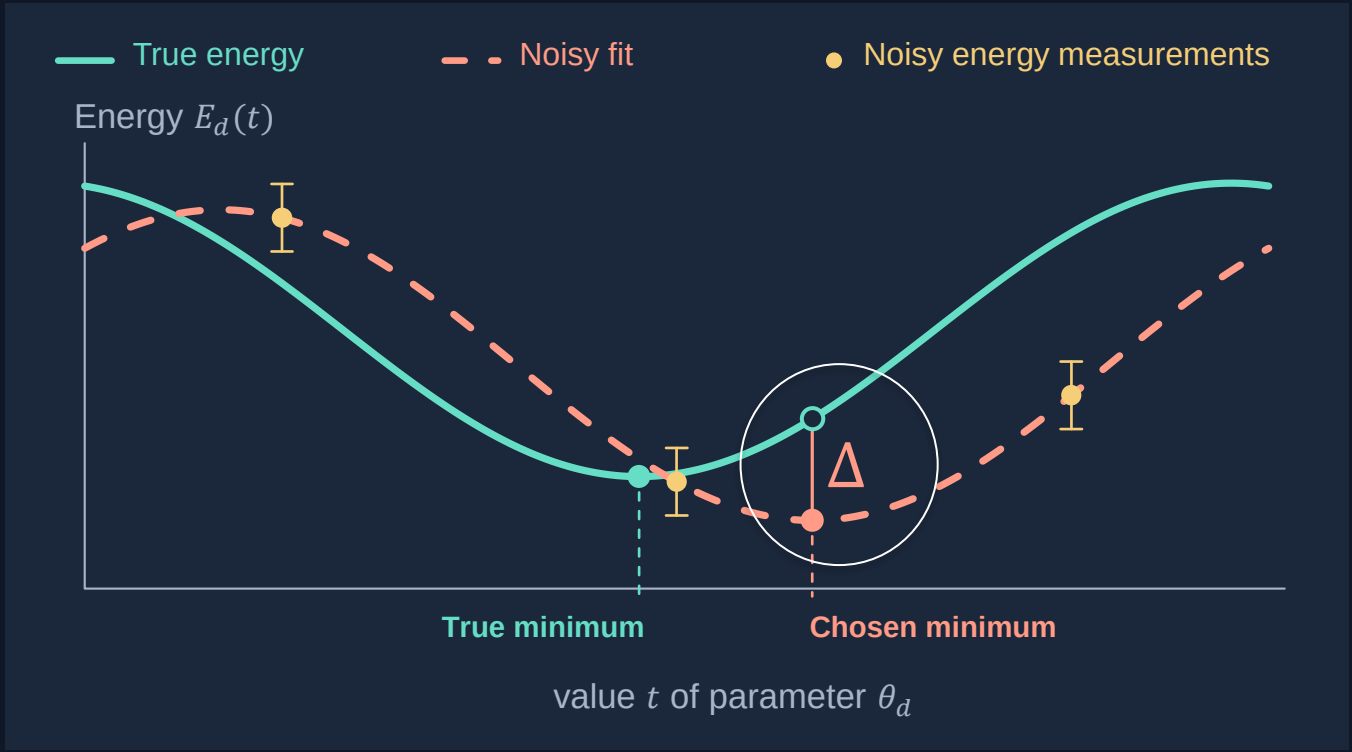

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Can past updates guide the measurement shifts to estimate the minimizing angle more precisely?

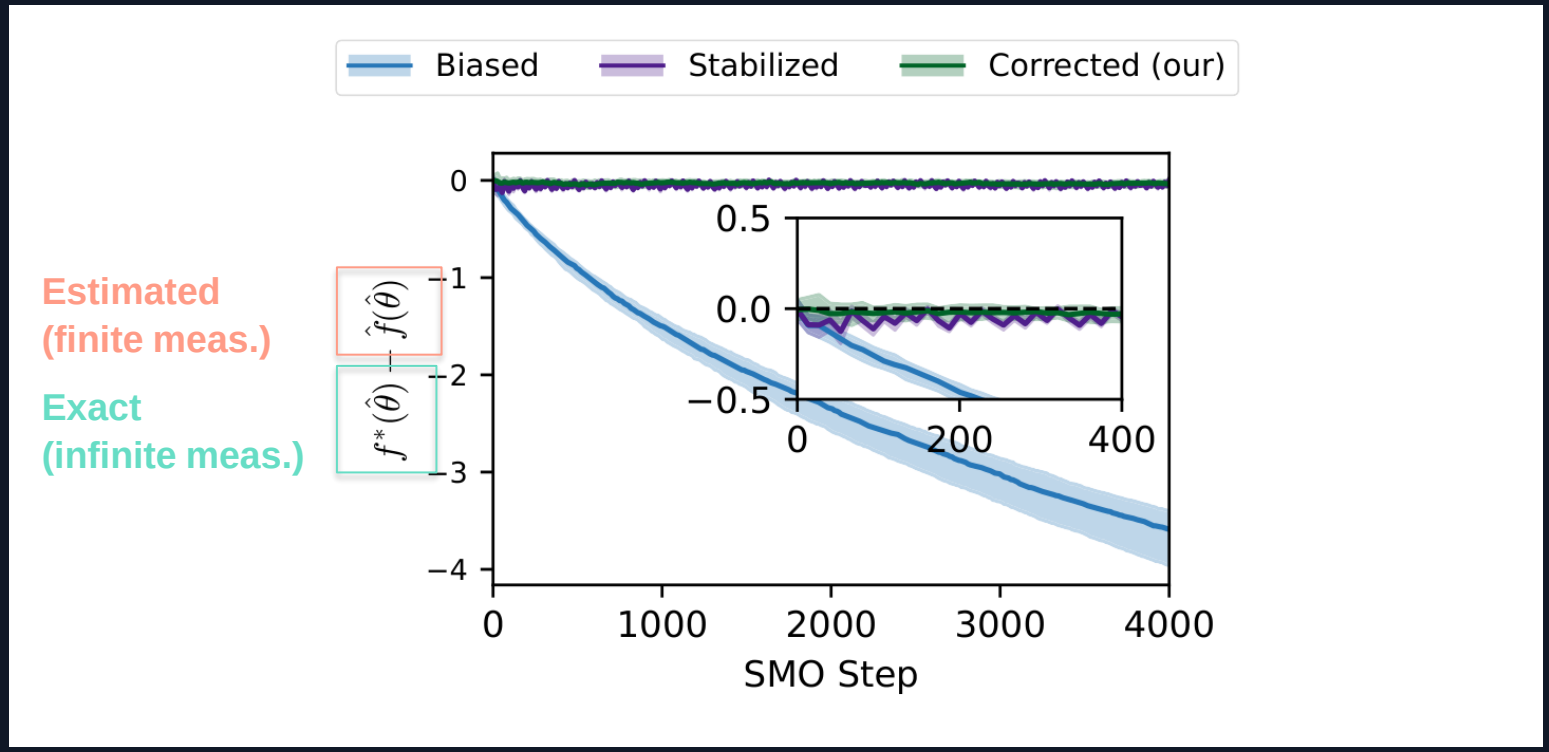
Bias: can we correct the energy estimate?

Our Work / SMO-NFT · Bias and Regularization



Energy reuse accumulates a systematic error

The reported energy gets lower and lower.



Pedrielli et al. · Bias, Fig. 1 · 100 trials

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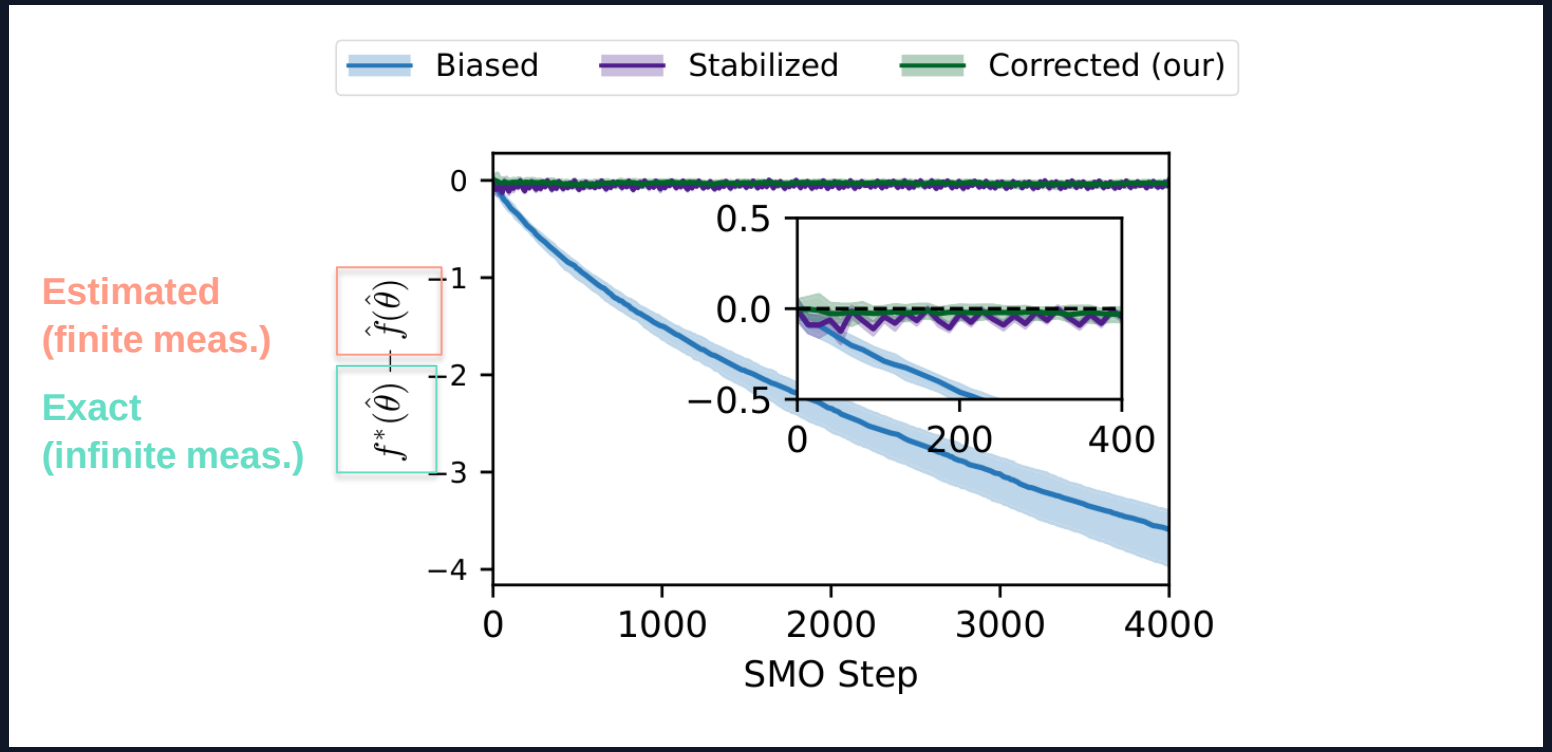

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Bayesian inference analysis → Δ

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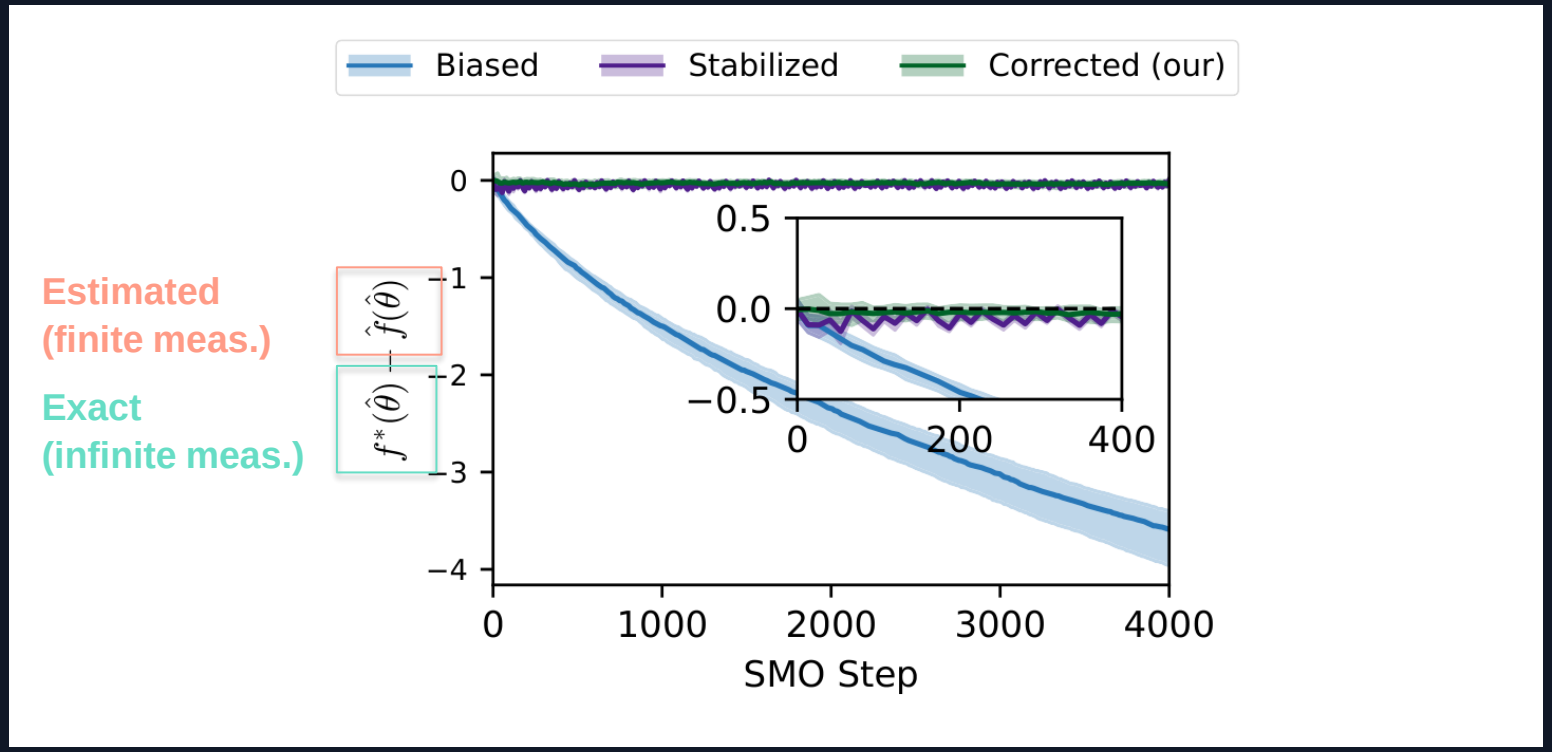

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1 Predict the downward bias

Bayesian inference analysis → Δ

2 Add back the predicted error

Corrected estimate

+ analytical correction Δ

Fitted minimum energy

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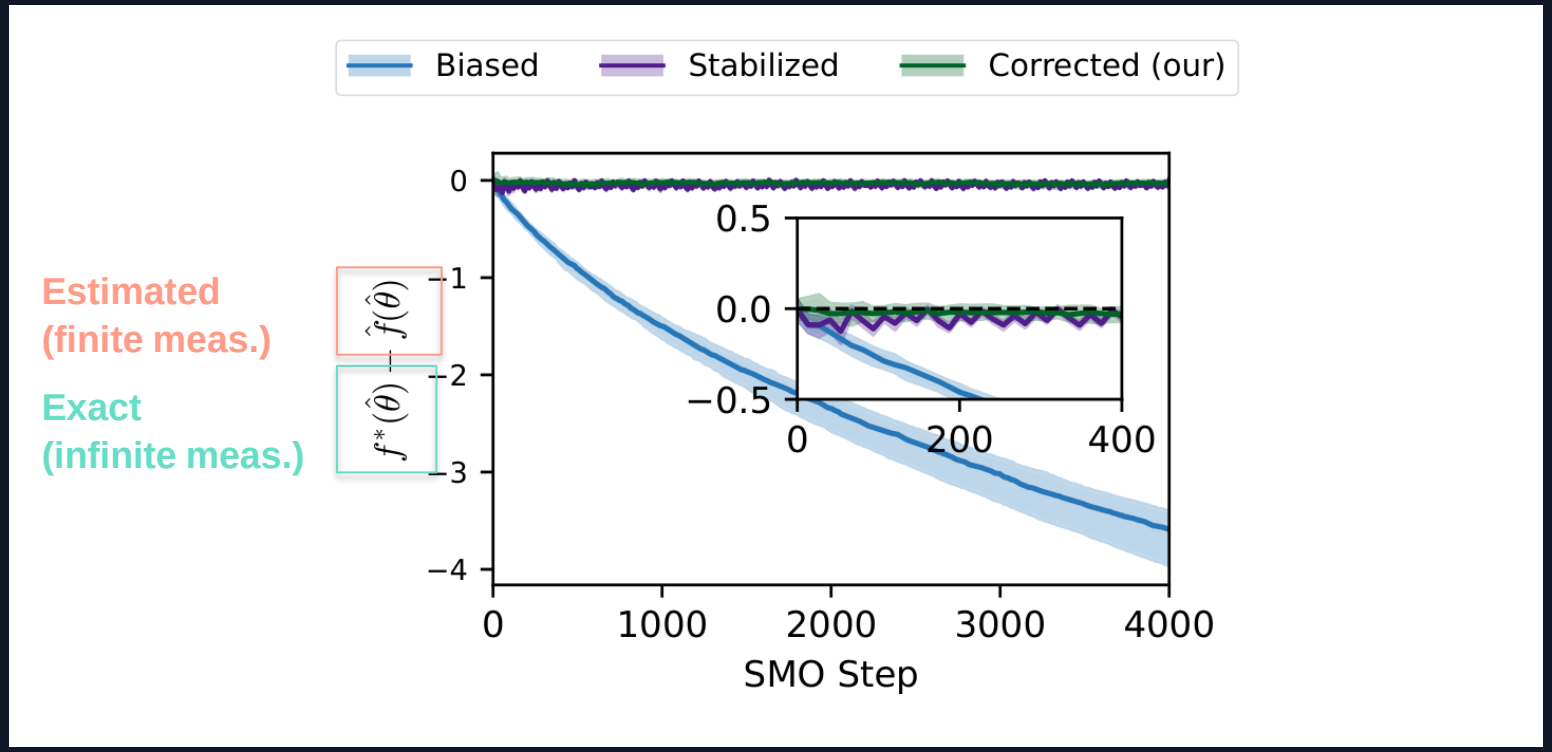

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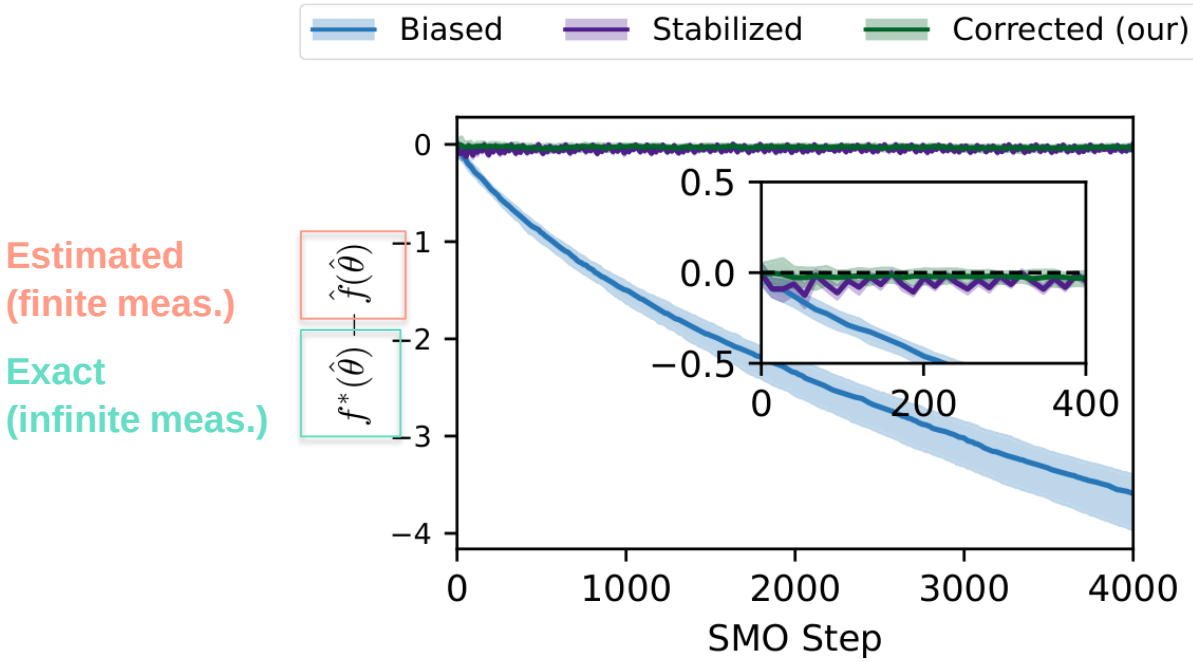

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Every update · no extra measurements

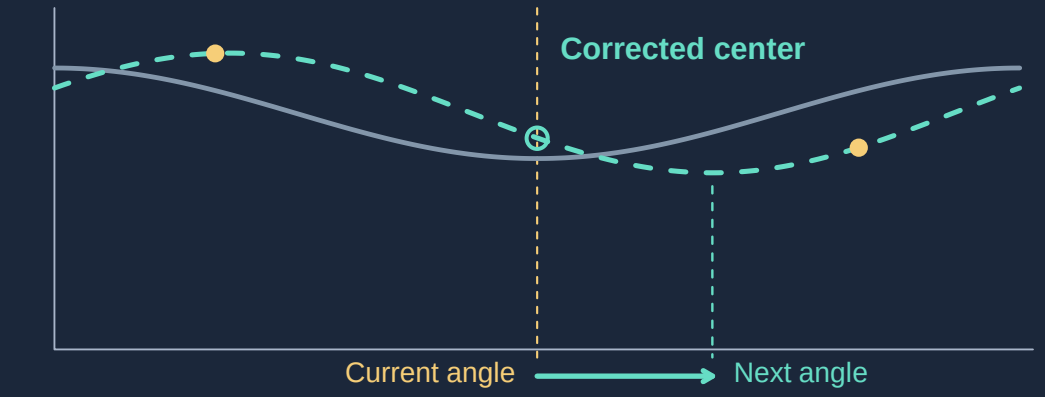
We can correct the leading bias, but this hinders performance. *Why?*

Correcting the estimate can destabilize the update

Near a flat minimum, a bias can suppress jumps driven by noise.

Correction

Use the corrected center in the fit.



True energy Corrected energy

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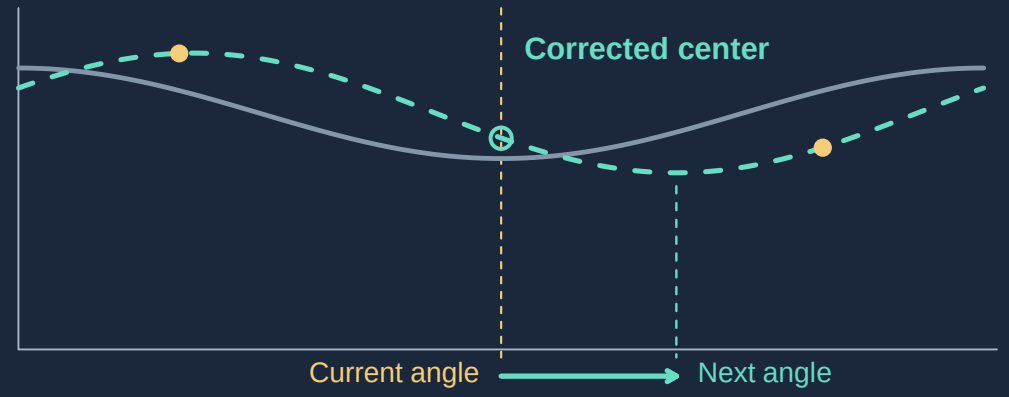
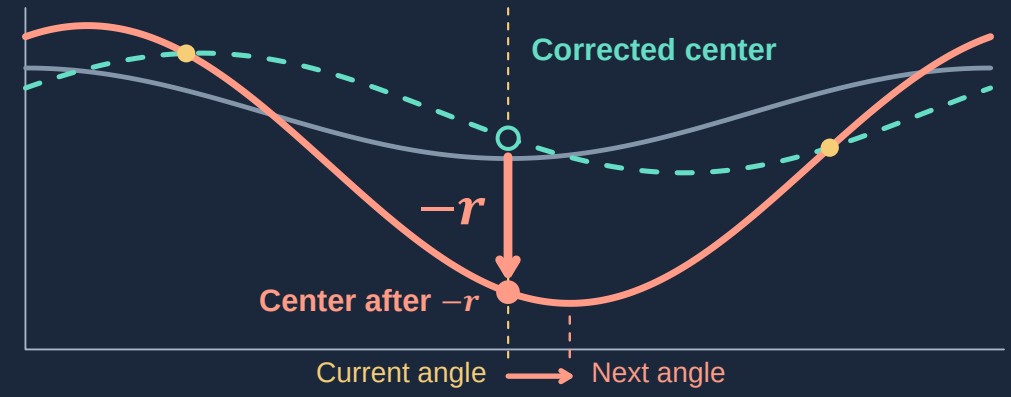


Regularization

Lower the corrected center by r, then refit.



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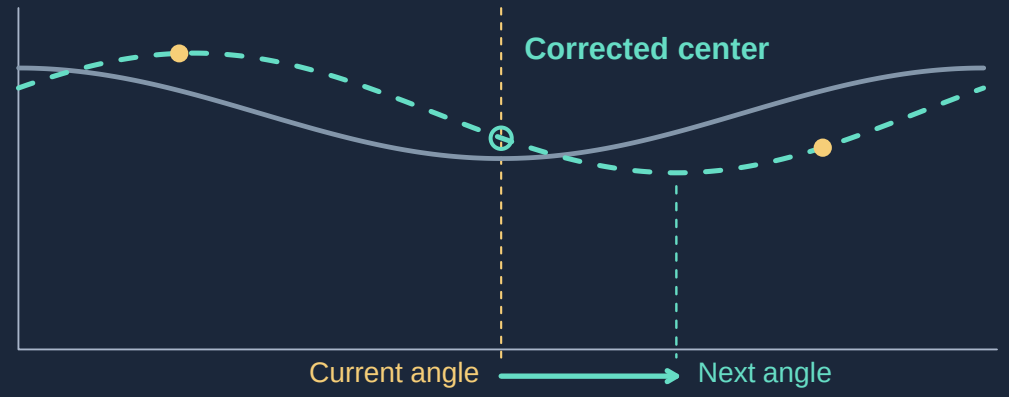

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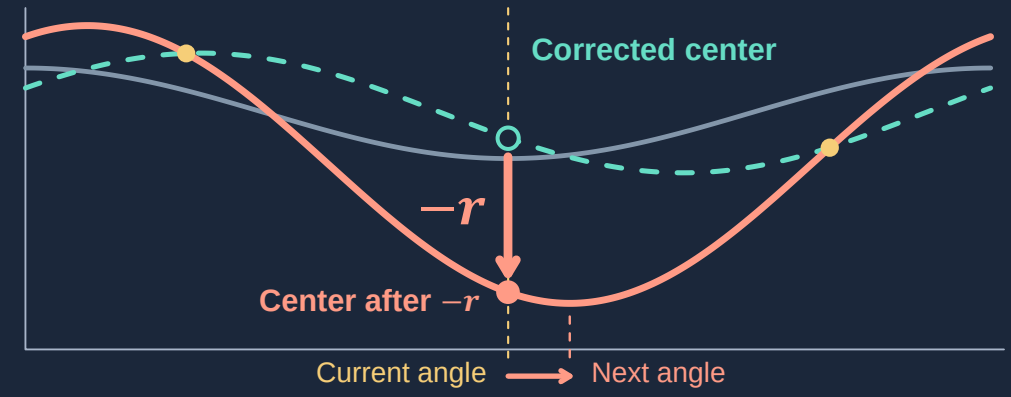
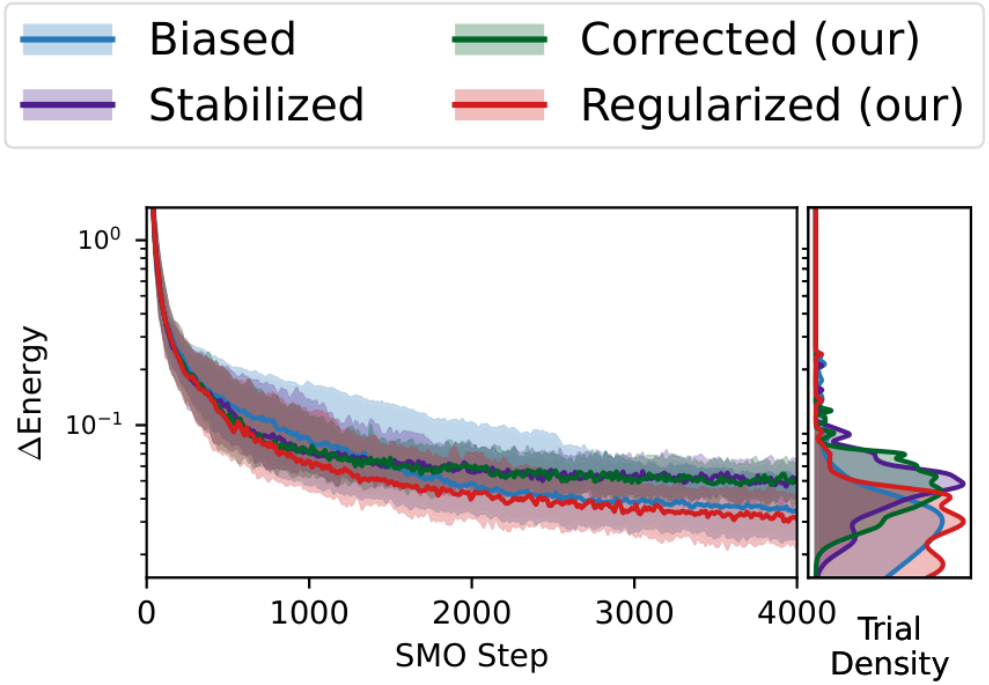


True energy — Corrected energy — Regularized energy

Replace spontaneous bias with a chosen regularizer; correct the reported energy.

Regularization improves the true energy reached

The corrected estimate alone does not produce the best optimization.



Bias paper, Fig. 2 (energy panel) · 100 sweeps / 4,000 updates · mean and one standard deviation

Red: regularized NFT

Lower true energy error than correction alone and the original NFT.

5 qubits · 3 layers
Ising model · 100 trials
900 shots / evaluation

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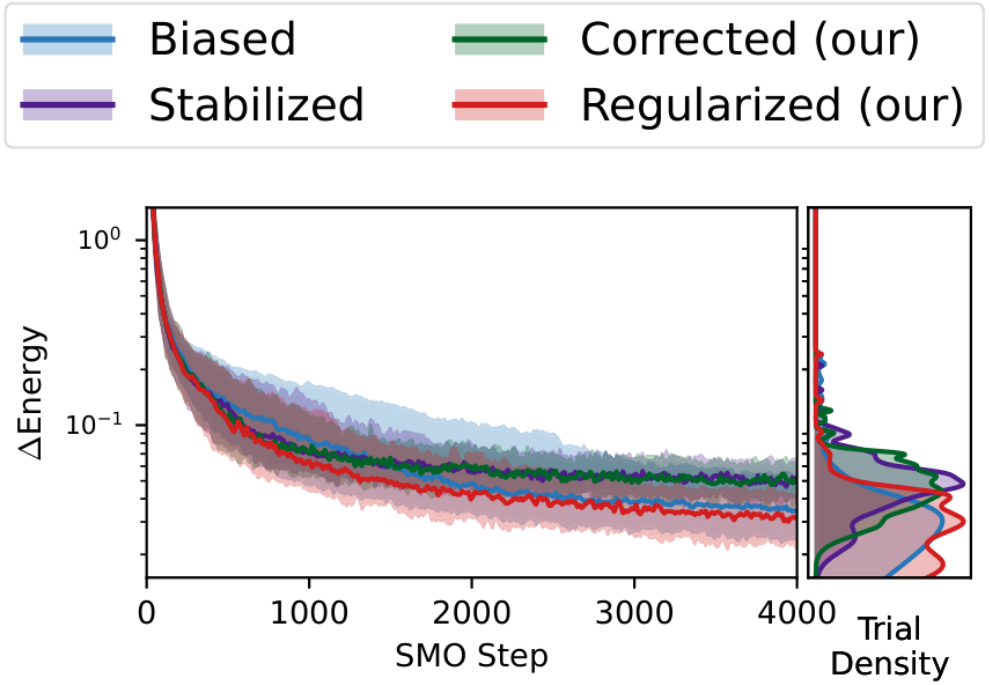

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The contribution: accurate energy estimation and a more stable coordinate update.

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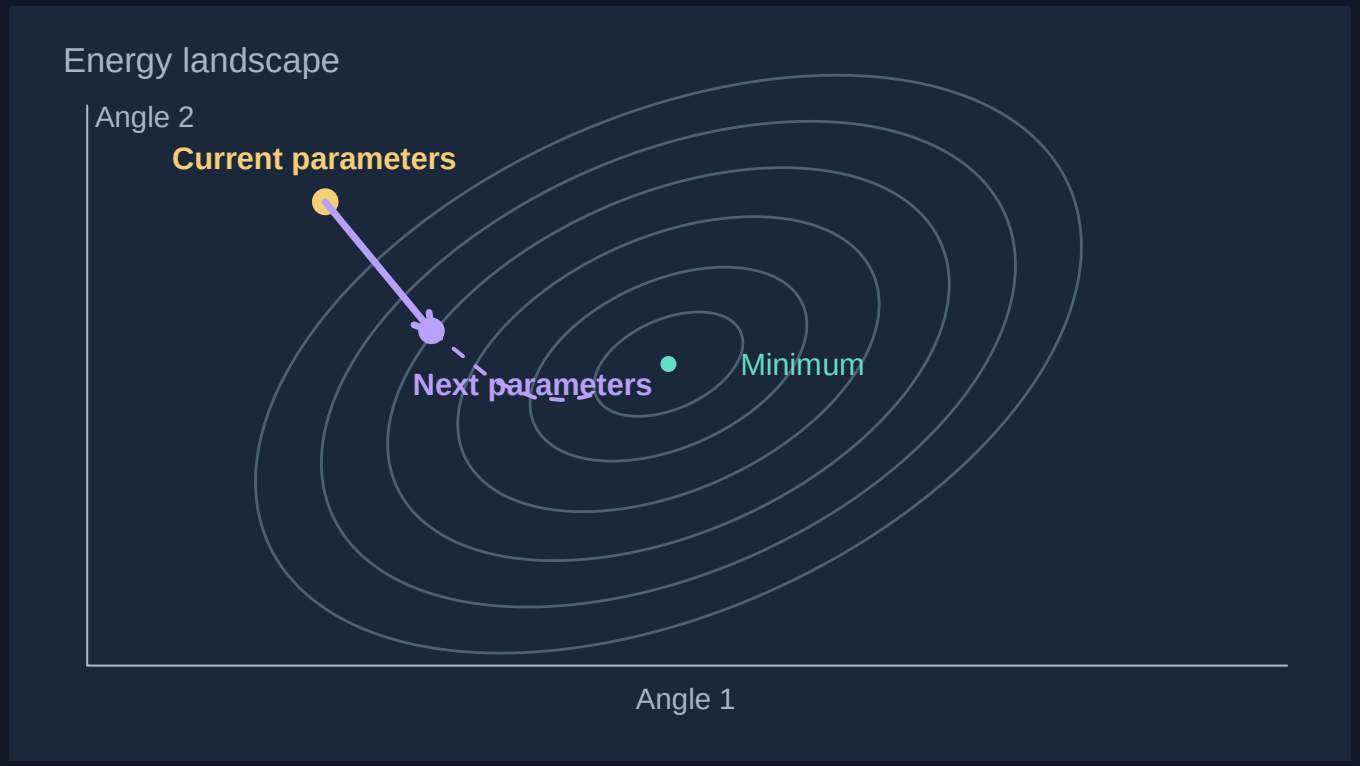
GradCoRe

Context / Gradient Descent



Gradient descent follows the local slopes

Estimate the gradient, take a controlled step in the full parameter space, then repeat.



Estimate the local slopes

One gradient component per parameter.

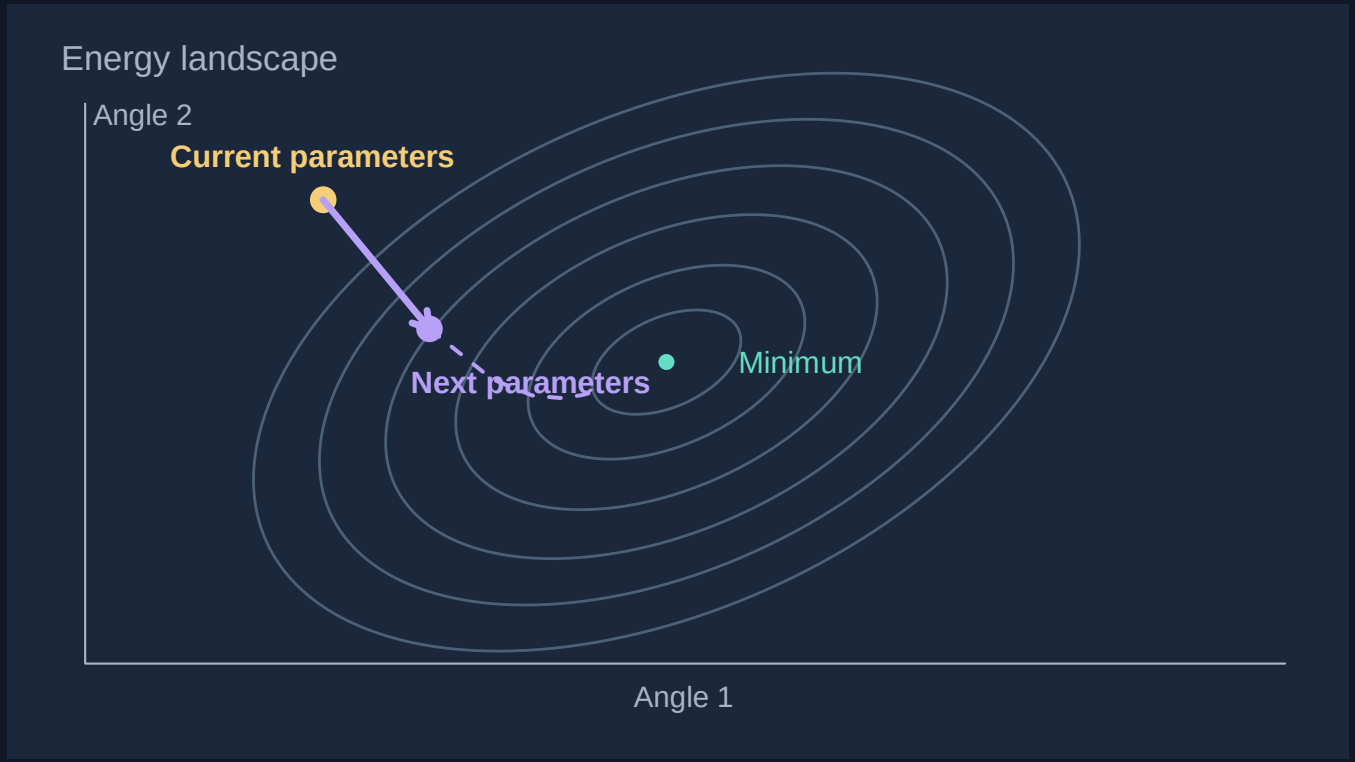
$$\theta^* = \theta - \eta \hat{g}$$

$\hat{g}$: estimated gradient
η: step size

Recompute after each update.

Gradient descent follows the local slopes

Estimate the gradient, take a controlled step in the full parameter space, then repeat.



Estimate the local slopes

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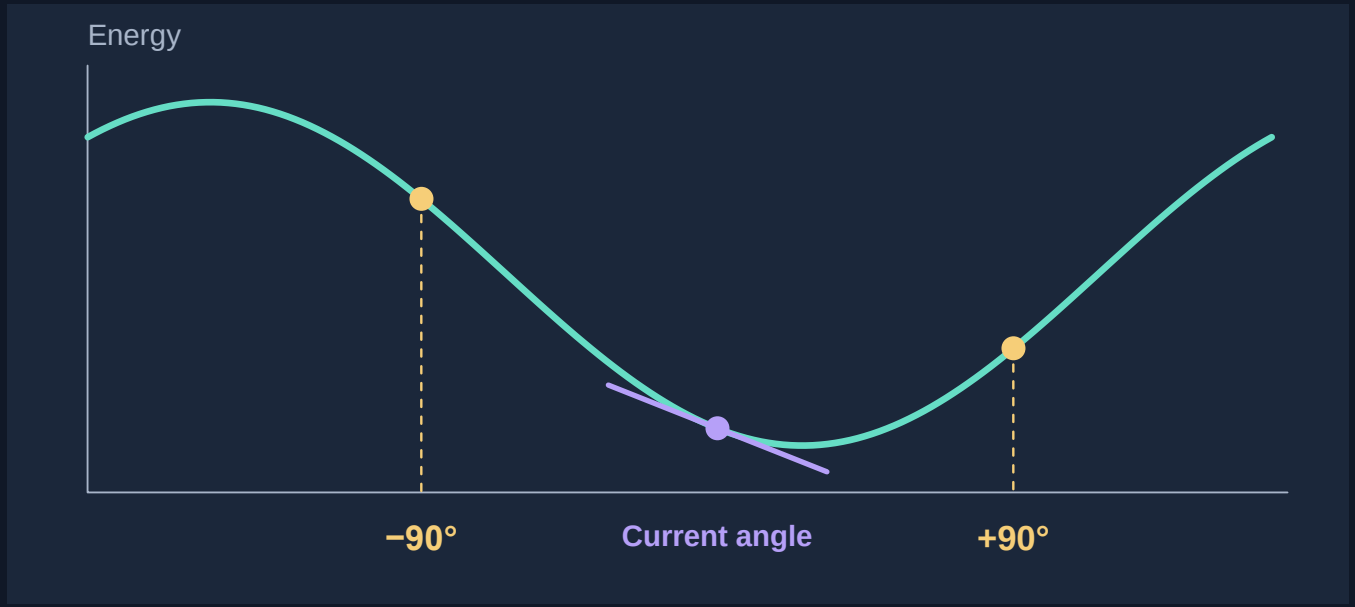
Recompute after each update.

Use the slopes to update the parameters together, rather than minimize one fitted slice.

The parameter-shift rule turns energies into slopes

The same sinusoidal structure on which SMO-NFT is based gives an exact derivative from two shifted energies.



$$E'_d(t) = \frac{E_d\left(t + \frac{\pi}{2}\right) - E_d\left(t - \frac{\pi}{2}\right)}{2}$$

Two circuit settings

Shift one angle by −90° and +90°.

Measure the energy at each shift.

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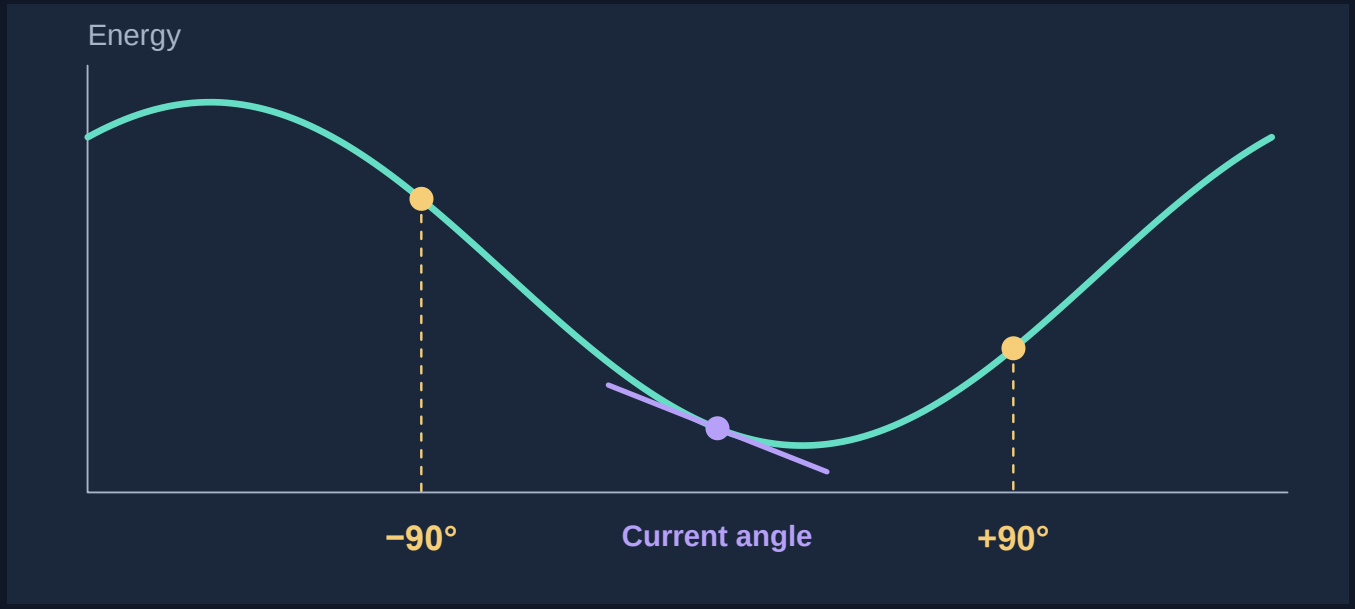

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Finite shots make the gradient estimate noisy. How precise must it be for a useful step?

Our Work / Bayesian PSR and GradCoRe

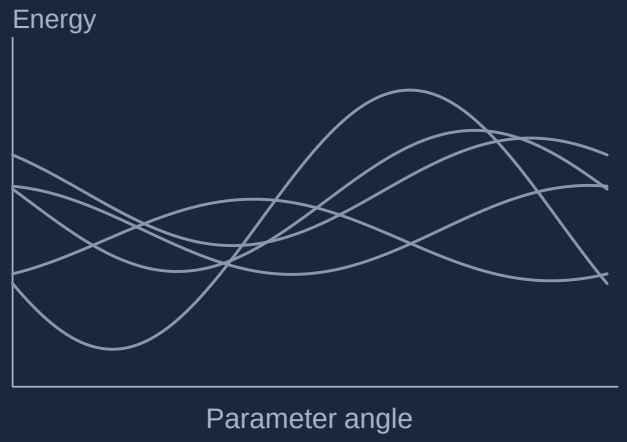


Bayesian inference: learn the gradient and its uncertainty

Gradient descent needs reliable slopes at the current parameters.

1 Start with structure

The known Fourier structure constrains the possible curves.



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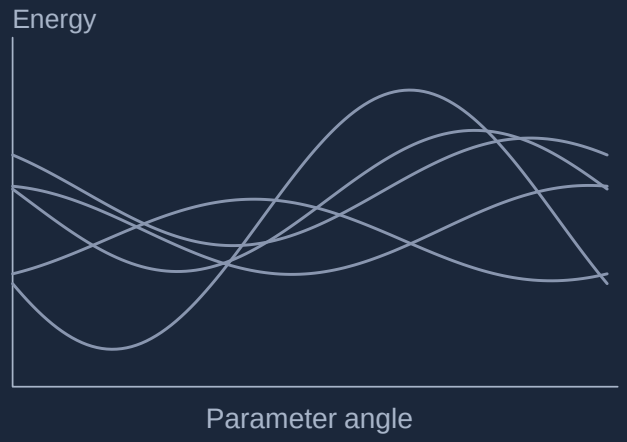
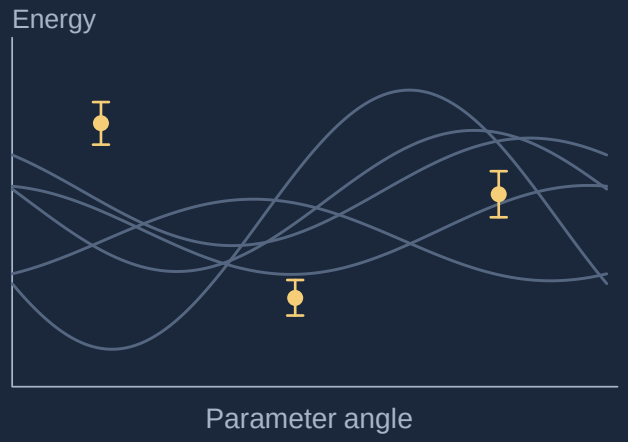


2 Add energy measurements

Past and new measurements refine the same GP model.



Bayesian inference: learn the gradient and its uncertainty

Gradient descent needs reliable slopes at the current parameters.

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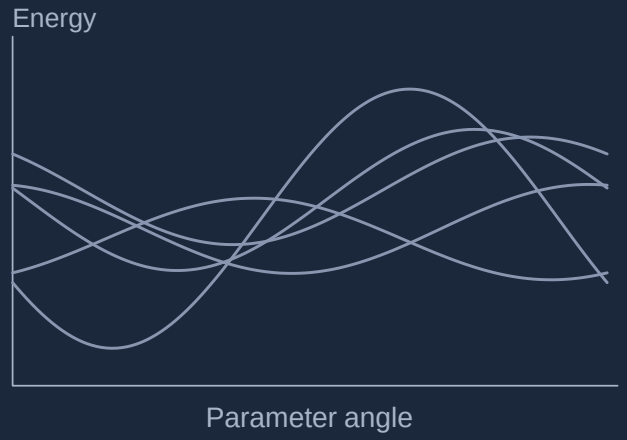

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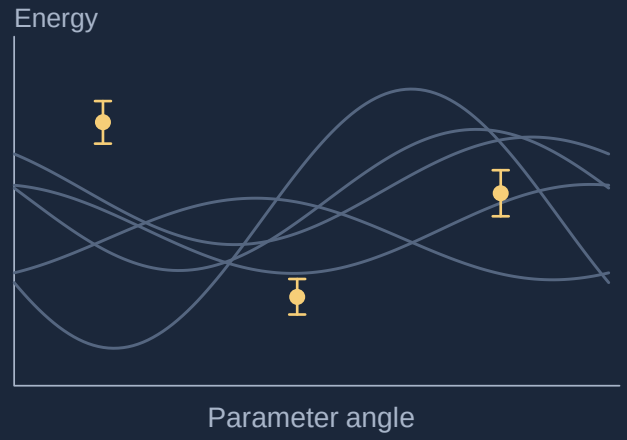
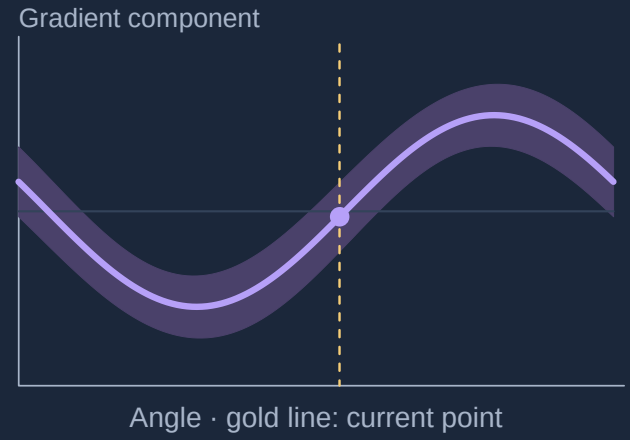


3 Infer the gradient

A slope estimate, plus how uncertain it remains.



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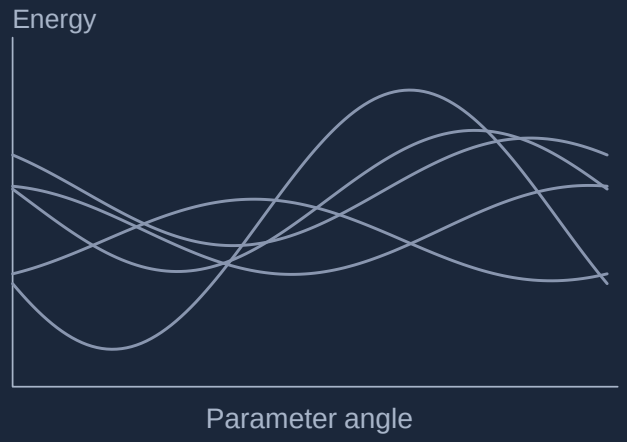

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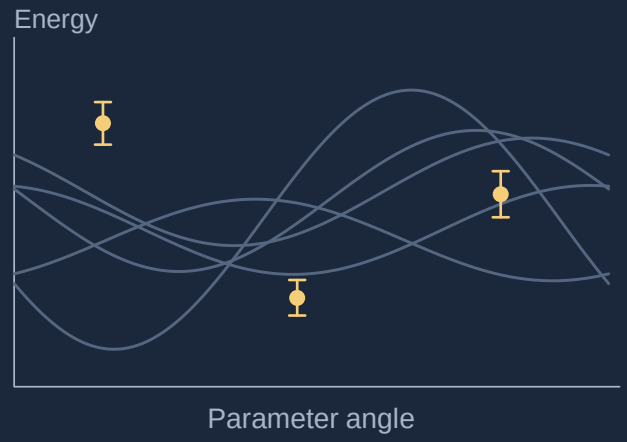

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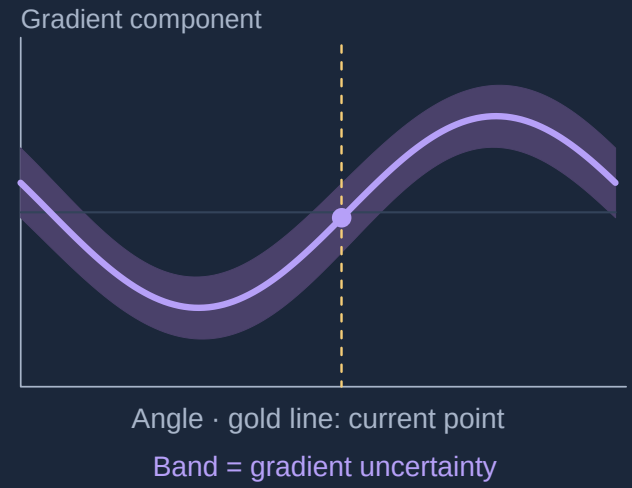

Energy observations → GP model → gradient estimate and uncertainty (Bayesian PSR).

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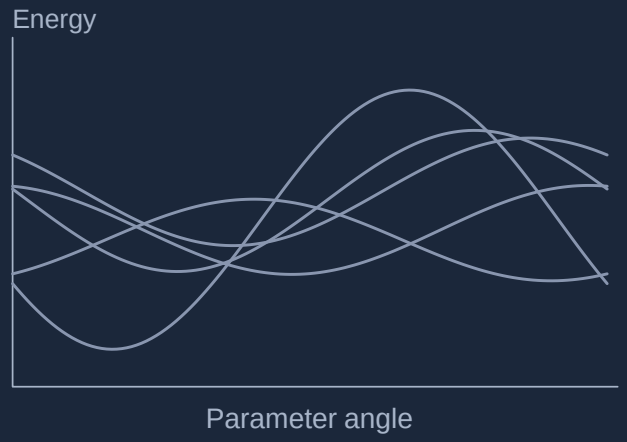

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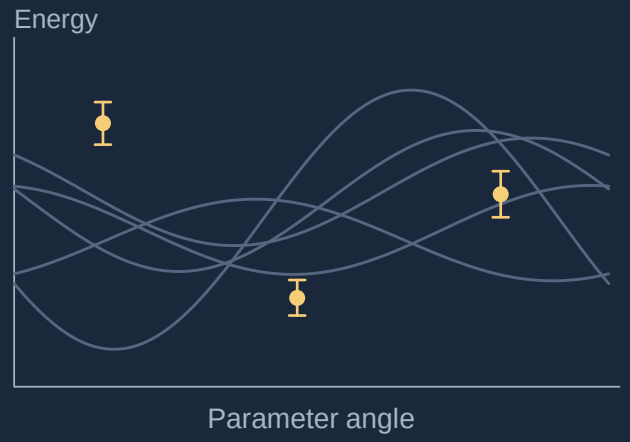

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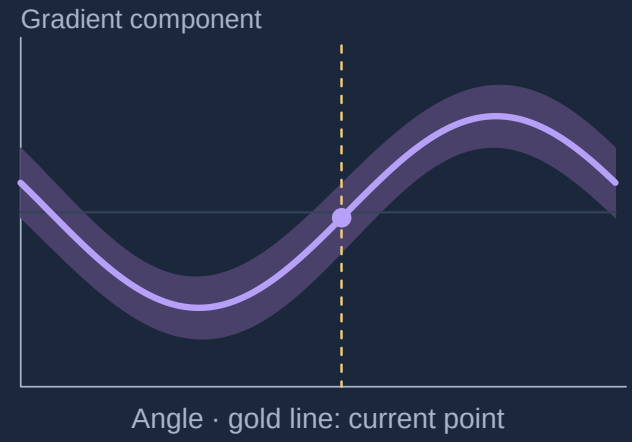
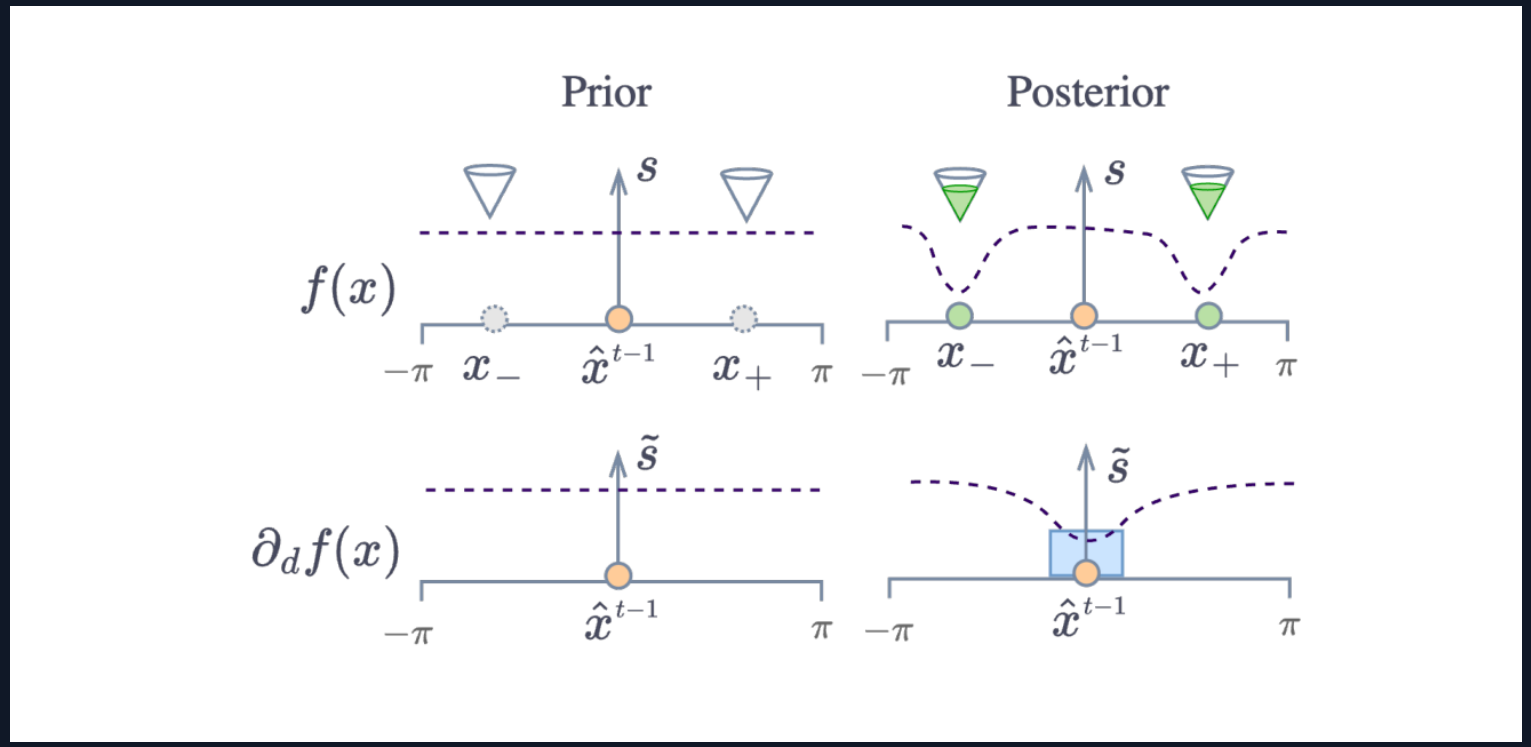


Energy observations → GP model → gradient estimate and uncertainty (Bayesian PSR).

GradCoRe leverages uncertainty in the gradient estimate to allocate resources in the next update.

GradCoRe spends shots on gradient precision

Choose a small measurement budget that makes the current gradient sufficiently certain.



Paper Fig. 1 · top: energy uncertainty · bottom: gradient uncertainty

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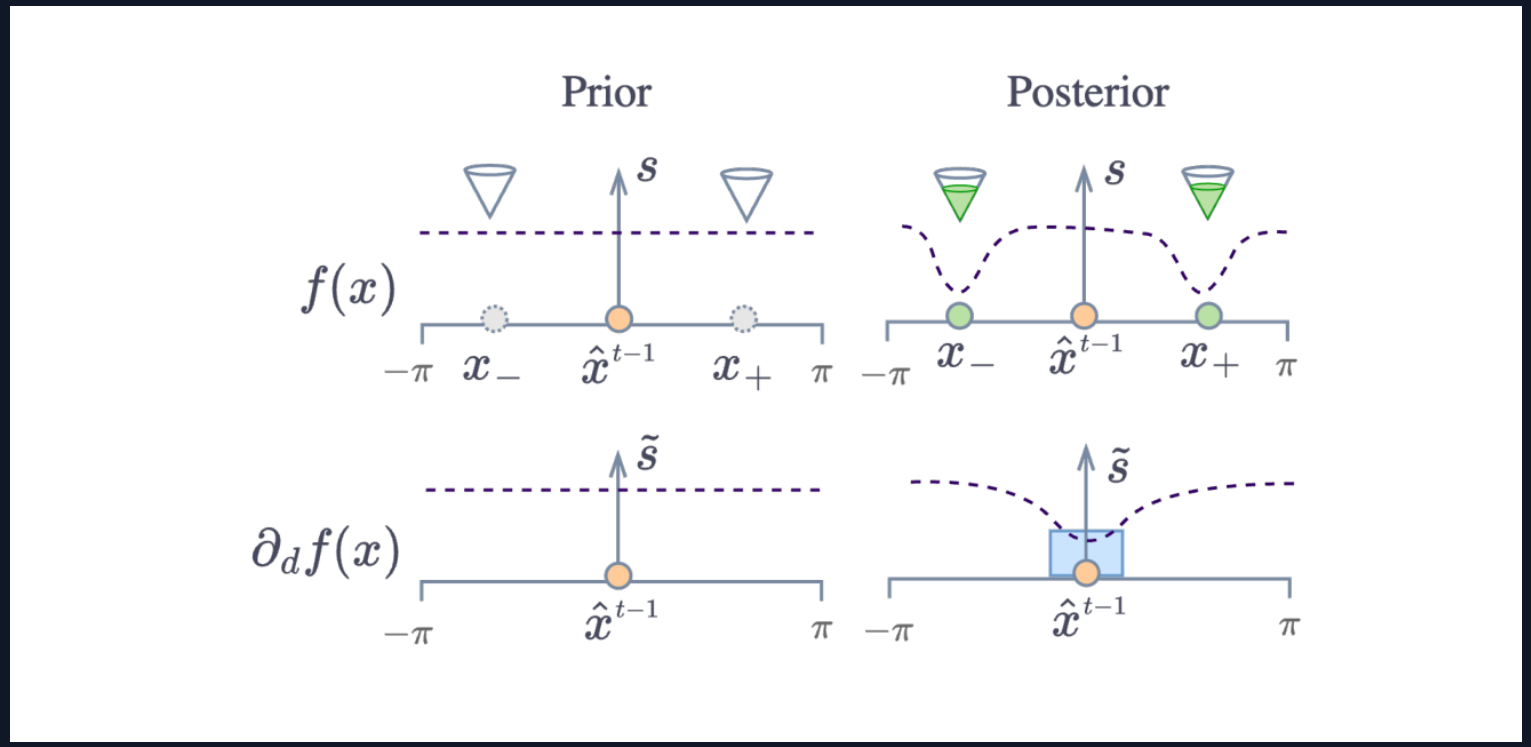

Paper Fig. 1 · top: energy uncertainty · bottom: gradient uncertainty

How do we choose the budget?

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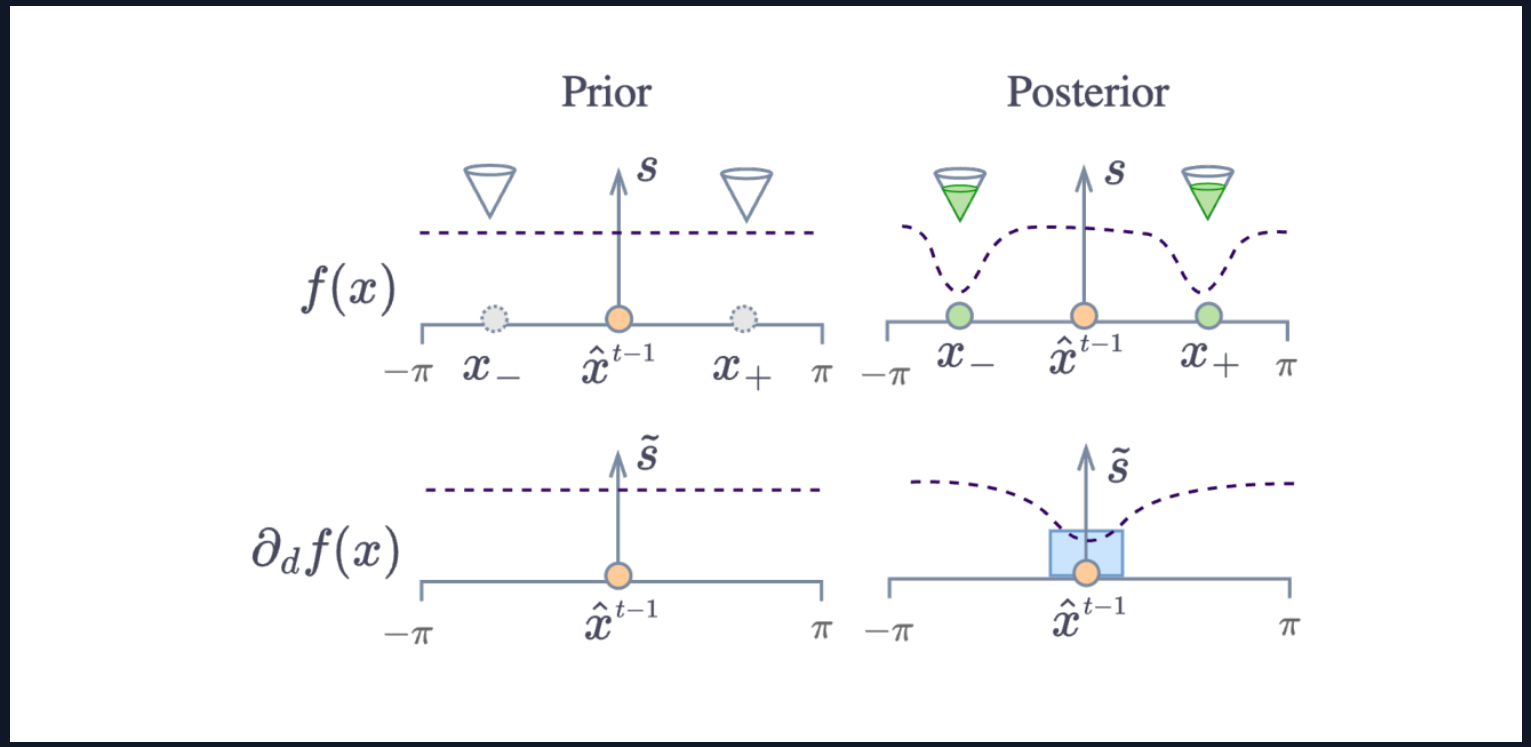


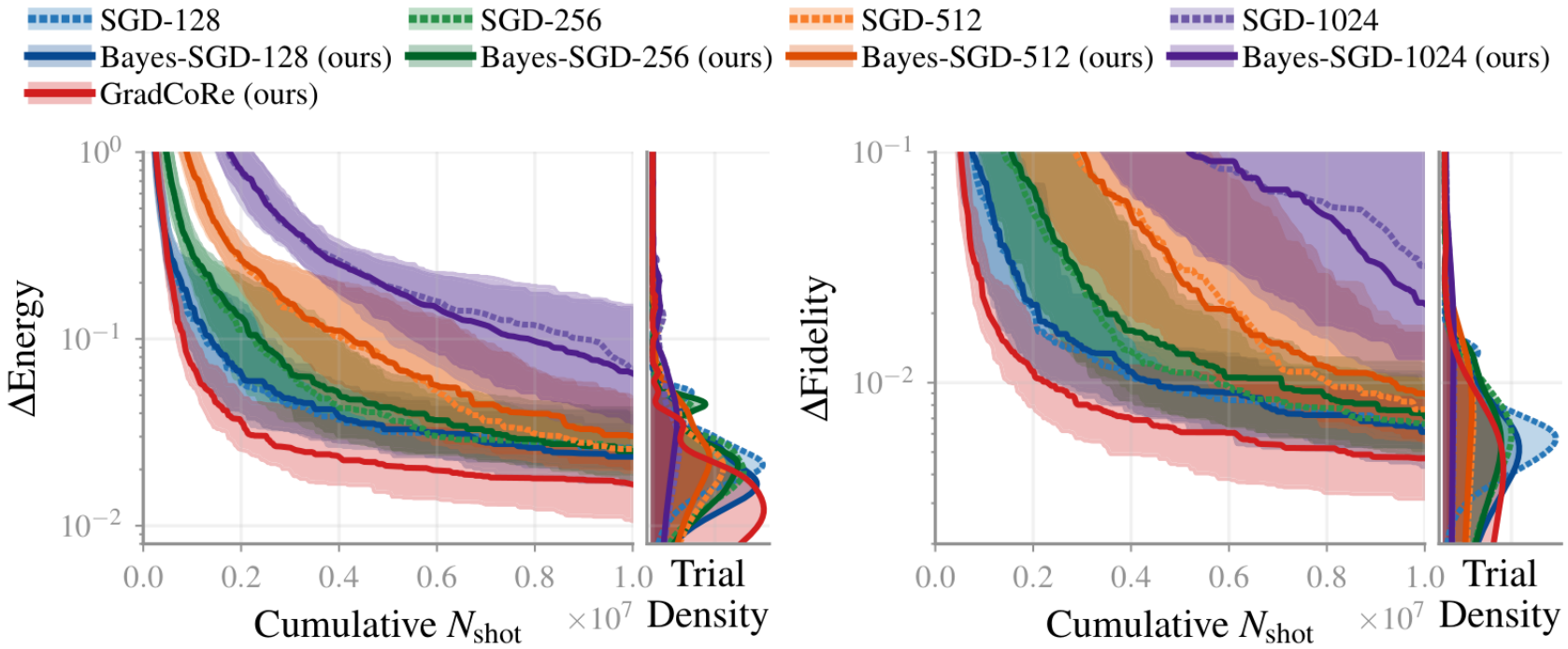
Paper Fig. 1 · top: energy uncertainty · bottom: gradient uncertainty

How do we choose the budget?

The need for precision increases as the optimization proceeds. GradCoRe calculates this and allocates.

Adaptive shots improve progress per measurement

Red: GradCoRe. Other curves: fixed shot budgets with standard or Bayesian PSR.



Paper Fig. 3 · Ising model · 5 qubits / 3 layers · 100 trials

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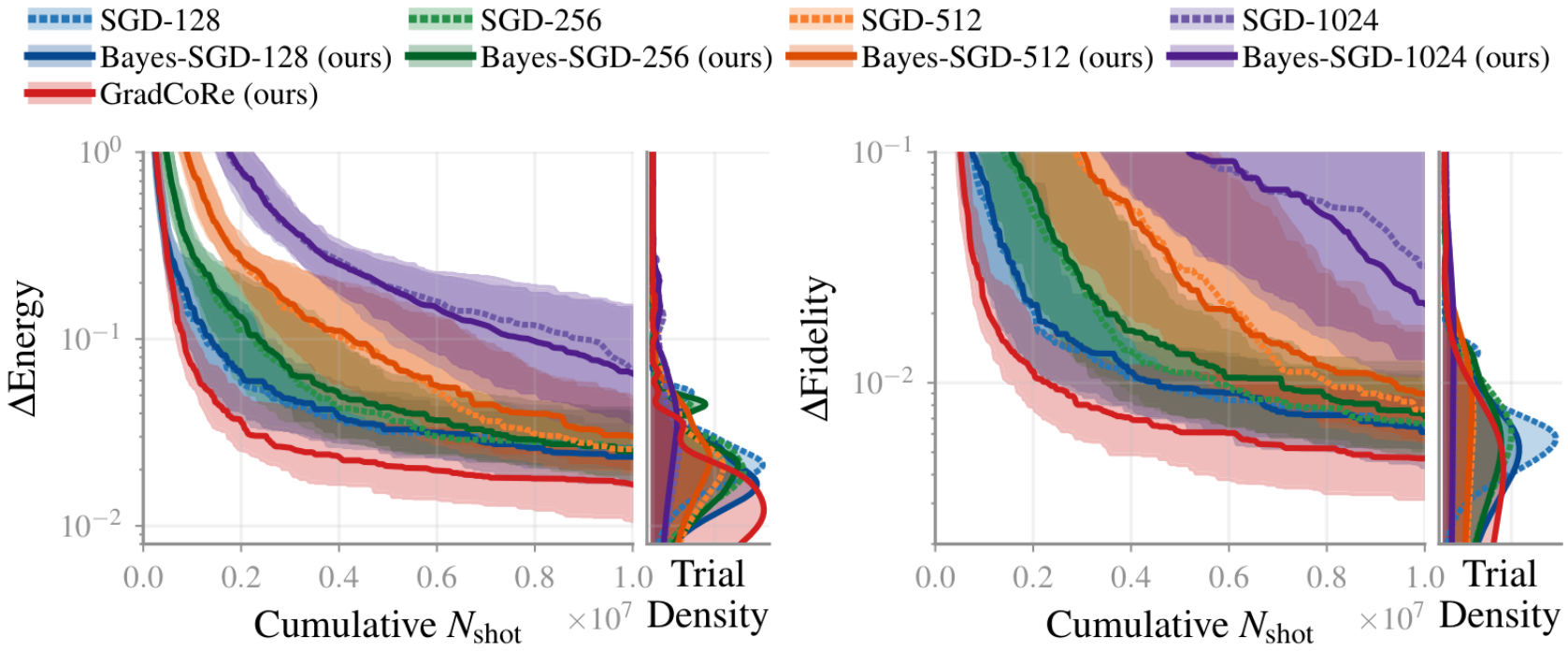
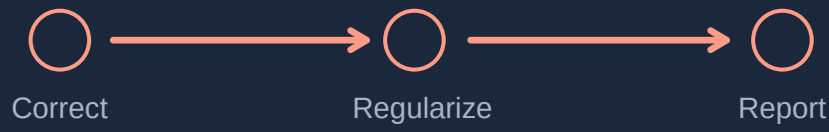


Paper Fig. 3 · Ising model · 5 qubits / 3 layers · 100 trials

Bayes-PSR gives gradient uncertainty. GradCoRe uses it to decide how much to measure.

Two optimizers, two uses of uncertainty

SMO–NFT · Bias



Correct and regularize the energy estimate.

Stabilize the coordinate update.

Gradient descent · GradCoRe

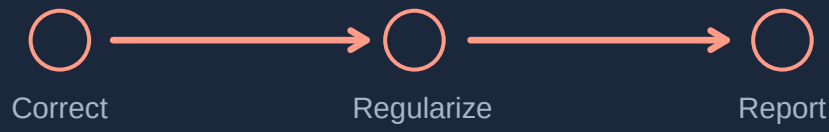


Infer the gradient and its uncertainty.

Adapt the measurement budget.

Two optimizers, two uses of uncertainty

SMO–NFT · Bias



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Thank you!