IBM Quantum Lab

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Qiskit | Global Summer School 2021

Training Parameterized Quantum Circuits

In this lab session we will have a closer look on how to train circuit-based models. At the end of this session you should know

- how to build variational quantum classifiers
- how to use different training techniques, especially gradient-based
- what restrictions the variational-based models have and how we might overcome them

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Where do we need to train parameterized circuits?

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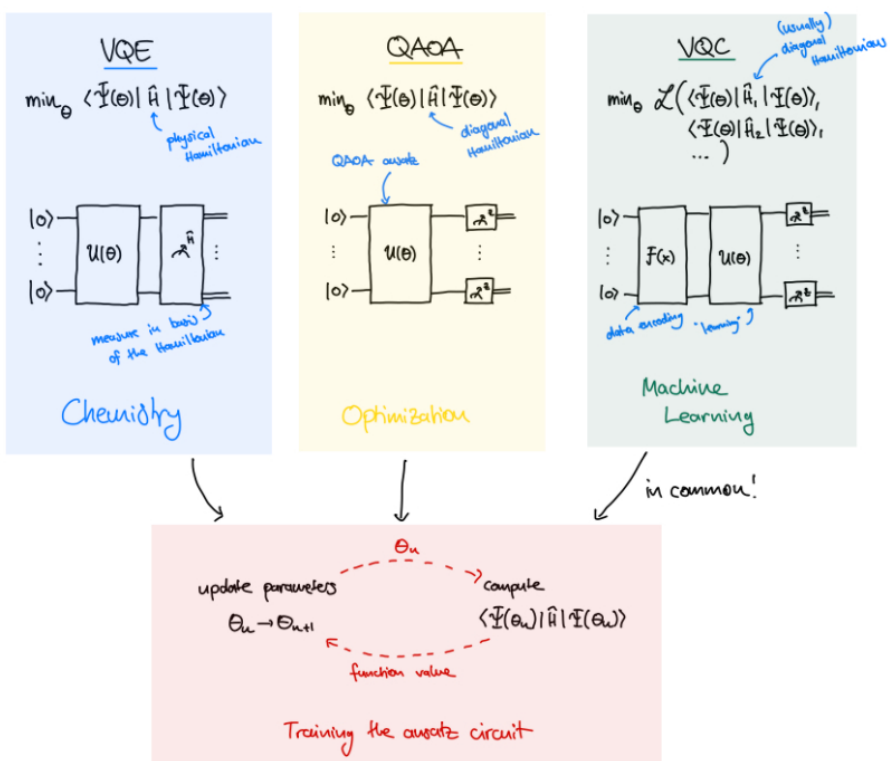


Our task

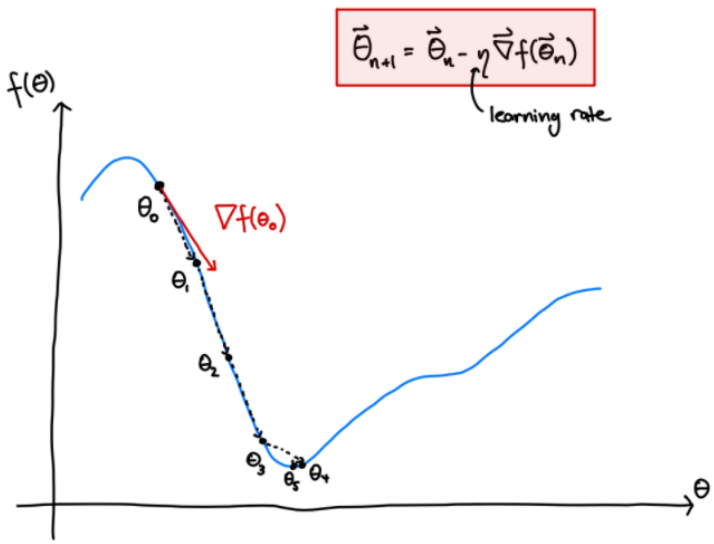
$$\vec{\theta}^* = \underset{\vec{\theta} \in \mathbb{R}^n}{\operatorname{argmin}} \; f(\vec{\theta})$$

VQE: $f(\vec{\theta}) = \langle \Psi(\vec{\theta}) | \hat{H} | \Psi(\vec{\theta}) \rangle$

QAOA: $f(\vec{\theta}) = \langle \Psi(\vec{\theta}) | \hat{H} | \Psi(\vec{\theta}) \rangle$

VQC: $f(\vec{\theta}) = \mathcal{L}(\langle \Psi(\vec{\theta}) | \hat{H}_1 | \Psi(\vec{\theta}) \rangle, \dots)$

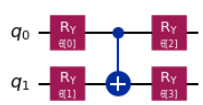
Gradients



Qiskit provides different methods to compute gradients of expectation values, let's explore them!

The parameterized ansatz state is $|\Psi(\vec\theta)\rangle = U(\vec\theta)|0\rangle$ where $U(\vec\theta)$ is given be the following circuit

In [1]:
```
from qiskit.circuit.library import RealAmplitudes

ansatz = RealAmplitudes(num_qubits=2, reps=1, entanglement='linear')
ansatz.draw('mpl', style='iqx')
```



and our Hamiltonian in this example is $\hat H = \hat Z \bigotimes \hat Z$

In [2]:
```
from qiskit.opflow import Z, I

hamiltonian = Z ^ Z
```

Plugged together to $\langle\Psi(\vec\theta) | \hat H | \Psi(\vec\theta)\rangle$:

In [3]:
```
from qiskit.opflow import StateFn

expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(ansatz)
```

To make things concrete, let's fix a point $\vec p$ and an index i and ask: What's the derivative of the expectation value with respect to parameter θ_i at point $\vec p$?

$$ \frac{\partial}{\partial \theta_i} \langle \Psi(\vec\theta) | \hat H | \Psi(\vec\theta) \rangle \bigg\vert_{\vec\theta = \vec p} $$

We'll choose a random point $\vec p$ and index $i=2$ (remember we start counting from 0).

In [4]:
```
import numpy as np

point = np.random.random(ansatz.num_parameters)
index = 2
```

Throughout this session we'll use a shot-based simulator with 8192 shots.

In [5]:
```
from qiskit import Aer
from qiskit.utils import QuantumInstance
```

```
backend = Aer.get_backend('qasm_simulator')
q_instance = QuantumInstance(backend, shots = 8192, seed_simulator = 2718, seed_transpiler = 2718)
```

Computing expectation values

We'll be using expectation values a lot, so let's recap how that worked in Qiskit.

With the `qiskit.opflow` module we can write and evaluate expectation values. The general structure for an expectation value where the state is prepared by a circuit is

```
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(circuit)
result = expectation.eval()
```

The above code uses plain matrix multiplication to evaluate the expected value, which is inefficient for large numbers of qubits. Instead, we can use a simulator (or a real quantum device) to evaluate the circuits by using a `CircuitSampler` in conjunction with an expectation converter like `PauliExpectation` as

```
sampler = CircuitSampler(q_instance)  # q_instance is the QuantumInstance from the beginning of the notebook
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(circuit)
in_pauli_basis = PauliExpectation().convert(expectation)
result = sampler.convert(in_pauli_basis).eval()
```

Exercise 1: Calculate the expected value of the following Hamiltonian `H` and state prepared by the circuit `U` with plain matrix multiplication.

In [6]:
```
from qiskit.circuit import QuantumCircuit
from qiskit.opflow import Z, X

H = X ^ X

U = QuantumCircuit(2)
U.h(0)
U.cx(0, 1)

# YOUR CODE HERE
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(U)
matmult_result = expectation.eval()
```

In [7]:
```
from qc_grader import grade_lab4_ex1

# Note that the grading function is expecting a complex number
grade_lab4_ex1(matmult_result)
```

```
Submitting your answer for lab4/ex1. Please wait...
Congratulations 🎉! Your answer is correct and has been submitted.
```

Exercise 2: Evaluate the expectation value with the QASM simulator by using the `QuantumInstance` object `q_instance` defined in the beginning of the notebook.

In [8]:
```
from qiskit.opflow import CircuitSampler, PauliExpectation

sampler = CircuitSampler(q_instance)

# YOUR CODE HERE
#sampler = CircuitSampler(q_instance)  # q_instance is the QuantumInstance from the beginning of the notebook
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(U)
in_pauli_basis = PauliExpectation().convert(expectation)
shots_result = sampler.convert(in_pauli_basis).eval()
```

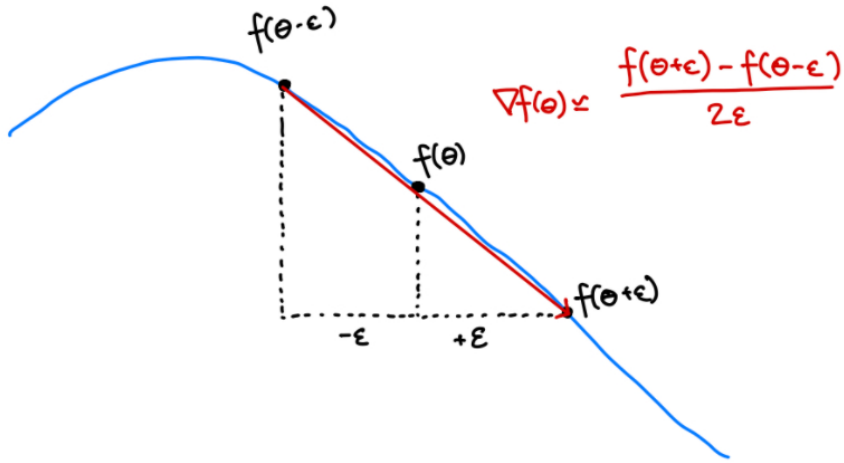
In [9]:
```
from qc_grader import grade_lab4_ex2

# Note that the grading function is expecting a complex number
grade_lab4_ex2(shots_result)
```

```
Submitting your answer for lab4/ex2. Please wait...
Congratulations 🎉! Your answer is correct and has been submitted.
```

Finite difference gradients

Arguably the simplest way to approximate gradients is with a finite difference scheme. This works independent of the function's inner, possibly very complex, structure

structure.



In [10]:
```
from qiskit.opflow import PauliExpectation, CircuitSampler

expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(ansatz)
in_pauli_basis = PauliExpectation().convert(expectation)
sampler = CircuitSampler(q_instance)

def evaluate_expectation(x):
    value_dict = dict(zip(ansatz.parameters, x))
    result = sampler.convert(in_pauli_basis, params=value_dict).eval()
    return np.real(result)
```

In [11]:
```
eps = 0.2
e_i = np.identity(point.size)[:, index]  # identity vector with a 1 at index ``index``, otherwise 0

plus = point + eps * e_i
minus = point - eps * e_i
```

In [12]:
```
finite_difference = (evaluate_expectation(plus) - evaluate_expectation(minus)) / (2 * eps)

print(finite_difference)
```

```
0.0531005859375
```

Instead of doing this manually, you can use Qiskit's `Gradient` class for this.

In [13]:
```
from qiskit.opflow import Gradient

expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(ansatz)
shifter = Gradient('fin_diff', analytic=False, epsilon=eps)
grad = shifter.convert(expectation, params=ansatz.parameters[index])
print(grad)
```

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```
SummedOp([
  2.5 * ComposedOp([
    OperatorMeasurement(ZZ),
    CircuitStateFn(
          ┌─────────┐     ┌─────────────┐
    q_0: ┤ RY(θ[0]) ├──■──┤ RY(θ[2] + 0.2) ├
          ├─────────┤┌─┴─┐└─────────────┘
    q_1: ┤ RY(θ[1]) ├┤ X ├──────────────
          └─────────┘└───┘
    )
  ]),
  -2.5 * ComposedOp([
    OperatorMeasurement(ZZ),
    CircuitStateFn(
          ┌─────────┐     ┌─────────────┐
    q_0: ┤ RY(θ[0]) ├──■──┤ RY(θ[2] - 0.2) ├
          ├─────────┤┌─┴─┐└─────────────┘
    q_1: ┤ RY(θ[1]) ├┤ X ├──────────────
```

Typesetting math: 100%

```
        )
      ])
    ])
```

In [14]:

```
value_dict = dict(zip(ansatz.parameters, point))
sampler.convert(grad, value_dict).eval().real
```

```
0.032958984375
```

Finite difference gradients can be volatile on noisy functions and using the exact formula for the gradient can be more stable.

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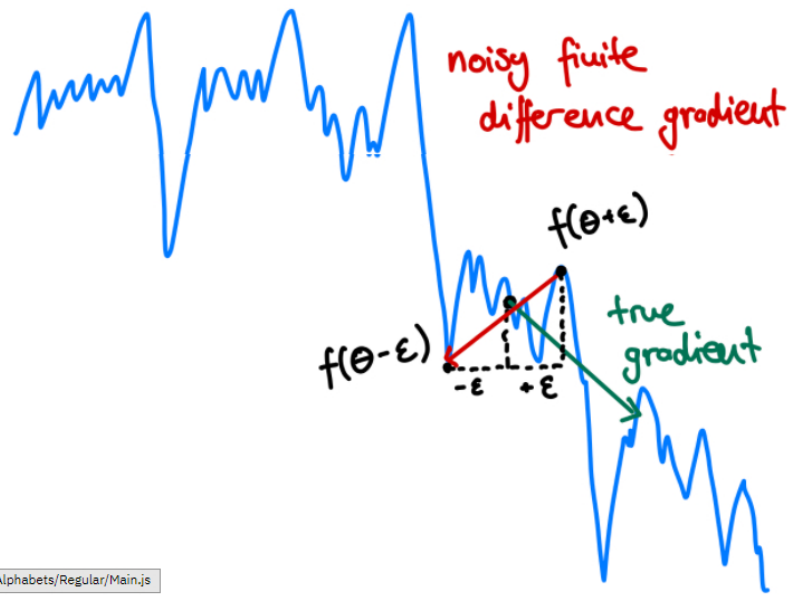

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Analytic gradients

Luckily there's a the *parameter shift* rule -- a simple formula for circuit-based gradients. (**Note:** here only stated for Pauli-rotations without coefficients, see [Evaluating analytic gradients on quantum hardware])

$$\boxed{\frac{\partial f}{\partial \theta_i} = \frac{f(\vec{\theta} + \frac{\pi}{2}\vec{e}_i) - f(\vec{\theta} - \frac{\pi}{2}\vec{e}_i)}{2}}$$

Parameter Shift Rule
(simplified)

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In [15]:

```
eps = np.pi / 2
e_i = np.identity(point.size)[:, index]  # identity vector with a 1 at index ``index``, otherwise 0

plus = point + eps * e_i
minus = point - eps * e_i

finite_difference = (evaluate_expectation(plus) - evaluate_expectation(minus)) / 2

print(finite_difference)
```

```
0.04455566406250002
```

In [16]:

```
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(ansatz)
shifter = Gradient()  # parameter-shift rule is the default
grad = shifter.convert(expectation, params=ansatz.parameters[index])
sampler.convert(grad, value_dict).eval().real
```

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```
0.03833007812500003
```

Based on the same principle, there's the *linear combination of unitaries* approach, that uses only one circuit but an additional auxiliary qubit.

In [17]:
```
expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(ansatz)
shifter = Gradient('lin_comb')  # parameter-shift rule is the default
grad = shifter.convert(expectation, params=ansatz.parameters[index])
sampler.convert(grad, value_dict).eval().real
```

```
0.0341796875
```

Let's try optimizing!

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We fixed an initial point for reproducibility.

In [18]:
```
# initial_point = np.random.random(ansatz.num_parameters)
initial_point = np.array([0.43253681, 0.09507794, 0.42805949, 0.34210341])
```

Similar to how we have a function to evaluate the expectation value, we'll need a function to evaluate the gradient.

In [19]:
```
expectation = StateFn(hamiltonian, is_measurement=True).compose(StateFn(ansatz))
gradient = Gradient().convert(expectation)
gradient_in_pauli_basis = PauliExpectation().convert(gradient)
sampler = CircuitSampler(q_instance)

def evaluate_gradient(x):
    value_dict = dict(zip(ansatz.parameters, x))
    result = sampler.convert(gradient_in_pauli_basis, params=value_dict).eval()  # add parameters in here!
    return np.real(result)
```

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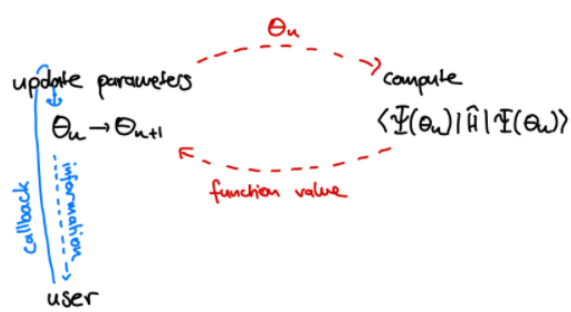
To compare the convergence of the optimizers, we can keep track of the loss at each step by using a callback function.



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In [20]:
```
# Note: The GradientDescent class will be released with Qiskit 0.28.0 and can then be imported as:
# from qiskit.algorithms.optimizers import GradientDescent
from qc_grader.gradient_descent import GradientDescent

gd_loss = []
def gd_callback(nfevs, x, fx, stepsize):
    gd_loss.append(fx)

gd = GradientDescent(maxiter=300, learning_rate=0.01, callback=gd_callback)
```

And now we start the optimization and plot the loss!

In [21]:
```
x_opt, fx_opt, nfevs = gd.optimize(initial_point.size,    # number of parameters
                                   evaluate_expectation,  # function to minimize
                                   gradient_function=evaluate_gradient,  # function to evaluate the gradient
                                   gradient_function=evaluate_gradient,  # function to evaluate the gradient
                                   initial_point=initial_point)  # initial point
```

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In [22]:
```
import matplotlib
import matplotlib.pyplot as plt
matplotlib.rcParams['font.size'] = 14

plt.figure(figsize=(12, 6))
plt.plot(gd_loss, label='vanilla gradient descent')
plt.axhline(-1, ls='--', c='tab:red', label='target')
plt.ylabel('loss')
```

```
plt.xlabel('iterations')
plt.legend();
```

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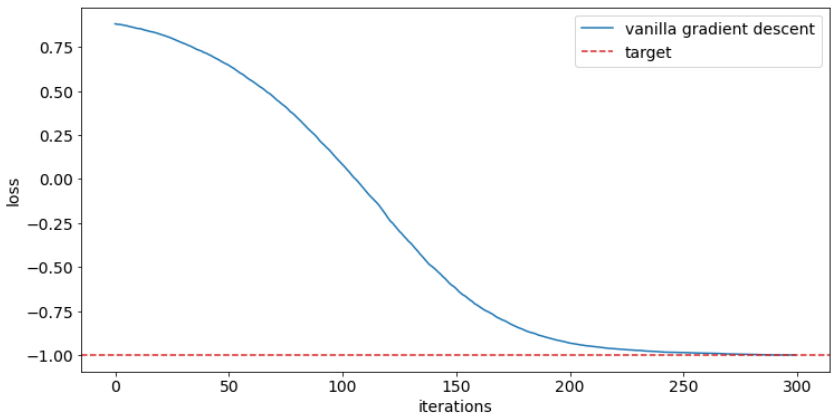
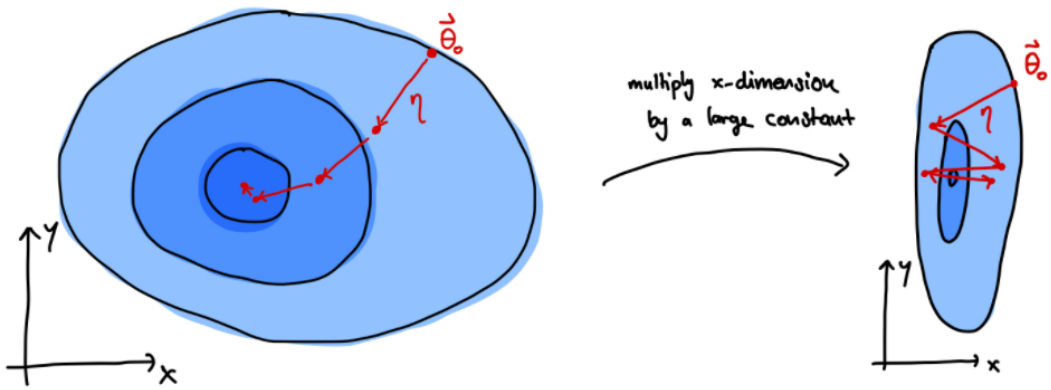
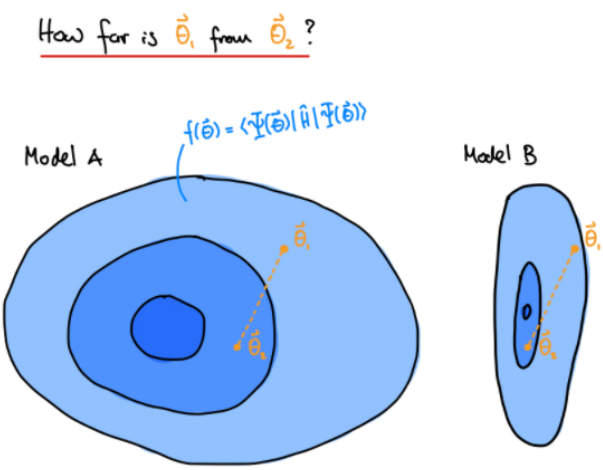


Does this always work?



Natural gradients



Vanilla gradients

$$\text{distance} = \| \vec{\theta}_1 - \vec{\theta}_2 \|_2$$

Euclidean distance

$\Rightarrow$ distance in A and B is the same

Natural gradients

Fidelity

$$\text{distance} = |\langle \Psi(\vec{\theta}_1) | \Psi(\vec{\theta}_2) \rangle|^2$$

$$= \| \vec{\theta}_1 - \vec{\theta}_2 \|_{g(\vec{\theta})}$$

$\Rightarrow$ distance depends on the model!

$$g_{ij}(\vec{\theta}) = \mathrm{Re}\left\{ \left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \Psi \right\rangle \left\langle \Psi \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle \right\}$$

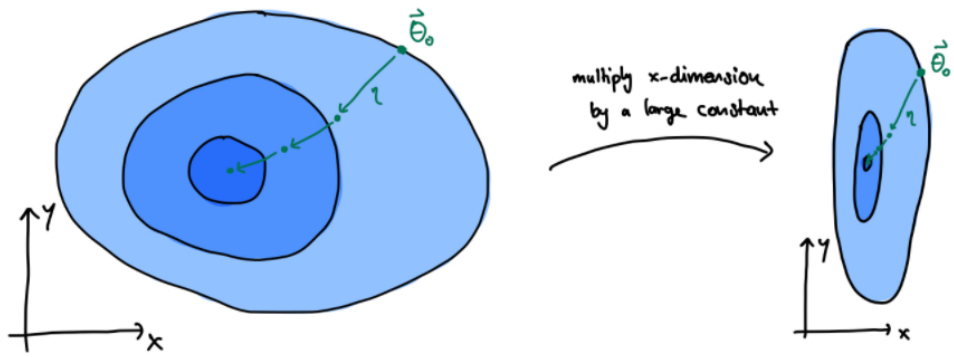
Quantum Fisher Information

Quantum Natural Gradient

$$\boxed{\vec{\theta} = \vec{\theta} - \eta\, g^{-1}(\vec{\theta})\, \vec{\nabla} f(\vec{\theta})}$$

$$\theta_{n+1} = \theta_n - \eta\, g^{-1}(\theta_n)\, \nabla f(\theta_n)$$

Quantum Natural Gradient



With Qiskit, we can evaluate the natural gradient by using the `NaturalGradient` class instead of the `Gradient`!

In [23]:
```
from qiskit.opflow import NaturalGradient
```

Analogously to the function to compute gradients, we can now write a function to evaluate the natural gradients.

In [24]:
```
expectation = StateFn(hamiltonian, is_measurement=True).compose(StateFn(ansatz))
natural_gradient = NaturalGradient(regularization='ridge').convert(expectation)
natural_gradient_in_pauli_basis = PauliExpectation().convert(natural_gradient)
sampler = CircuitSampler(q_instance, caching="all")

def evaluate_natural_gradient(x):
    value_dict = dict(zip(ansatz.parameters, x))
    result = sampler.convert(natural_gradient, params=value_dict).eval()
    return np.real(result)
```

And as you can see they do indeed differ!

In [25]:
```
print('Vanilla gradient:', evaluate_gradient(initial_point))
print('Natural gradient:', evaluate_natural_gradient(initial_point))
```

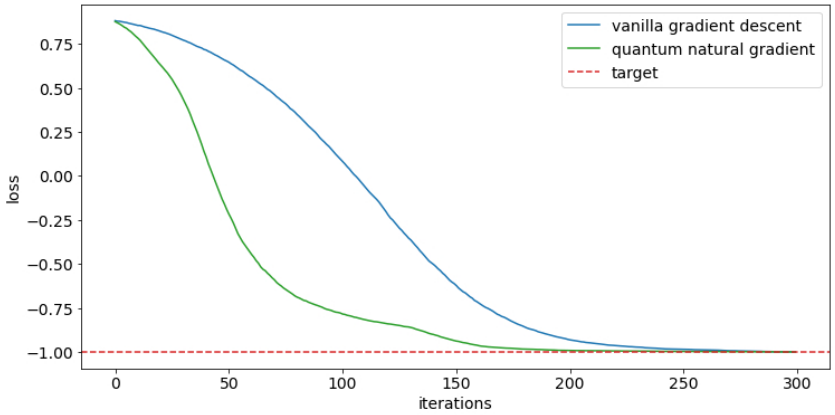
```
Vanilla gradient: [ 0.13989258 -0.35095215 -0.25402832 -0.22497559]
Natural gradient: [ 0.71587182 -0.86457185 -0.98086271 -0.33820243]
```

Let's look at how this influences the convergence.

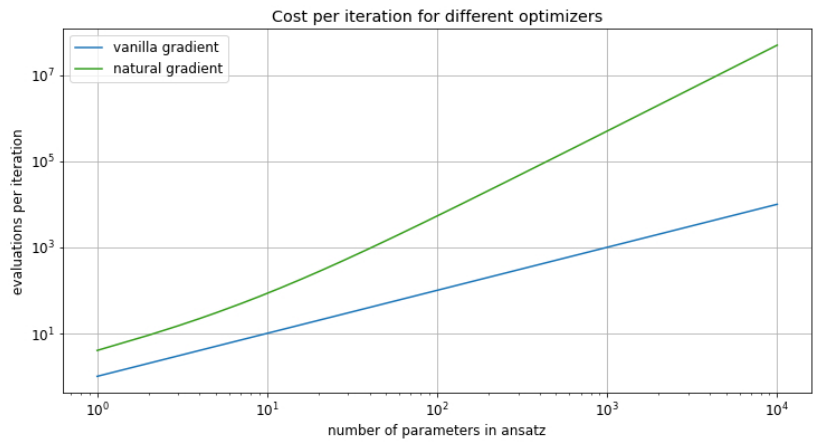
In [26]:
```
qng_loss = []
def qng_callback(nfevs, x, fx, stepsize):
    qng_loss.append(fx)

qng = GradientDescent(maxiter=300, learning_rate=0.01, callback=qng_callback)
```

In [27]:
```
x_opt, fx_opt, nfevs = qng.optimize(initial_point.size,
                                    evaluate_expectation,
                                    gradient_function=evaluate_natural_gradient,
                                    initial_point=initial_point)
```

In [28]:
```
def plot_loss():
    plt.figure(figsize=(12, 6))
    plt.plot(gd_loss, 'tab:blue', label='vanilla gradient descent')
    plt.plot(qng_loss, 'tab:green', label='quantum natural gradient')
    plt.axhline(-1, c='tab:red', ls='--', label='target')
    plt.ylabel('loss')
    plt.xlabel('iterations')
    plt.legend()

plot_loss()
```

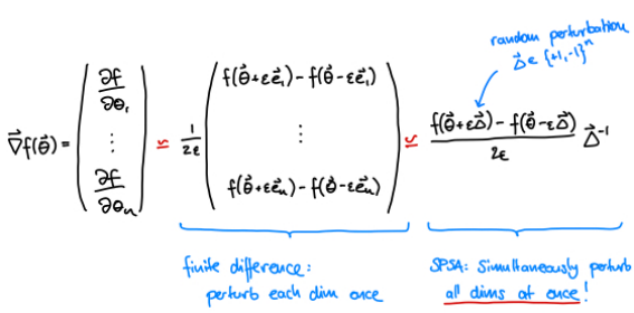


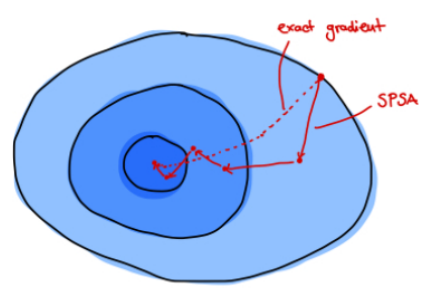
This sounds great! But if we think about how many circuits we need to evaluate these gradients can become costly!



Simultaneous Perturbation Stochastic Approximation

Idea: avoid the expensive gradient evaluation by sampling from the gradients. Since we don't care about the exact values but only about convergence, an unbiased sampling should on average work equally well!



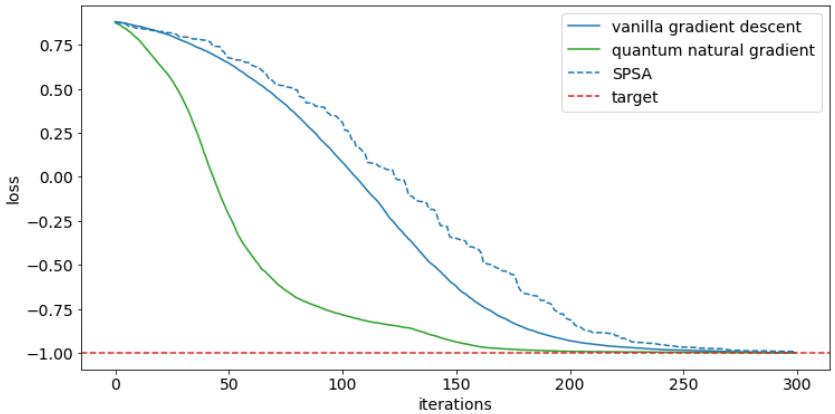


This optimization technique is known as SPSA. How does it perform?

In [29]:
```
from qc_grader.spsa import SPSA

spsa_loss = []
def spsa_callback(nfev, x, fx, stepsize, accepted):
    spsa_loss.append(fx)

spsa = SPSA(maxiter=300, learning_rate=0.01, perturbation=0.01, callback=spsa_callback)

x_opt, fx_opt, nfevs = spsa.optimize(initial_point.size,
                                     evaluate_expectation,
                                     initial_point=initial_point)
```

In [30]:
```
def plot_loss():
```

```
    plt.figure(figsize=(12, 6))
    plt.plot(gd_loss, 'tab:blue', label='vanilla gradient descent')
    plt.plot(qng_loss, 'tab:green', label='quantum natural gradient')
    plt.plot(spsa_loss, 'tab:blue', ls='--', label='SPSA')
    plt.axhline(-1, c='tab:red', ls='--', label='target')
    plt.ylabel('loss')
    plt.xlabel('iterations')
    plt.legend()

plot_loss()
```



And just at a fraction of the cost!

Can we do the same for natural gradients?

1

$$g_{ij}(\vec{\theta}) = \mathrm{Re}\left\{ \left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \Psi}{\partial \theta_i} \middle| \Psi \right\rangle\!\left\langle \Psi \middle| \frac{\partial \Psi}{\partial \theta_j} \right\rangle \right\} = -\frac{1}{2} \frac{\partial^2}{\partial \theta_i \partial \theta_j} \left| \langle \Psi(\vec{\theta}') | \Psi(\vec{\theta}) \rangle \right|^2 \Big|_{\vec{\theta}' = \vec{\theta}}$$

Hessian of the Fidelity!

2

SPSA: Gradient → 1 perturbation $(\vec{\Delta})$ —derive again→ Hessian → 2 perturbations $(\vec{\Delta}_1, \vec{\Delta}_2)$

Simultaneous Perturbation Stochastic Approximation of the Quantum Fisher Information

It turns out -- yes, we can!

We'll skip the details here, but the idea is to sample not only from the gradient but to extend this to the quantum Fisher information and thus to the natural gradient.

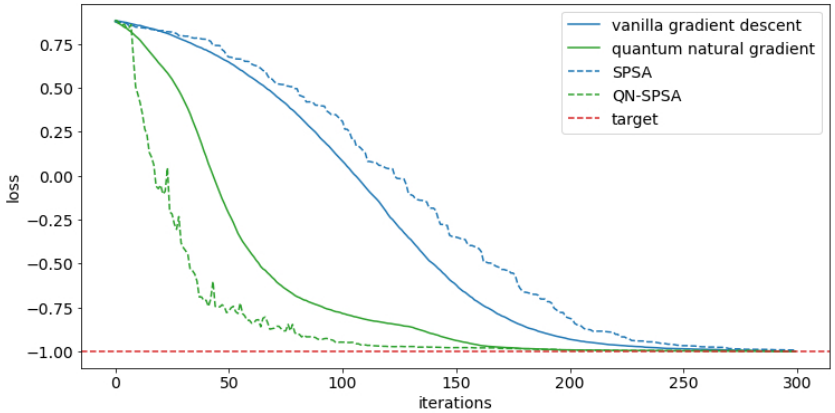
In [31]:

```
# Note: The QNSPSA class will be released with Qiskit 0.28.0 and can then be imported as:
# from qiskit.algorithms.optimizers import QNSPSA
from qc_grader.qnspsa import QNSPSA

qnspsa_loss = []
def qnspsa_callback(nfev, x, fx, stepsize, accepted):
    qnspsa_loss.append(fx)

fidelity = QNSPSA.get_fidelity(ansatz, q_instance, expectation=PauliExpectation())
qnspsa = QNSPSA(fidelity, maxiter=300, learning_rate=0.01, perturbation=0.01, callback=qnspsa_callback)

x_opt, fx_opt, nfevs = qnspsa.optimize(initial_point.size,
                                       evaluate_expectation,
                                       initial_point=initial_point)
```

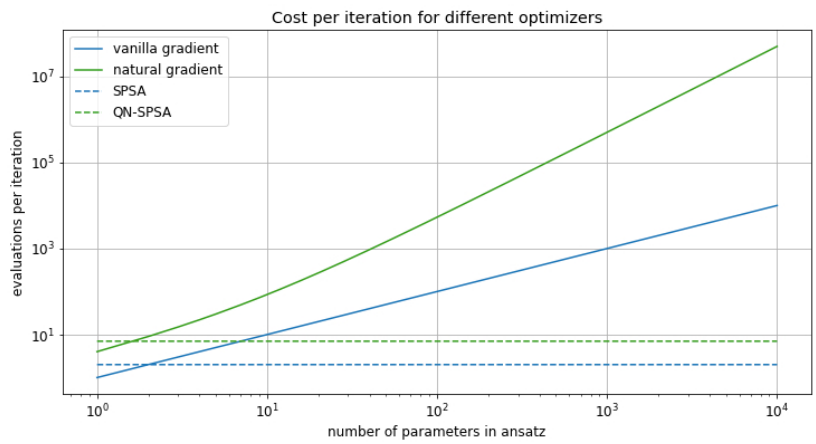
In [32]:

```
def plot_loss():
    plt.figure(figsize=(12, 6))
    plt.plot(gd_loss, 'tab:blue', label='vanilla gradient descent')
    plt.plot(qng_loss, 'tab:green', label='quantum natural gradient')
    plt.plot(spsa_loss, 'tab:blue', ls='--', label='SPSA')
    plt.plot(qnspsa_loss, 'tab:green', ls='--', label='QN-SPSA')
    plt.axhline(-1, c='tab:red', ls='--', label='target')
```

```
    plt.ylabel('loss')
    plt.xlabel('iterations')
    plt.legend()

plot_loss()
```

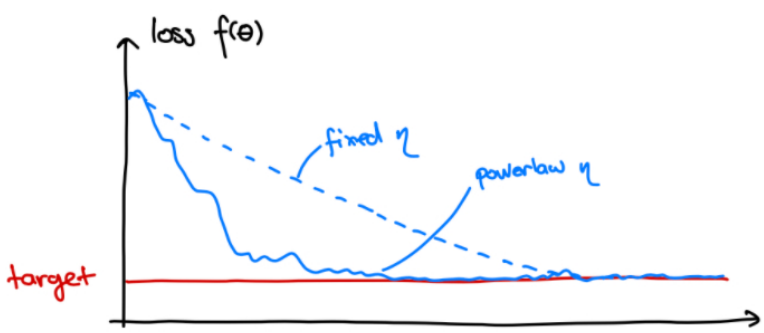


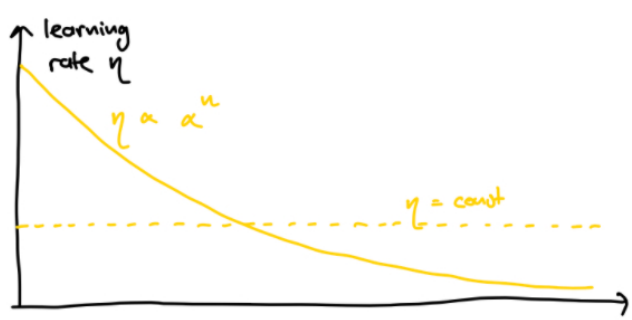
What are the costs?



Training in practice

Today, evaluating gradients is really expensive and the improved accuracy is not that valuable since we have noisy readout anyways. Therefore, in practice, people often resort to using SPSA. To improve convergence, we do however not use a constant learning rate, but an exponentially decreasing one.

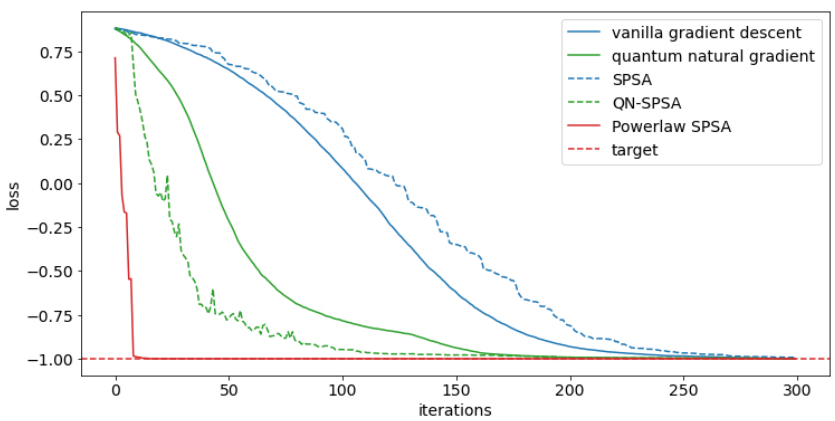




Qiskit will try to automatically calibrate the learning rate to the model if you don't specify the learning rate.

In [33]:
```
autospsa_loss = []
def autospsa_callback(nfev, x, fx, stepsize, accepted):
    autospsa_loss.append(fx)

autospsa = SPSA(maxiter=300, learning_rate=None, perturbation=None, callback=autospsa_callback)

x_opt, fx_opt, nfevs = autospsa.optimize(initial_point.size,
                                         evaluate_expectation,
                                         initial_point=initial_point)
```

In [34]:
```
def plot_loss():
    plt.figure(figsize=(12, 6))
    plt.plot(gd_loss, 'tab:blue', label='vanilla gradient descent')
    plt.plot(qng_loss, 'tab:green', label='quantum natural gradient')
    plt.plot(spsa_loss, 'tab:blue', ls='--', label='SPSA')
    plt.plot(qnspsa_loss, 'tab:green', ls='--', label='QN-SPSA')
    plt.plot(autospsa_loss, 'tab:red', label='Powerlaw SPSA')
    plt.axhline(-1, c='tab:red', ls='--', label='target')
    plt.ylabel('loss')
    plt.xlabel('iterations')
    plt.legend()

plot_loss()
```



Training a new loss function.

In this exercise we'll train a different loss function than before: A transverse field Ising Hamiltonian on a linear chain with 3 spins

$$ \hat H = -Z_0 Z_1 - Z_1 Z_2 - X_0 - X_1 - X_2 $$ *or, spelling out all operations* $$ \hat H = -Z \otimes Z \otimes I - I \otimes Z \otimes Z - X \otimes I \otimes I - I \otimes X \otimes I - I \otimes I \otimes X. $$

Exercise 3: Define the Hamiltonian with Opflow's operators. Make sure to add brackets around the tensors, e.g. `(X ^ X) + (Z ^ I)` *for $X \otimes X + Z \otimes I$.*

In [35]:
```
H_tfi = - (Z ^ Z ^ I) - (I ^ Z ^ Z) - (X ^ I ^ I) - (I ^ X ^ I) - (I ^ I ^ X) # TODO
```

In [36]:
```
from qc_grader import grade_lab4_ex3

# Note that the grading function is expecting a Hamiltonian
grade_lab4_ex3(H_tfi)
```

```
Submitting your answer for lab4/ex3. Please wait...
Congratulations 🎉! Your answer is correct and has been submitted.
```

Exercise 4: We'll use the `EfficientSU2` *variational form as ansatz, since now we care about complex amplitudes. Use the* `evaluate_tfi` *function, which evaluates the energy of the transverse-field Ising Hamiltonian, to find the optimal parameters with* `SPSA`.

In [37]:

```python
from qiskit.circuit.library import EfficientSU2

efficient_su2 = EfficientSU2(3, entanglement="linear", reps=2)
tfi_sampler = CircuitSampler(q_instance)

def evaluate_tfi(parameters):
    exp = StateFn(H_tfi, is_measurement=True).compose(StateFn(efficient_su2))
    value_dict = dict(zip(efficient_su2.parameters, parameters))
    result = tfi_sampler.convert(PauliExpectation().convert(exp), params=value_dict).eval()
    return np.real(result)
```

In this cell, use the SPSA optimizer to find the minimum.

Hint: Use the autocalibration (by not specifying the learning rate and perturbation) and 300 iterations to get close enough to the minimum.

In [39]:

```python
# target energy
tfi_target = -3.4939592074349326

# initial point for reproducibility
tfi_init = np.array([0.95667807, 0.06192812, 0.47615196, 0.83809827, 0.89022282,
                     0.27140831, 0.9540853 , 0.41374024, 0.92595507, 0.76150126,
                     0.8701938 , 0.05096063, 0.25476016, 0.71807858, 0.85661325,
                     0.48311132, 0.43623886, 0.6371297 ])

tfi_result = SPSA.optimize(tfi_init.size,  evaluate_tfi, initial_point=tfi_init)# TODO optimize with SPSA (300 iterations with a
tfi_minimum = tfi_result[1]
```

```
Traceback (most recent call last):
  File "<ipython-input-39-cbbb7cd57d54>", line 10, in <module>
    tfi_result = tfi_result.optimize(tfi_init.size,  evaluate_tfi, initial_point=tfi_init)# TODO optimize with SPSA (300 iterat
ions with automatic calibration should be fine)
NameError: name 'tfi_result' is not defined

Use %tb to get the full traceback.
```

Search for solution online

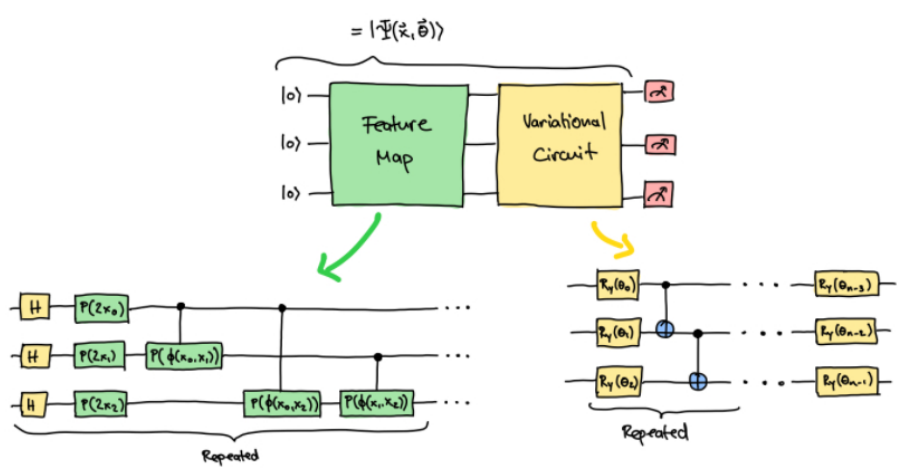
In [ ]:

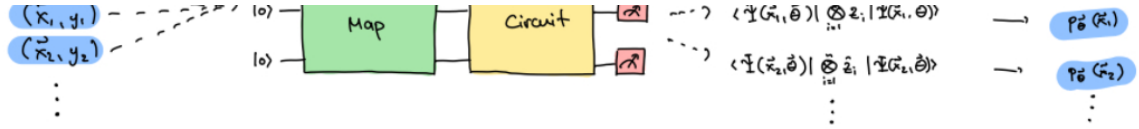
```python
print("Error:", np.abs(tfi_result[1] - tfi_target))
```

In [ ]:

```python
from qc_grader import grade_lab4_ex4

# Note that the grading function is expecting a floating point number
grade_lab4_ex4(tfi_minimum)
```

How can you use it in VQC/QNNs?



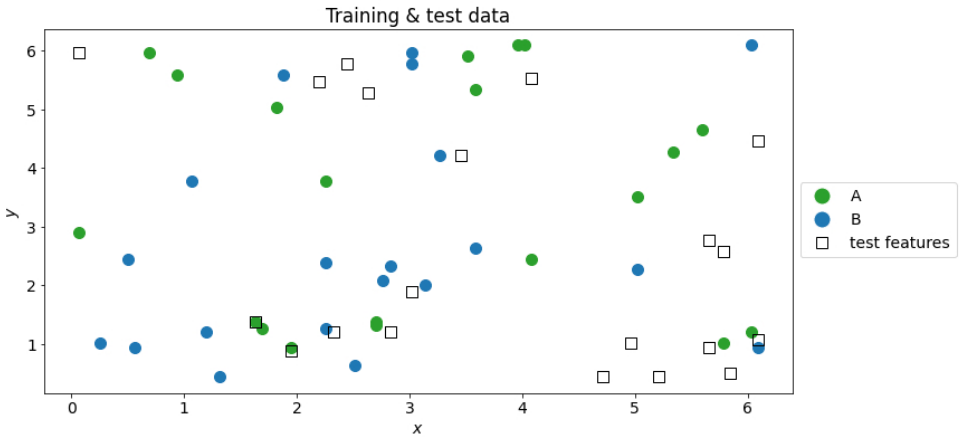


Generating data

We're using some artificial dataset provided by Qiskit's ML package. There are other datasets available, like Iris or Wine, but we'll keep it simple and 2D so we can plot the data.

In [32]:
```
from qiskit_machine_learning.datasets import ad_hoc_data

training_features, training_labels, test_features, test_labels = ad_hoc_data(
    training_size=20, test_size=10, n=2, one_hot=False, gap=0.5
)

# the training labels are in {0, 1} but we'll use {-1, 1} as class labels!
training_labels = 2 * training_labels - 1
test_labels = 2 * test_labels - 1
```

In [33]:
```
def plot_sampled_data():
    from matplotlib.patches import Patch
    from matplotlib.lines import Line2D
    import matplotlib.pyplot as plt

    plt.figure(figsize=(12,6))

    for feature, label in zip(training_features, training_labels):
        marker = 'o'
        color = 'tab:green' if label == -1 else 'tab:blue'
        plt.scatter(feature[0], feature[1], marker=marker, s=100, color=color)

    for feature, label in zip(test_features, test_labels):
        marker = 's'
        plt.scatter(feature[0], feature[1], marker=marker, s=100, facecolor='none', edgecolor='k')

    legend_elements = [
        Line2D([0], [0], marker='o', c='w', mfc='tab:green', label='A', ms=15),
        Line2D([0], [0], marker='o', c='w', mfc='tab:blue', label='B', ms=15),
        Line2D([0], [0], marker='s', c='w', mfc='none', mec='k', label='test features', ms=10)
    ]

    plt.legend(handles=legend_elements, bbox_to_anchor=(1, 0.6))

    plt.title('Training & test data')
    plt.xlabel('$x$')
    plt.ylabel('$y$')

plot_sampled_data()
```



Building a variational quantum classifier

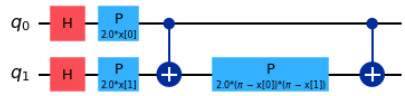
Let's get the constituents we need:

- a Feature Map to encode the data

- an Ansatz to train
- an Observable to evaluate

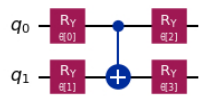
We'll use a standard feature map from the circuit library.

In [34]:
```
from qiskit.circuit.library import ZZFeatureMap

dim = 2
feature_map = ZZFeatureMap(dim, reps=1)  # let's keep it simple!
feature_map.draw('mpl', style='iqx')
```



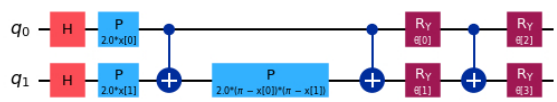
We don't care about complex amplitudes so let's use an ansatz with only real amplitudes.

In [35]:
```
ansatz = RealAmplitudes(num_qubits=dim, entanglement='linear', reps=1)  # also simple here!
ansatz.draw('mpl', style='iqx')
```



Put together our circuit is

In [36]:
```
circuit = feature_map.compose(ansatz)
circuit.draw('mpl', style='iqx')
```



And we'll use global $\bigotimes_{i} \hat Z_i$ operators for the expectation values.

In [37]:
```
hamiltonian = Z ^ Z  # global Z operators
```

Classifying our data

Now we understood all the parts, it's time to classify the data. We're using Qiskit's ML package for that and it's `OpflowQNN` class to describe the circuit and expectation value along with a `NeuralNetworkClassifier` for the training.

First, we'll do vanilla gradient descent.

In [38]:
```
gd_qnn_loss = []
def gd_qnn_callback(*args):
    gd_qnn_loss.append(args[2])

gd = GradientDescent(maxiter=100, learning_rate=0.01, callback=gd_qnn_callback)
```

In [39]:
```
from qiskit_machine_learning.neural_networks import OpflowQNN

qnn_expectation = StateFn(hamiltonian, is_measurement=True) @ StateFn(circuit)

qnn = OpflowQNN(qnn_expectation,
                input_params=list(feature_map.parameters),
                weight_params=list(ansatz.parameters),
                exp_val=PauliExpectation(),
                gradient=Gradient(),  # <-- Parameter-Shift gradients
```

```
                 quantum_instance=q_instance)
```

Now we can define the classifier, which takes the QNN, the loss and the optimizer.

In [40]:
```
from qiskit_machine_learning.algorithms import NeuralNetworkClassifier
#initial_point = np.array([0.2, 0.1, 0.3, 0.4])
classifier = NeuralNetworkClassifier(qnn, optimizer=gd)
```

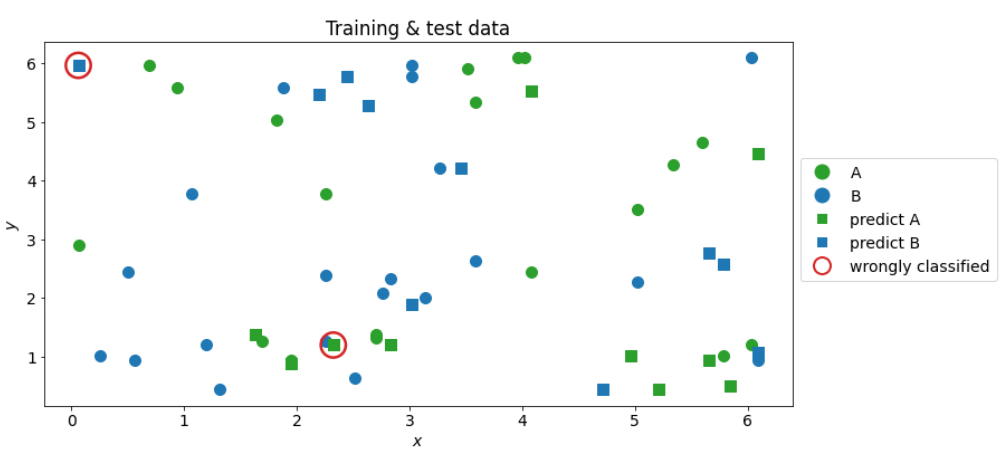
... and train!

In [41]:
```
classifier.fit(training_features, training_labels);
```

To predict the new labels for the test features we can use the `predict` method.

In [42]:
```
predicted = classifier.predict(test_features)
```

In [43]:
```
def plot_predicted():
    from matplotlib.lines import Line2D
    plt.figure(figsize=(12, 6))

    for feature, label in zip(training_features, training_labels):
        marker = 'o'
        color = 'tab:green' if label == -1 else 'tab:blue'
        plt.scatter(feature[0], feature[1], marker=marker, s=100, color=color)

    for feature, label, pred in zip(test_features, test_labels, predicted):
        marker = 's'
        color = 'tab:green' if pred == -1 else 'tab:blue'
        if label != pred:  # mark wrongly classified
            plt.scatter(feature[0], feature[1], marker='o', s=500, linewidths=2.5,
                        facecolor='none', edgecolor='tab:red')

        plt.scatter(feature[0], feature[1], marker=marker, s=100, color=color)

    legend_elements = [
        Line2D([0], [0], marker='o', c='w', mfc='tab:green', label='A', ms=15),
        Line2D([0], [0], marker='o', c='w', mfc='tab:blue', label='B', ms=15),
        Line2D([0], [0], marker='s', c='w', mfc='tab:green', label='predict A', ms=10),
        Line2D([0], [0], marker='s', c='w', mfc='tab:blue', label='predict B', ms=10),
        Line2D([0], [0], marker='o', c='w', mfc='none', mec='tab:red', label='wrongly classified', mew=2, ms=15)
    ]

    plt.legend(handles=legend_elements, bbox_to_anchor=(1, 0.7))

    plt.title('Training & test data')
    plt.xlabel('$x$')
    plt.ylabel('$y$')

plot_predicted()
```



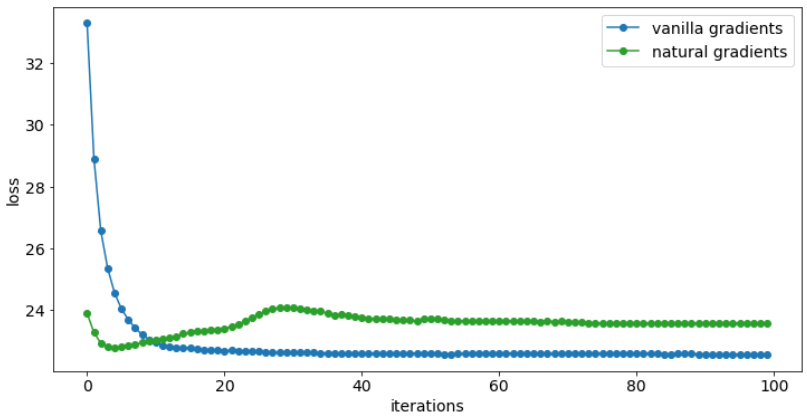
And since we know how to use the natural gradients, we can now train with the QNN with natural gradient descent by replacing `Gradient` with `NaturalGradient`.

In [44]:
```
qng_qnn_loss = []
def qng_qnn_callback(*args):
    qng_qnn_loss.append(args[2])

gd = GradientDescent(maxiter=100, learning_rate=0.01, callback=qng_qnn_callback)
```

In [45]:
```
qnn = OpflowQNN(qnn_expectation,
                input_params=list(feature_map.parameters),
                weight_params=list(ansatz.parameters),
                gradient=NaturalGradient(regularization='ridge'),  # <-- using Natural Gradients!
                quantum_instance=q_instance)
classifier = NeuralNetworkClassifier(qnn, optimizer=gd)#, initial_point=initial_point)
```

In [46]:
```
classifier.fit(training_features, training_labels);
```

In [47]:
```
def plot_losses():

    plt.figure(figsize=(12, 6))
    plt.plot(gd_qnn_loss, 'tab:blue', marker='o', label='vanilla gradients')
    plt.plot(qng_qnn_loss, 'tab:green', marker='o', label='natural gradients')
    plt.xlabel('iterations')
    plt.ylabel('loss')
    plt.legend(loc='best')

plot_losses()
```



Limits in training circuits

Nothing in life is for free... that includes sufficiently large gradients for all models!

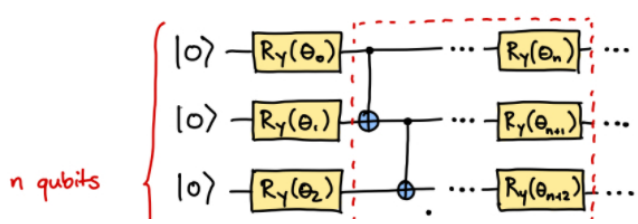
We've seen that training with gradients works well on the small models we tested. But can we expect the same if we increase the number of qubits? To investigate that we measure the variance of the gradients for different model sizes. The idea is simple: if the variance is really small, we don't have enough information to update our parameters.

Exponentially vanishing gradients (Barren plateaus)

[Barren plateaus in quantum neural network training landscapes]

[Cost Function Dependent Barren Plateaus in Shallow Parametrized Quantum Circuits]

Let's pick our favorite example from the gradients and see what happens if we increase the number of qubits and layers.

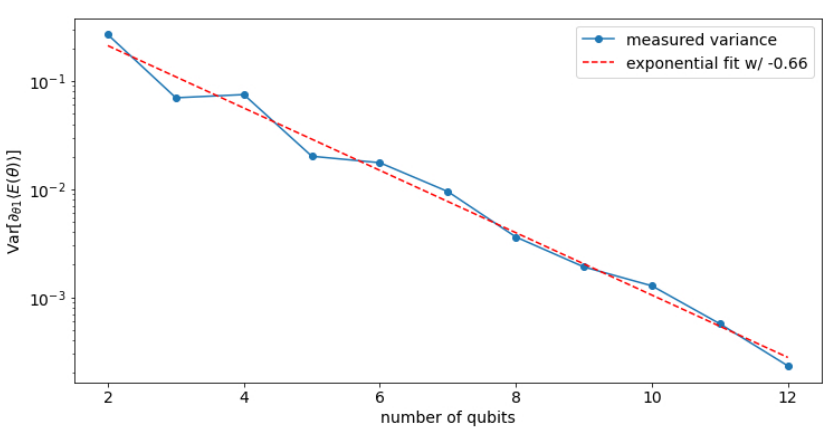


In [48]:
```
from qiskit.opflow import I

def sample_gradients(num_qubits, reps, local=False):
    """Sample the gradient of our model for ``num_qubits`` qubits and ``reps`` repetitions.

    We sample 100 times for random parameters and compute the gradient of the first RY rotation gate.
    """
    index = num_qubits - 1

    # you can also exchange this for a local operator and observe the same!
    if local:
        operator = Z ^ Z ^ (I ^ (num_qubits - 2))
    else:
        operator = Z ^ num_qubits

    # real amplitudes ansatz
    ansatz = RealAmplitudes(num_qubits, entanglement='linear', reps=reps)

    # construct Gradient we want to evaluate for different values
    expectation = StateFn(operator, is_measurement=True).compose(StateFn(ansatz))
    grad = Gradient().convert(expectation, params=ansatz.parameters[index])

    # evaluate for 100 different, random parameter values
    num_points = 100
    grads = []
    for _ in range(num_points):
        # points are uniformly chosen from [0, pi]
        point = np.random.uniform(0, np.pi, ansatz.num_parameters)
        value_dict = dict(zip(ansatz.parameters, point))
        grads.append(sampler.convert(grad, value_dict).eval())

    return grads
```

Let's plot from 2 to 12 qubits.

In [49]:
```
num_qubits = list(range(2, 13))
reps = num_qubits  # number of layers = numbers of qubits
gradients = [sample_gradients(n, r) for n, r in zip(num_qubits, reps)]
```

In [51]:
```
fit = np.polyfit(num_qubits, np.log(np.var(gradients, axis=1)), deg=1)
x = np.linspace(num_qubits[0], num_qubits[-1], 200)

plt.figure(figsize=(12, 6))
plt.semilogy(num_qubits, np.var(gradients, axis=1), 'o-', label='measured variance')
plt.semilogy(x, np.exp(fit[0] * x + fit[1]), 'r--', label=f'exponential fit w/ {fit[0]:.2f}')
plt.xlabel('number of qubits')
plt.ylabel(r'$\mathrm{Var}[\partial_{\theta 1} \langle E(\theta) \rangle]$')
plt.legend(loc='best');
```



Oh no! The variance decreases exponentially! This means our gradients contain less and less information and we'll have a hard time to train the model. This is known as the *Barren plateau* problem or *exponentially vanishing gradients*.

Exploratory Exercise: Do Natural Gradient suffer from vanishing gradients?

Repeat the Barren plateau plot for natural gradients instead of standard gradients. For this, write a new function `sample_natural_gradients` *that computes the natural gradient instead of the gradient.*

In [ ]:
```
from qiskit.opflow import NaturalGradient

def sample_natural_gradients(num_qubits, reps):
    index = num_qubits - 1

    operator = Z ^ num_qubits

    ansatz = RealAmplitudes(num_qubits, entanglement='linear', reps=reps)

    expectation = StateFn(operator, is_measurement=True).compose(StateFn(ansatz))
    grad = # TODO: ``grad`` should be the natural gradient for the parameter at index ``index``.
    # Hint: Check the ``sample_gradients`` function, this one is almost the same.
    grad = NaturalGradient().convert(expectation, params=ansatz.parameters[index])

    num_points = 100
    grads = []
    for _ in range(num_points):
        point = np.random.uniform(0, np.pi, ansatz.num_parameters)
        value_dict = dict(zip(ansatz.parameters, point))
        grads.append(sampler.convert(grad, value_dict).eval())
    return grads
```

Now we'll repeat the experiment to check the variance of the gradients (this cell takes some time to run!)

In [ ]:
```
num_qubits = list(range(2, 13))
reps = num_qubits  # number of layers = numbers of qubits
natural_gradients = [sample_natural_gradients(n, r) for n, r in zip(num_qubits, reps)]
```

and plot the results. What do you observe?

In [ ]:
```
fit = np.polyfit(num_qubits, np.log(np.var(natural_gradients, axis=1)), deg=1)
x = np.linspace(num_qubits[0], num_qubits[-1], 200)

plt.figure(figsize=(12, 6))
plt.semilogy(num_qubits, np.var(gradients, axis=1), 'o-', label='vanilla gradients')
plt.semilogy(num_qubits, np.var(natural_gradients, axis=1), 's-', label='natural gradients')
plt.semilogy(x, np.exp(fit[0] * x + fit[1]), 'r--', label=f'exponential fit w/ {float(fit[0]):.2f}')
plt.xlabel('number of qubits')
plt.ylabel(r'$\mathrm{Var}[\partial_{\theta 1} \langle E(\theta) \rangle]$')
plt.legend(loc='best');
```

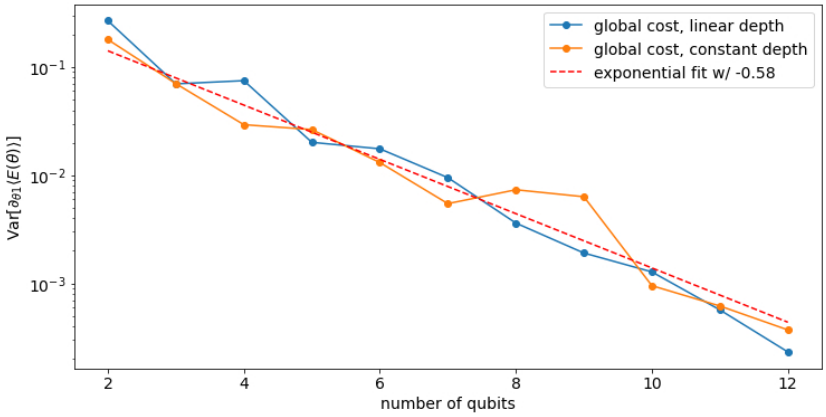
What about shorter circuits?

Is there something we can do about these Barren plateaus? It's a hot topic in current research and there are some proposals to mitigate Barren plateaus.

Let's have a look on how global and local cost functions and the depth of the ansatz influences the Barren plateaus.

In [52]:
```
num_qubits = list(range(2, 13))
fixed_depth_global_gradients = [sample_gradients(n, 1) for n in num_qubits]
```

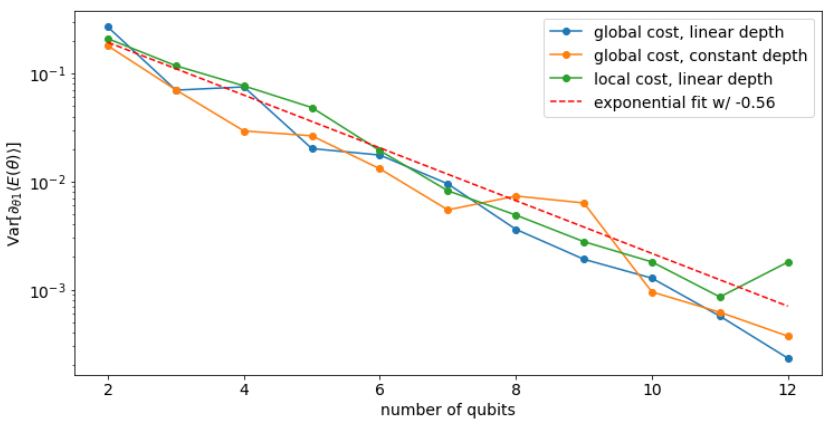
In [53]:
```
fit = np.polyfit(num_qubits, np.log(np.var(fixed_depth_global_gradients, axis=1)), deg=1)
x = np.linspace(num_qubits[0], num_qubits[-1], 200)

plt.figure(figsize=(12, 6))
plt.semilogy(num_qubits, np.var(gradients, axis=1), 'o-', label='global cost, linear depth')
plt.semilogy(num_qubits, np.var(fixed_depth_global_gradients, axis=1), 'o-', label='global cost, constant depth')
plt.semilogy(x, np.exp(fit[0] * x + fit[1]), 'r--', label=f'exponential fit w/ {fit[0]:.2f}')
plt.xlabel('number of qubits')
plt.ylabel(r'$\mathrm{Var}[\partial_{\theta 1} \langle E(\theta) \rangle]$')
plt.legend(loc='best');
```



And what if we use *local* operators?

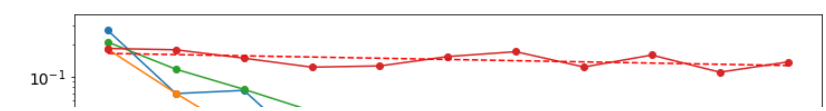
In [54]:
```
num_qubits = list(range(2, 13))
linear_depth_local_gradients = [sample_gradients(n, n, local=True) for n in num_qubits]
```

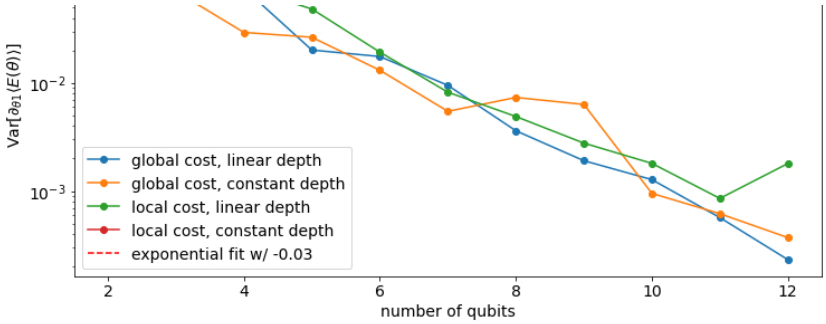
In [55]:
```
fit = np.polyfit(num_qubits, np.log(np.var(linear_depth_local_gradients, axis=1)), deg=1)
x = np.linspace(num_qubits[0], num_qubits[-1], 200)

plt.figure(figsize=(12, 6))
plt.semilogy(num_qubits, np.var(gradients, axis=1), 'o-', label='global cost, linear depth')
plt.semilogy(num_qubits, np.var(fixed_depth_global_gradients, axis=1), 'o-', label='global cost, constant depth')
plt.semilogy(num_qubits, np.var(linear_depth_local_gradients, axis=1), 'o-', label='local cost, linear depth')
plt.semilogy(x, np.exp(fit[0] * x + fit[1]), 'r--', label=f'exponential fit w/ {fit[0]:.2f}')
plt.xlabel('number of qubits')
plt.ylabel(r'$\mathrm{Var}[\partial_{\theta 1} \langle E(\theta) \rangle]$')
plt.legend(loc='best');
```



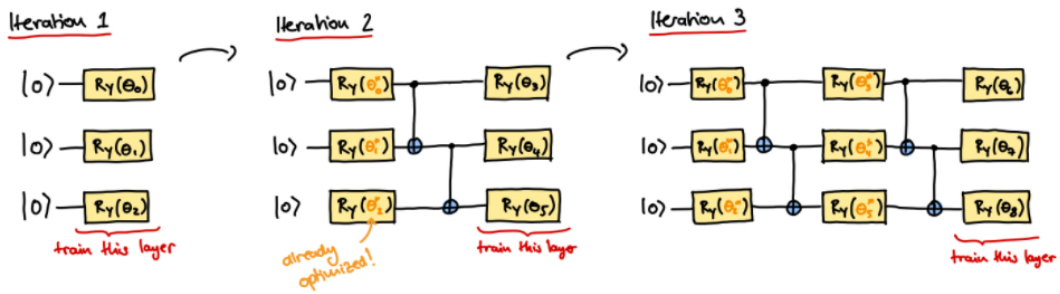
In [56]:
```
num_qubits = list(range(2, 13))
fixed_depth_local_gradients = [sample_gradients(n, 1, local=True) for n in num_qubits]
```

In [57]:
```
fit = np.polyfit(num_qubits, np.log(np.var(fixed_depth_local_gradients, axis=1)), deg=1)
x = np.linspace(num_qubits[0], num_qubits[-1], 200)

plt.figure(figsize=(12, 6))
plt.semilogy(num_qubits, np.var(gradients, axis=1), 'o-', label='global cost, linear depth')
plt.semilogy(num_qubits, np.var(fixed_depth_global_gradients, axis=1), 'o-', label='global cost, constant depth')
plt.semilogy(num_qubits, np.var(linear_depth_local_gradients, axis=1), 'o-', label='local cost, linear depth')
plt.semilogy(num_qubits, np.var(fixed_depth_local_gradients, axis=1), 'o-', label='local cost, constant depth')
plt.semilogy(x, np.exp(fit[0] * x + fit[1]), 'r--', label=f'exponential fit w/ {fit[0]:.2f}')
plt.xlabel('number of qubits')
plt.ylabel(r'$\mathrm{Var}[\partial_{\theta 1} \langle E(\theta) \rangle]$')
plt.legend(loc='best');
```





Layerwise training



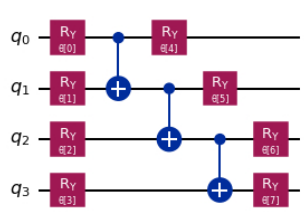
In [58]:

```
num_qubits = 6
operator = Z ^ Z ^ (I ^ (num_qubits - 4))

def minimize(circuit, optimizer):
    initial_point = np.random.random(circuit.num_parameters)

    exp = StateFn(operator, is_measurement=True) @ StateFn(circuit)
    grad = Gradient().convert(exp)

    # pauli basis
    exp = PauliExpectation().convert(exp)
    grad = PauliExpectation().convert(grad)

    sampler = CircuitSampler(q_instance, caching="all")

    def loss(x):
        values_dict = dict(zip(circuit.parameters, x))
        return np.real(sampler.convert(exp, values_dict).eval())

    def gradient(x):
        values_dict = dict(zip(circuit.parameters, x))
        return np.real(sampler.convert(grad, values_dict).eval())

    return optimizer.optimize(circuit.num_parameters, loss, gradient, initial_point=initial_point)
```

Useful feature: Qiskit's ansatz circuits are mutable!

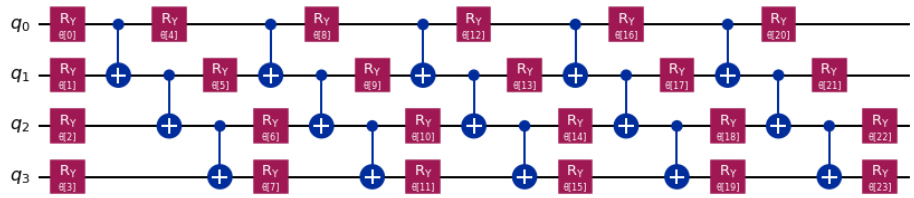
In [59]:

```
circuit = RealAmplitudes(4, reps=1, entanglement='linear')
circuit.draw('mpl', style='iqx')
```



In [60]:

```
circuit.reps = 5
circuit.draw('mpl', style='iqx')
```



In [64]:

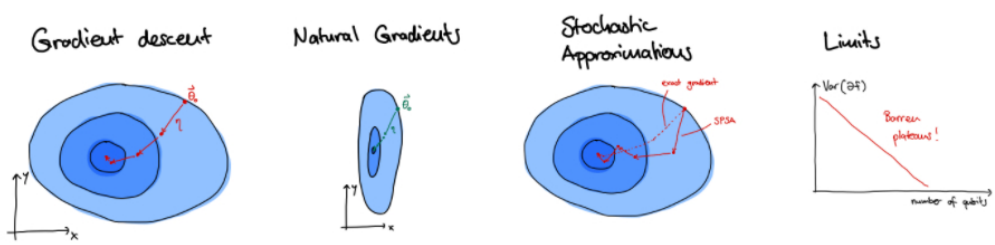
```
def layerwise_training(ansatz, max_num_layers, optimizer):
    optimal_parameters = []
    fopt = None
    for reps in range(1, max_num_layers):
        ansatz.reps = reps

        # bind already optimized parameters
        values_dict = dict(zip(ansatz.parameters, optimal_parameters))
        partially_bound = ansatz.bind_parameters(values_dict)

        xopt, fopt, _ = minimize(partially_bound, optimizer)
        print('Circuit depth:', ansatz.depth(), 'best value:', fopt)
        optimal_parameters += list(xopt)

    return fopt, optimal_parameters
```

In [65]:

```
ansatz = RealAmplitudes(4, entanglement='linear')
optimizer = GradientDescent(maxiter=50)
```

In [66]:

```
np.random.seed(12)
fopt, optimal_parameters = layerwise_training(ansatz, 4, optimizer)
```

```
Circuit depth: 5 best value: 0.2421875
Circuit depth: 8 best value: -0.14428710937499992
Circuit depth: 11 best value: -0.513427734375
```

Summary