Investigating Control Channel Noise Resilience

David Goodwin, Ilya Kuprov

dg1g13@soton.ac.uk, University of Southampton, Southampton, UK.

Introduction

Although optimal control of NMR systems has been reported successful for large spin systems [1], practical systems contain a level of noise inherent in any electronic system [2] and the resilience of the system to noise is sensitive to the size of the spin system. These investigations are implemented using gradient ascent pulse engineering in the Spinach library [3, 4] and optimisation by the (limited memory) BFGS algorithm.

We show the level of noise a state transfer simulation can withstand to obtain an acceptable fidelity in comparison of initial and target states using a number of averaged control channels; denying the optimization algorithm a 'cheat' in finding a path through a specific noise instance yet still allowing the character of the noise to become part of the objective function. The change in fidelity at different noise levels is shown for a number of systems, including state transfer through HCF and a typical protein backbone, and a test of noise resilience being a 'freeze-pulse' to freeze the system in an initial state over a designated time period.

Model

We consider transfer of megnetisation in two different systems, chosen as a small and medium sized simulation rather than the science they produce:

- $^1H^{13}C^{19}F$ from ^1H to ^{19}F

- $^{15}N^1H^{13}C^{13}C^{13}C^{15}N$ from ^1H to 2nd ^{15}N

Their optimal set of control pulses are simulated within 20ms and 100ms pulse durations with 128 and 256 time steps, for HCF and NHCCCN respectively. Optimisation is run to 256 iterations and is expected to reach a level of convergence if one can be reached.

An additive noise term applied to the objective function at each step of the optimisation. The additive noise is applied as a number of different instances over an ensemble as the system is controlled. The waveform (x_n) to be the argument of the objective function is the arithmetic mean of the local waveforms, being the previous waveform summed with the noise level (A) multiplied with the Gaussian noise (W);

$$x_{i,n} = x_{i-1} + AW_n$$

$$x_i = \frac{1}{N} \sum_{n=1}^{N} x_{i,n}$$

References

[1] I. Kuprov, J. Magn. Reson., 233, 107-112 (2013)
[2] S. Kallush, M. Khasin, and R. Kosloff, New J Phys., 16, 015008 (2014)
[3] P. de Fouquieres, S.G. Schirmer, S.J. Glaser, I. Kuprov. J. Magn. Reson., 212, 412-417 (2011)
[4] H.J. Hogben, M. Krzystyniak, G.T.P. Charnock, P.J. Hore, and I. Kuprov. J. Magn. Reson., 208, 179-194 (2011)

All random numbers were seeded with `rng(128,'v4')` from within a matlab session.
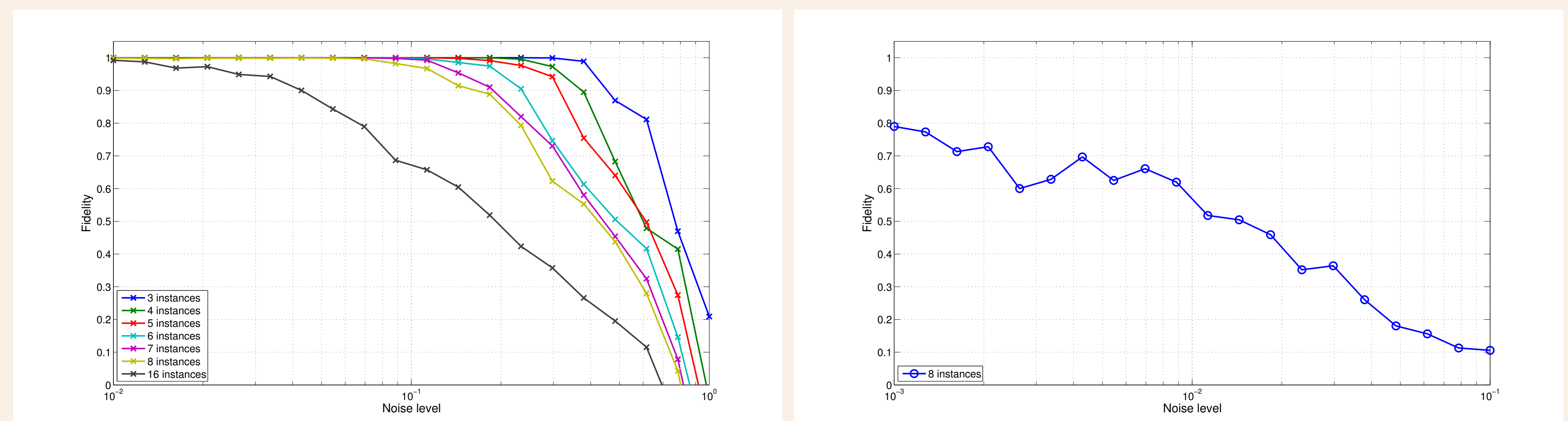
"Freeze-pulse"

As a test of the application of noise to the optimisation algorithm, we set the target state of the evolution to the same as the initial state; the control pulses named a "freeze-pulse". Other than a different target state, all other parts of the simulation as the state transfer simulations.

Below are the results of the HCF freeze-pulse simulation (left) and the protein-backbone freeze-pulse simulation (right).
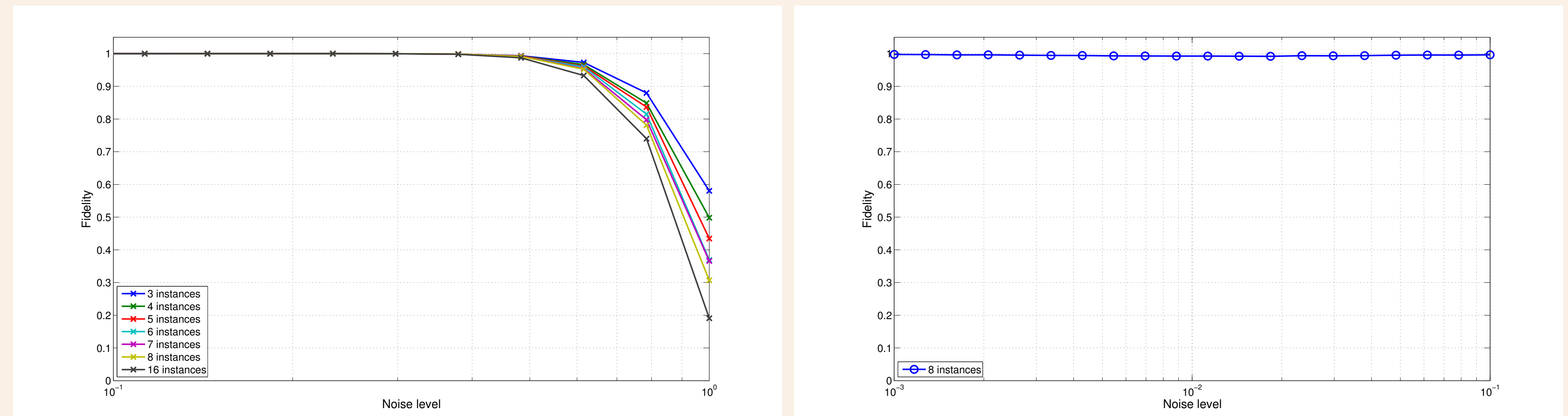

In the HCF simulation a decent level of fidelity is found for noise levels less than 0.6 of the signal. After this level, the noise becomes more difficult for the optimisation to handle, with lesser fidelities achieved. Here, the more local noise instances we simulate, the more pronounced the fidelity loss. The protein-backbone simulation show excellent fidelity over the noise levels investigated. We used a smaller noise level set on the protein-backbone simulation as it was expected that a larger system would be more susceptible to noise [2], comprising a more 'delicate' system.

State Transfer

Below are the results of the HCF state transfer simulation (left) and the protein-backbone state transfer simulation (right).


Comparing the HCF simulation to it's freeze-pulse, we see the same system being less resilient to the noise instances as we transfer the magnetisation over two bonds. Similarly, the protein-backbone is less resilient to the noise instances, but the effect is more pronounced; expected to be a result of the complicated arrangement of ^{13}C isotopes making a more difficult and precise route for the optimisation to find: the effect of noise being pronounced at this modest level. An example of an l-BFGS-GRAPE state transfer simulation is show below, without any noise or relaxation:
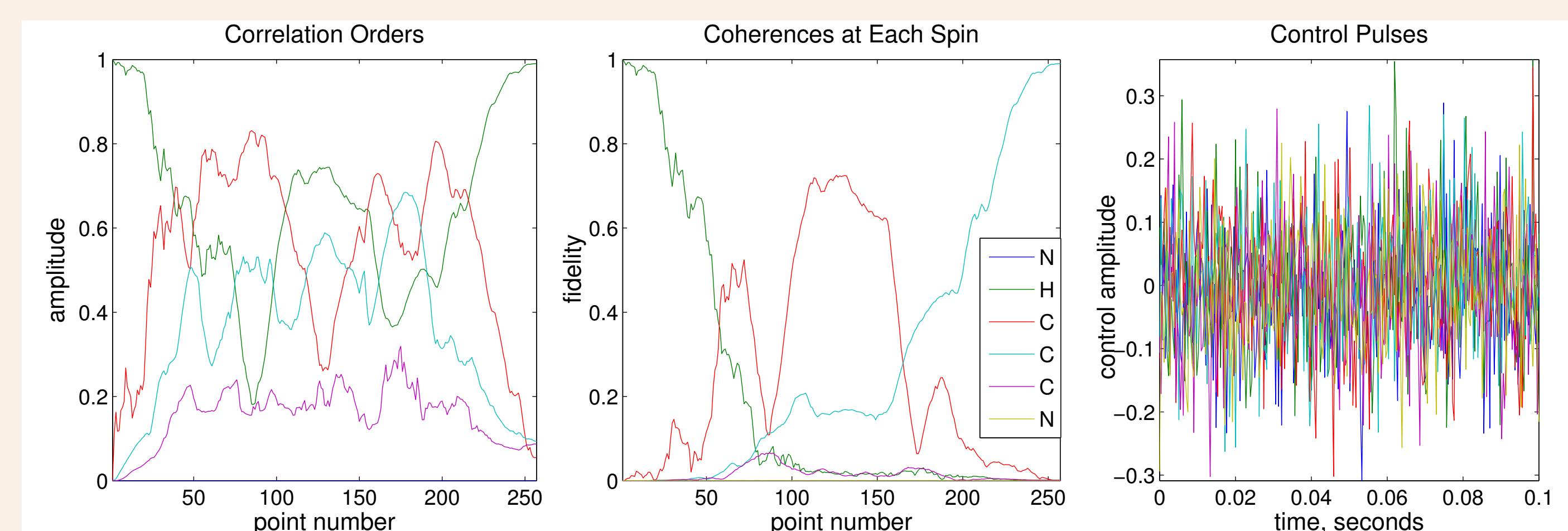
State Transfer with Relaxation

Results of the HCF state transfer simulation with T1/T2 relaxation with rates of 0.5 Hz for R1 and 2.5 Hz for R2 are show below. The dotted lines are for comparison to the HCF state transfer simulation above.
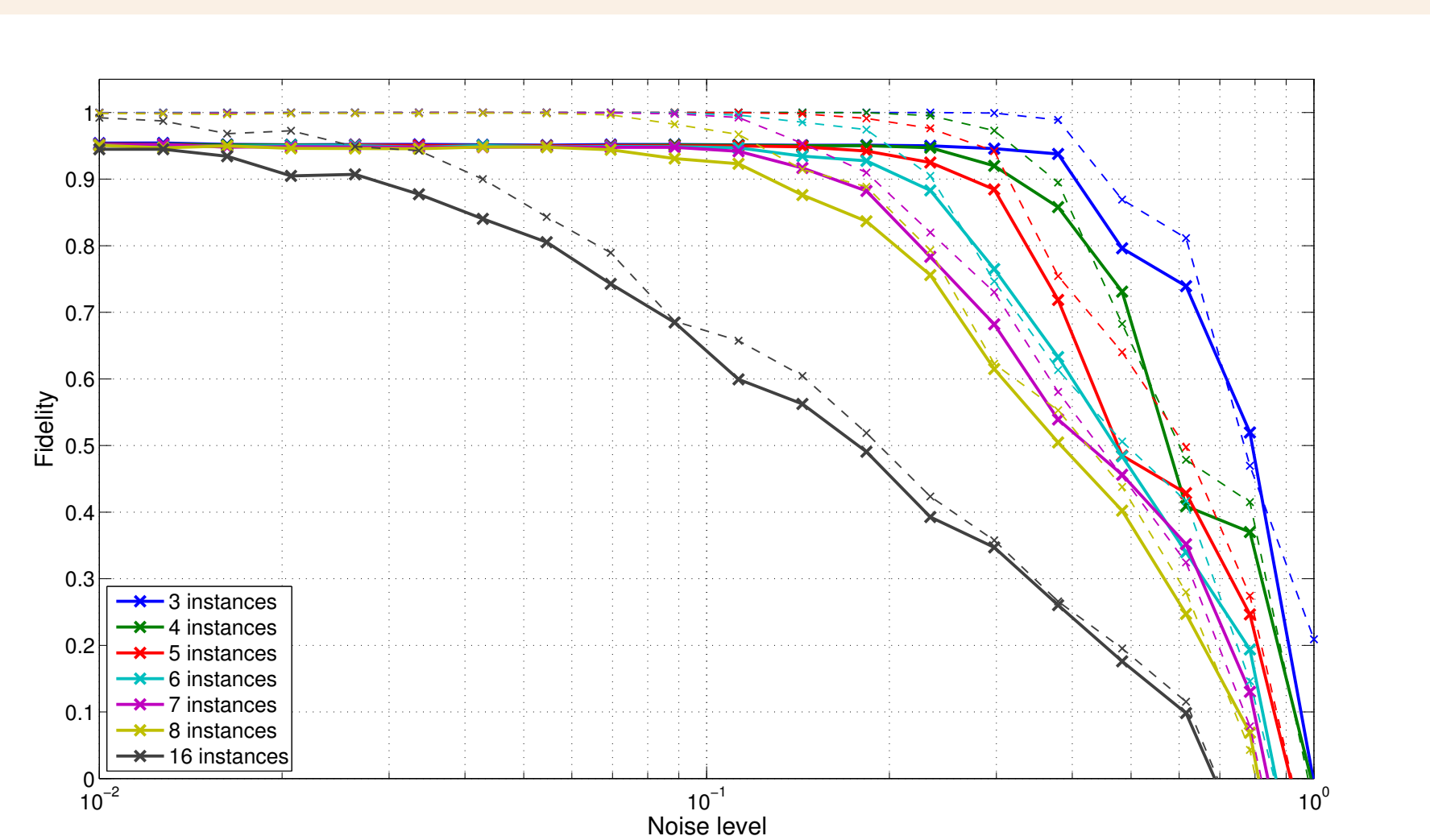
In this case, the relaxation acts as a damping rate for the whole system, translating the whole of the plot downwards to slightly less fidelity.

An interesting observation is that the relaxation seems less of a dominant term as higher noise levels are experienced; for all numbers of noise instances fidelity is similar with or without relaxation.