

## Alpha divergence minimization...

- 1 generalizes existing inference methods (VB and EP).
- 2 better than any of them in regression problems with neural nets.

## Distributed Thompson sampling...

- 1 Allows to handle large batch sizes and large molecule libraries.
- 2 By using exploration it produces improvements over greedy approaches.

## Data-driven molecule optimization...

- 1 New compounds generated by optimizing in latent space.
- 2 Can leverage large lists of unlabeled chemical compounds.