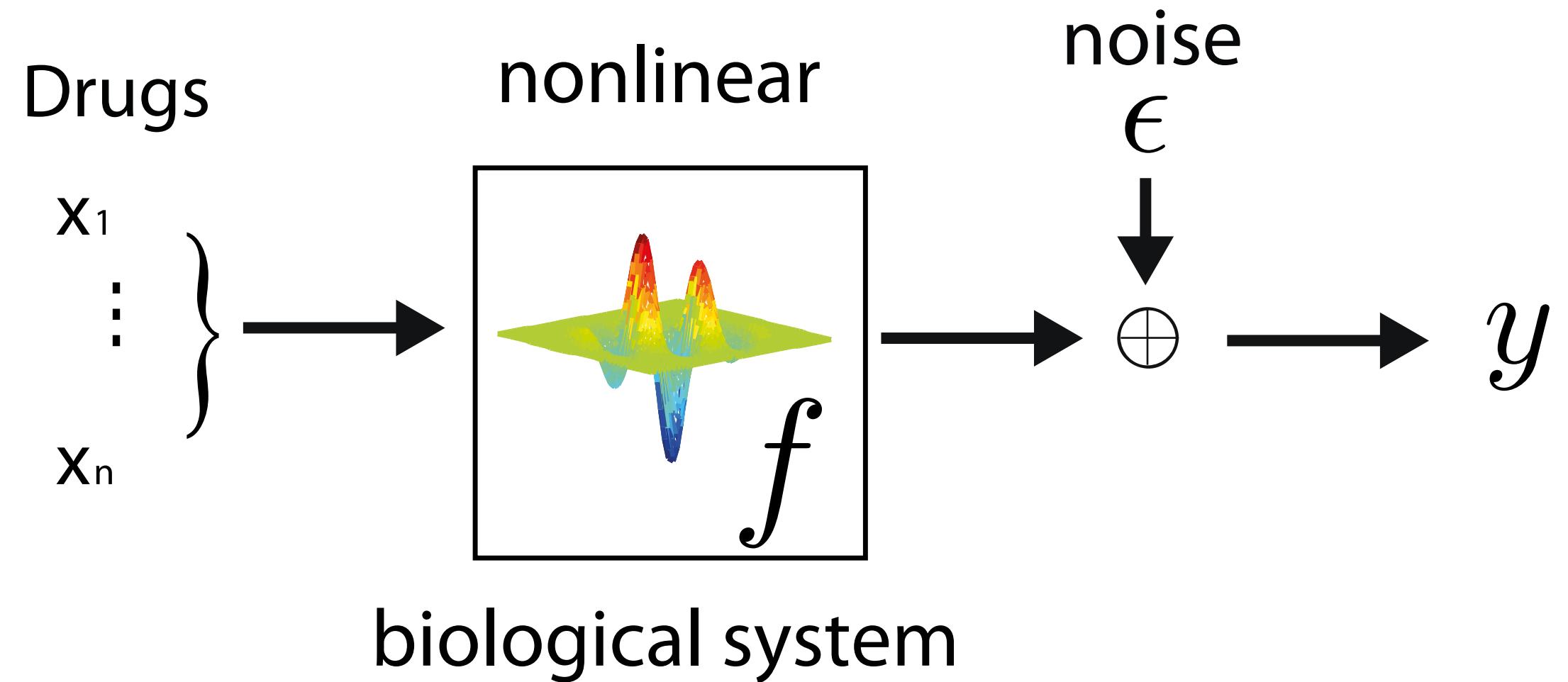


Adaptive Experimental Design For Drug Combinations

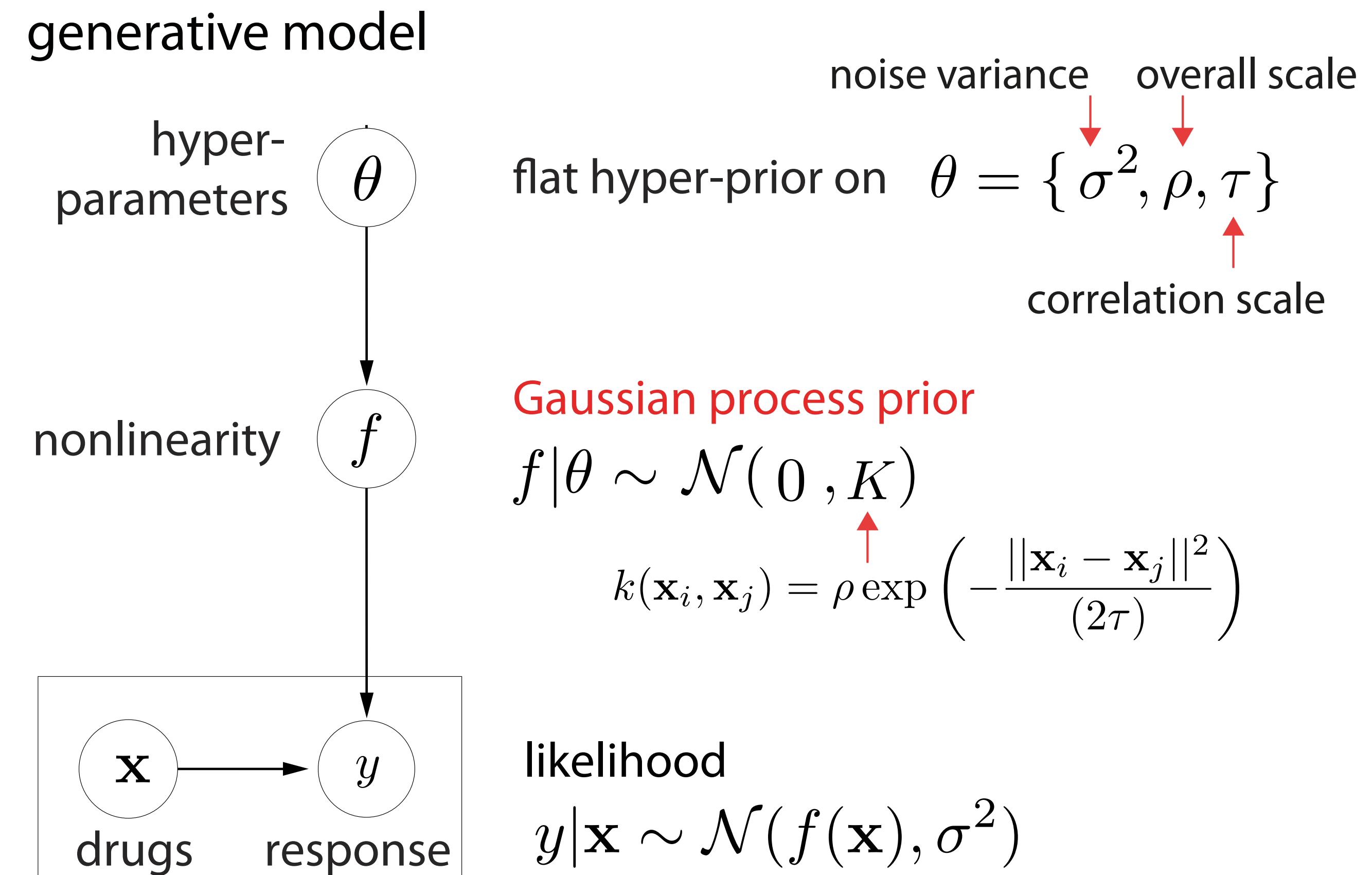
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1. Drug combinations problem



2. Response modeling using Gaussian processes



MAP inference:
at test points $P(\mathbf{f}^* | X^*, X, \mathbf{y}, \theta) \sim \mathcal{N}(\mu, \Sigma)$

$$\mu = K(X^*, X)(K + \sigma^2 I)^{-1}\mathbf{y}$$

$$\Sigma = K(X^*, X^*) - K(X^*, X)(K + \sigma^2 I)^{-1}K(X, X^*)$$

Hyperparameter estimation:

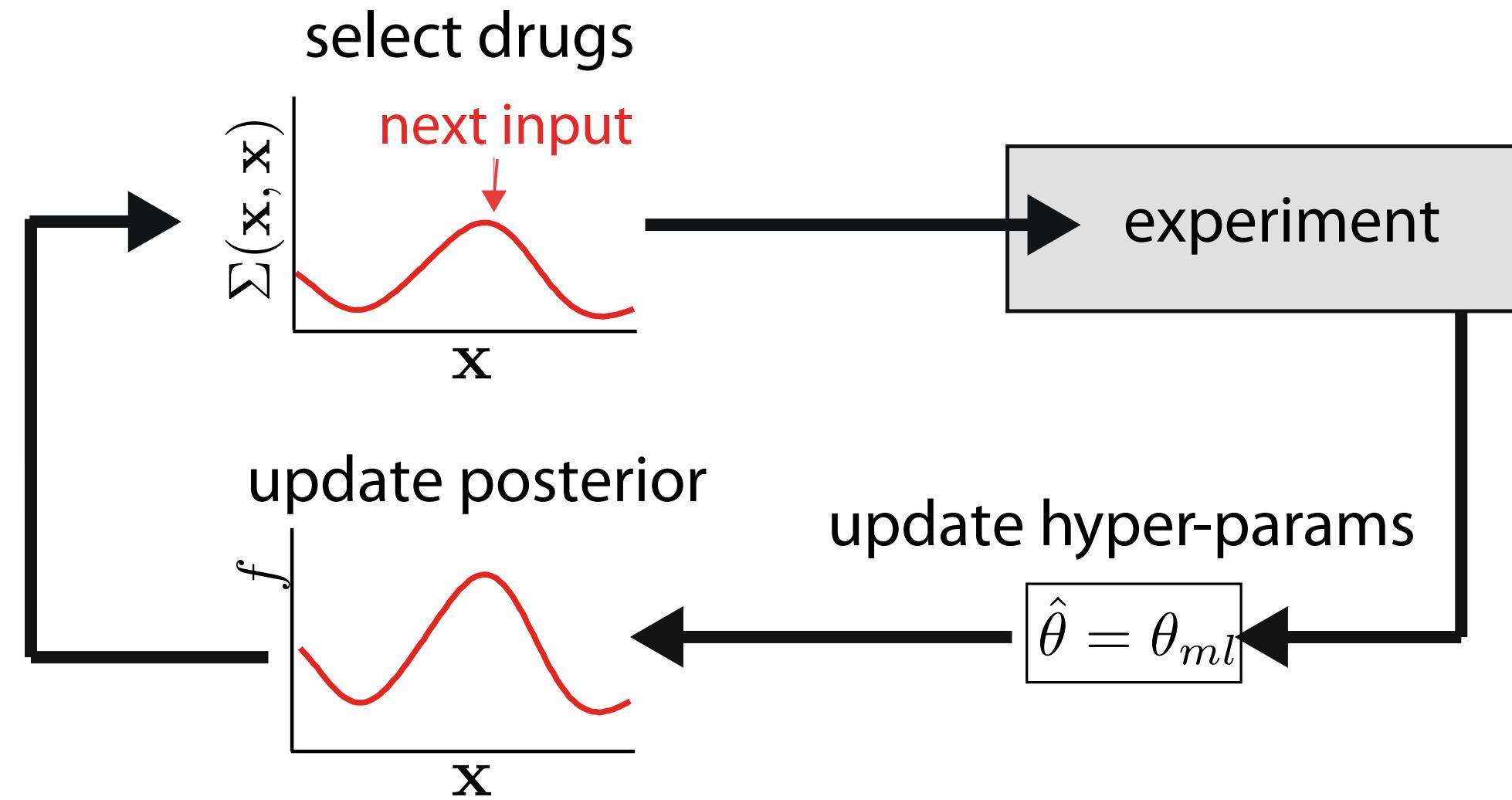
$$\theta_{ml} = \arg \max_{\theta} P(\mathbf{y}|\theta) = \int P(\mathbf{y}|X, \mathbf{f})P(\mathbf{f}|X, \theta)d\mathbf{f}.$$

3. Info-theoretic Active Learning

- maximize expected info gain about f

$$\begin{aligned} \mathbf{x}^* &= \arg \max_{\mathbf{x}} \mathbb{E}_{p(y|\mathbf{x}, D_t)} [H(\mathbf{f}|D_t) - H(\mathbf{f}|D_t, \mathbf{x}, y)] \\ &= \arg \max_{\mathbf{x}} \Sigma(\mathbf{x}, \mathbf{x}) \quad \text{uncertainty sampling} \end{aligned}$$

- sequential active learning

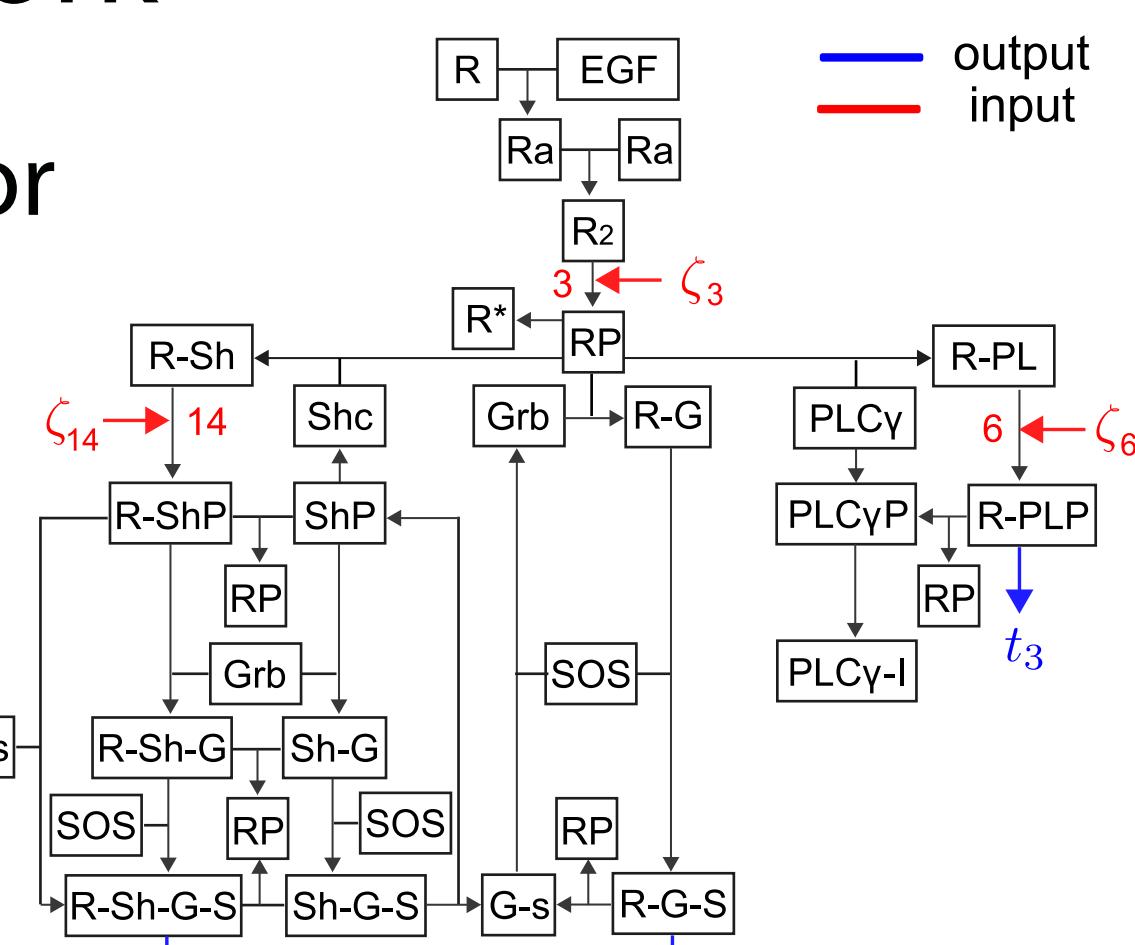


4. Application to EGFR network

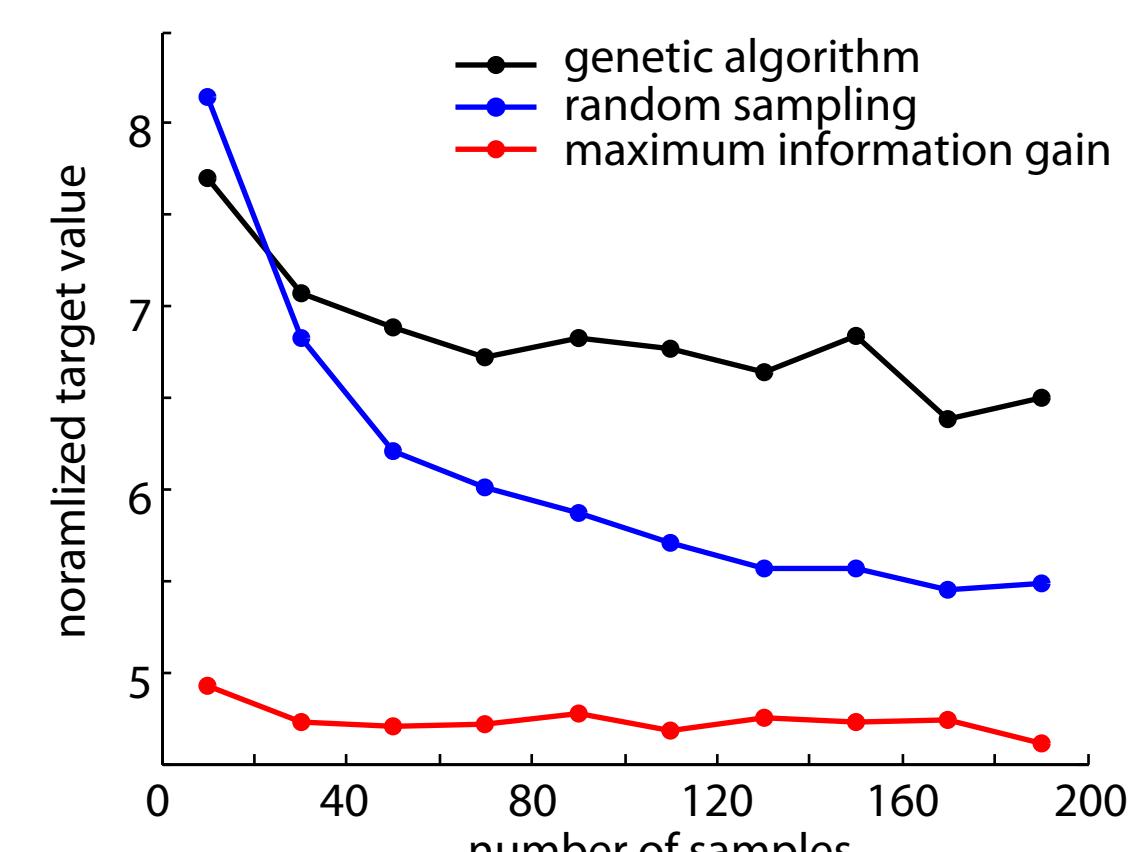
- Epidermal Growth Factor Receptor
- Inhibiting EGFR desired

select drugs

$$\text{minimizing target: } t = \exp\left(\sum_{i=1}^3 t_i\right)$$



5. Results



t_1, t_2, t_3 with best combinations

