Learn Something New

Supervised Learning -- Revisited

A **supervised** model has following parts:

- **Data**: X and Y
- **Parameters**: some variables you are trying to learn/fit/optimize.
- **Hyper-parameters**: some **pre-set** macros which controls model complexity and/or model behavior. For example
  - **Polynomial regression**: order n
  - **Multi-dimensional linear regression**: kernels, regularization parameter λ, regularization type L1/L2
  - **Random Forest**: `n_estimators`, `max_depth`, etc.
  - **Neural Network**: learning rate, activation functions, drop-out ratio, etc.
- **Algorithm**: i.e., which model? **A hyper-parameter**. Examples:
  - Additive or multiplicative
  - Decision tree
  - Support vector machine
  - Ensembles
  - ...
- **Loss function**: **Also a hyper-parameter**. Common loss function:
  - Mean square error: regression
  - Mean absolute error: regression
  - Cross entropy: classification
  - negative log-Likelihood function: probabilistic models
  - Gram matrix: style transfer
  - Regularization (can be add to any loss)
    - **AIC/BIC**: $||\beta||_0$ for simpliness
    - **L1**: $||\beta||_1$ for sparse-ness
    - **L2**: $||\beta||_2$ for small, non-zero coefficient
    - **Early stopping**: regularization in time
    - **Share parameter**: e.g., recurrent/convolutional network
    - ...
- **Optimizer**: **Again, a hyper-parameter**. How to find the best numerical solutions? For

example:

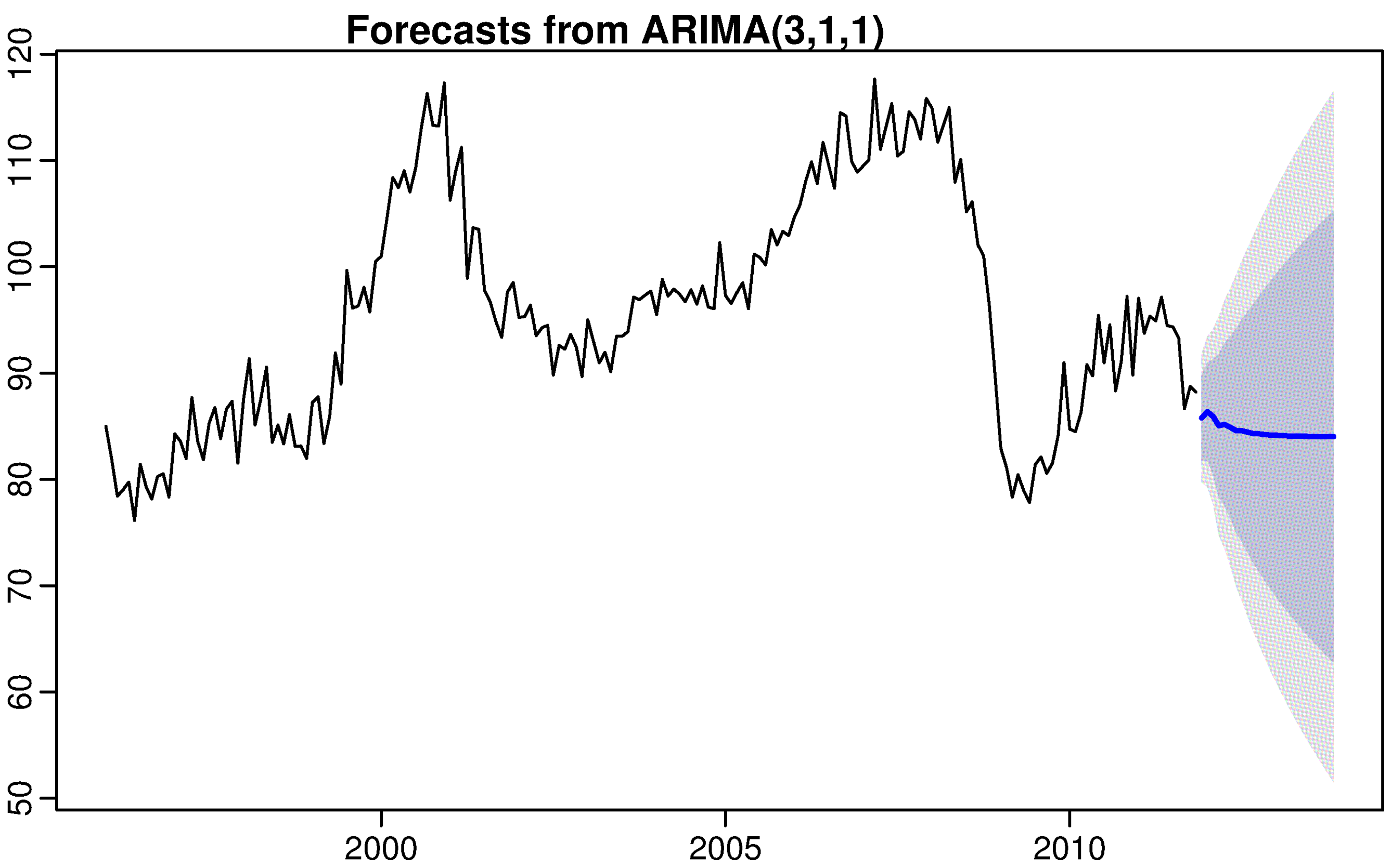
- Random guess
- Closed-form solution
- Gradient-based optimization
- Genetic algorithm

Long-term Forecasting in Machine Learning World

Question: Given a time-series y_t, What if we have want to forecast H steps further in the future?

Seasonal ARIMA?

- well-suited for short-term forecasts, not for longer term forecasts
- convergence of the autoregressive part



Let's use ML

Still assume **assume** y_t follows some additive autoregressive models:

$$y_{t+1} = f(y_t, \ldots, y_{t-n+1}) + \epsilon_t$$

- **Note I didn't assume stationarity here.** (Why?)
- $f(\cdot)$ can be any machine learning model with
    - $X = [\vec{y}_t, \ldots, \vec{y}_{t-n+1}]$
    - $Y = \vec{y}_{t+1}$
    - To be more specific:

$$X = \begin{bmatrix} y_t & y_{t-1} & \cdots & y_{t-n+1} \\ y_{t-1} & y_{t-2} & \cdots & y_{t-n} \\ \vdots & \vdots & \ddots & \vdots \\ y_n & y_{n-1} & \cdots & y_1 \end{bmatrix}, Y = \begin{bmatrix} y_{t+1} \\ y_t \\ \vdots \\ y_{n+1} \end{bmatrix}$$

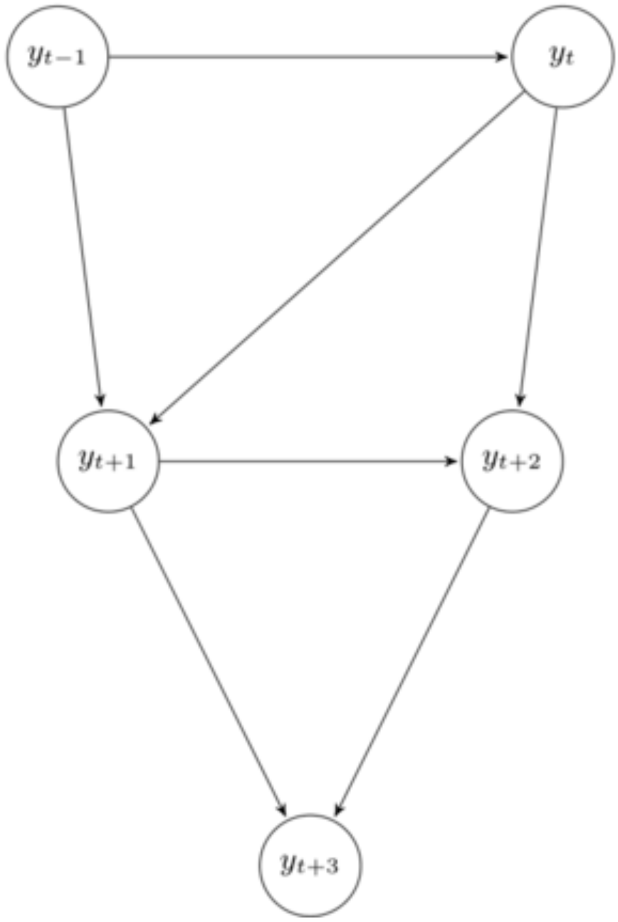
    - Using Sklearn syntax: `f = model.fit(X, Y)`
- When $H = 1$, any ML models can take care of.
- When $H > 1$, things become more interesting. Three possible solutions presented here.
- **Assume $n = 2$ from now on.**

Solution 1: Iterated forecasting

We forecast y's one at a time.

$$\hat{y}_{t+1} = f(y_t, y_{t-1}) \hat{y}_{t+2} = f(y_{t+1}, y_t) \vdots \hat{y}_{t+H} = f(y_{t+H-1}, y_{t+H-2})$$

Conditional dependency structure in time series

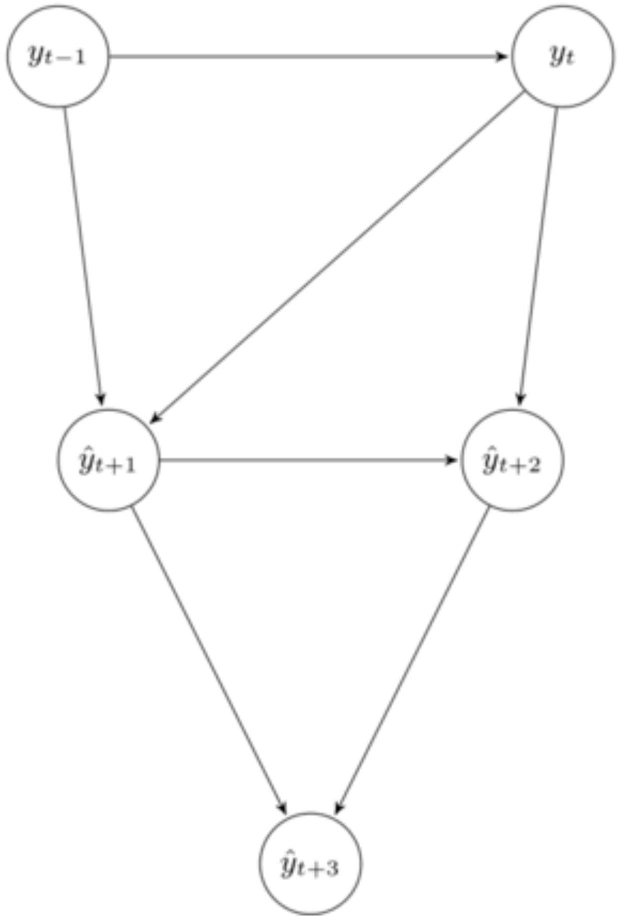


However, we are standing at time t. We don't know anything at $t+1$!

We need to replace the future by our estimates!

$$\hat{y}_{t+1} = f(y_t, y_{t-1}) \hat{y}_{t+2} = f(\hat{y}_{t+1}, y_t) \vdots \hat{y}_{t+H} = f(\hat{y}_{t+H-1}, \hat{y}_{t+H-2})$$

Iterated modelling of conditional dependencies

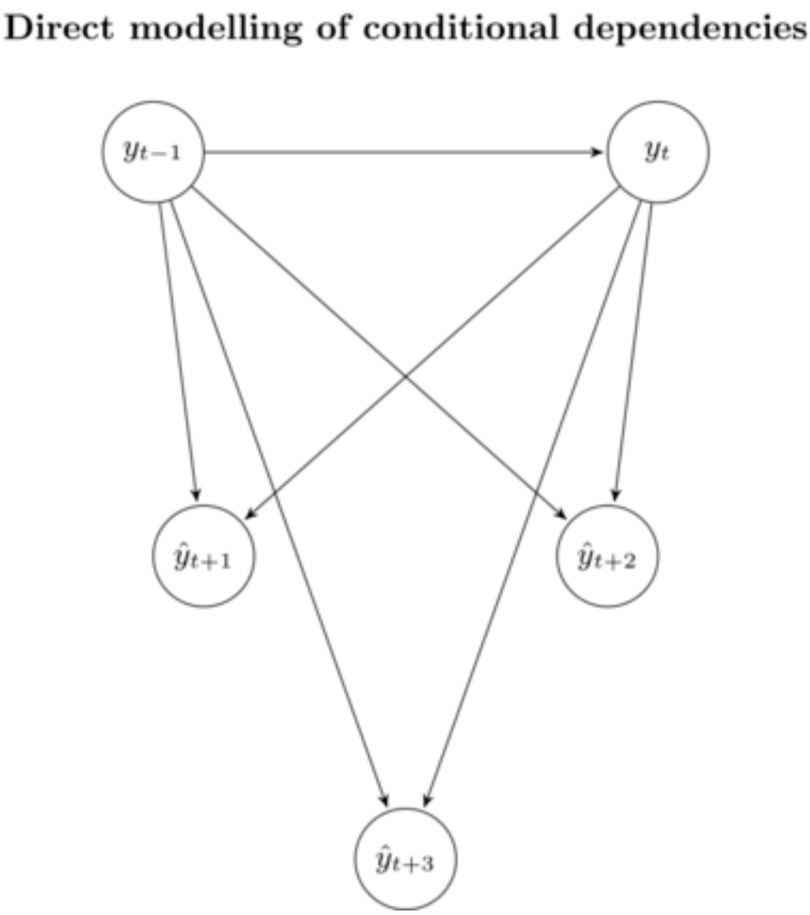


- **An unbiased estimator of** $\mathrm{E}[y_{t+1:(t+H)} \mid y_t]$, since it preserves the stochastic dependencies of the underlying data.
- **Bias-variance trade-off**: suffers from high variance due to the **accumulation of error in the individual forecasts.**
- Low performance over longer time horizons H.
- When we have additional inputs, x_t, we need to forecast $\hat{x}_{t+h}$ as well!

Solution 2: H-step ahead forecasting

Learn H different models:

$$\hat{y}_{t+1} = f_1(y_t, y_{t-1}) \hat{y}_{t+2} = f_1(y_t, y_{t-1}) \vdots \hat{y}_{t+H} = f_H(y_t, y_{t-1})$$



- Does NOT suffer from the accumulation of error.
- **Models are trained independently**, no statistical dependencies between the predicted values y_{t+h} are guaranteed.

Solution 3: Multiple input multiple output (MIMO) models

One model fits all.

$$[\hat{y}_{t+H}, \ldots, \hat{y}_{t+1}] = f(y_t, y_{t-1})$$

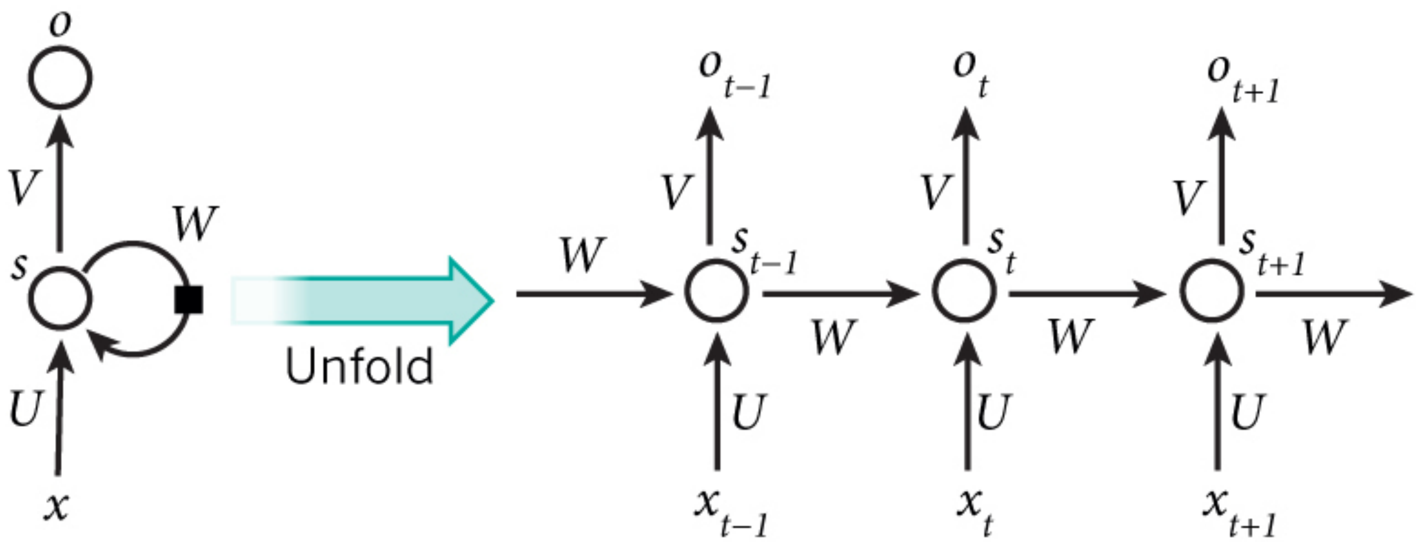
- No conditional independence assumptions are made.
- No accumulation of error of individual forecasts.
- All horizons H are forecasted with the same model, which **limits flexibility**.

Summary

- No free lunch.
- Going to traditional ML means no uncertainty estimates.
- Work-around: bootstrap or Bayesian regression (computationally $$)

How to decide n?

- **Small n**: simpler model, restricted explainability. Unlikely to capture the full seasonality.
- **Big n**: complex model, easy to overfit, don't know where to stop.
- n usually is a hyper-parameter to tune.
- Or, use a recurrent model (i.e., $n = \infty$)



Hyperparameter Tuning

The most time-costly thing you will ever encounter in ML!

Model training

When you hear

> Let's train a model ... -- Your future boss

it means:

1. Choose a set of hyper-parameter:
   - **Regularizer** λ
   - **Model** $f(\cdot)$
   - **Loss** $L(y, \hat{y})$
   - **Optimizer**
2. Prepare dataset, X and Y
3. A supervised model, with parameters θ, can be thus defined as

$$\hat{Y} = f_\lambda(X, \theta)$$

4. Use optimizer to solve

$$\theta^* = \text{argmin}_\theta L(Y, \hat{Y})$$

Model evaluations

Hyper-parameter space is (almost) infinite and non-convex. There will always be a better model:

- Impossible to achieve global maximum
- Gradient-base method cannot be used at hyper-parameter level (not always true -- Learning to learn by gradient descent by gradient descent)

Given we have some models (with their own hyper-parameters), **how do we compare them?**

- Define an evaluation metric
  - Sharpe Ratio
  - PnL
  - Accuracies
  - Click-through rate (recommendation system)
  - ETA (dispatch system)
  - ...
- Train these models on a training set
- Evaluate on a validation set
- Pick the best model(s) with best performance on the validation set
- (Optional) Re-train the model(s) on train + validation set

Question: How do we choose finite models out of the infinite model domain?

Time is money

Some benchmarks of training a model (i.e., a set of hyper-parameter) with < 10G of data:

- **Linear regressions**: gradient method, parallelizable, <1min
- **Random forest**: gradient method, parallelizable, ~10min
- **Boostings**: gradient method, cannot be parallelized, <1h

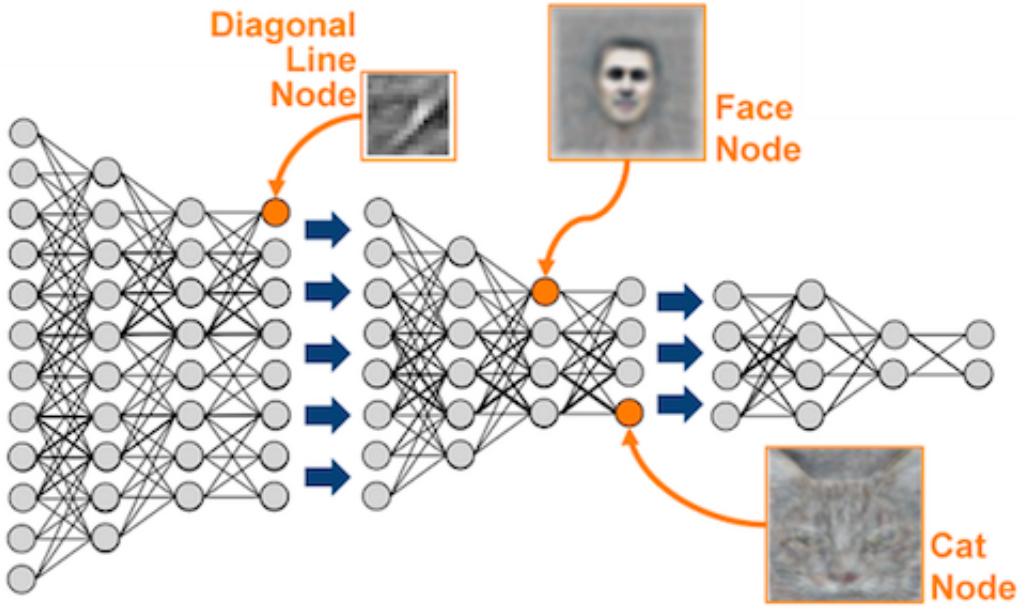
Above have well-defined functional forms. What if

- $f(\cdot)$ is explicitly unknown and multimodal.
- Evaluations of $f(\cdot)$ may be perturbed (non-convex).

- Evaluations of $f(\cdot)$ are expensive.

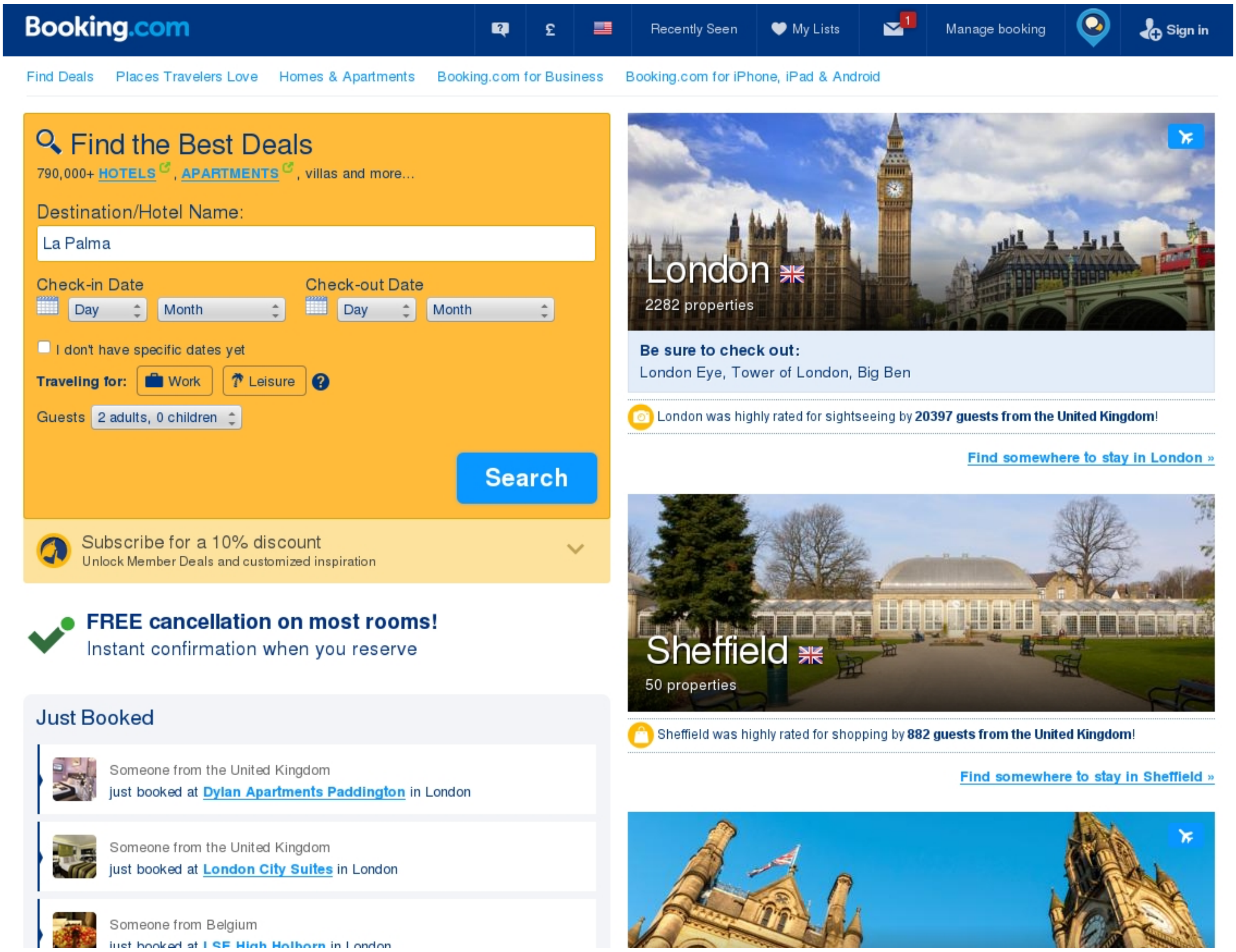
Such as

- **Neural networks**: hours ~ days

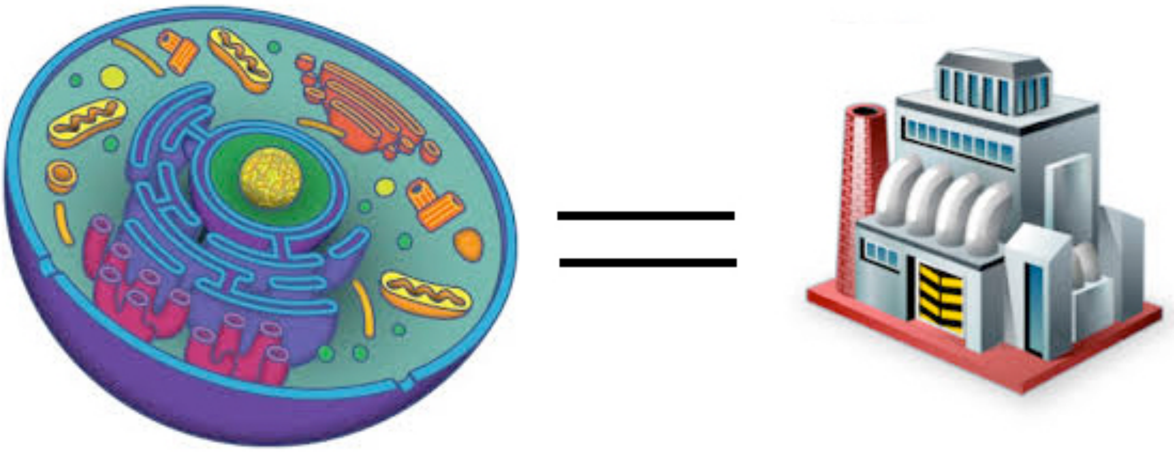


- **Dispatch algo**: hours

- **A/B Testing**: days



- **Design of experiments: gene optimization**: years?



What are we aiming for: Get a **good-enough model** with as fewer try as possible

Option 1: Use previous knowledge

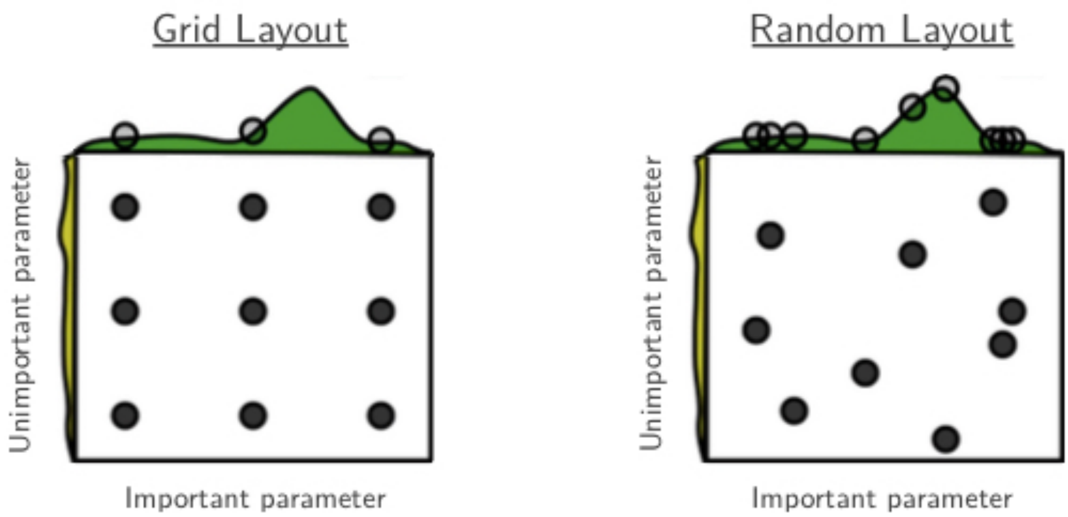
To select the parameters at hand. Perhaps not very scientific but still in use...

Option 2: Grid search

- A brute force way to iterate through all possibilities.
- Sklearn API
- How to grid search?
  - discrete variables: simple iterate
  - continuous variable
    - uniform grid (e.g., hidden dimensions)
    - log grid (e.g., learning rate)
- **Curse of dimensionality!**

Option 3: Random search

- Some hyper-parameters are useless (won't improve model performace)
- Better than grid search in various senses but still expensive to guarantee good coverage.



Question: Can we do better?

Option 4: Bayesian optimization

Given fixed data-set, X and Y, and pre-specified evaluation metric, $L[f_\lambda(x, \theta), y]$, **hyper-parameter and model performance is a mapping**.

Goal: fit a function (i.e., another model), $g : \lambda \to L(f_\lambda(X_{val}, \theta), Y_{val})$

- g is a non-parametric **meta-model**.
- We can only afford very few "training data" (i.e., hyper-param search) to fit g -- **Bayesian**

models are better.
- **State-of-art**: Gaussian Process
- **Illustration** here
  - **Simple idea**: p8-17
  - **Simple algo**: p34-40
  - **Why doesn't everyone use this**: p41

Proper Backtesting

> A **quantitative trading strategy** is indeed a **hyper-parameter** -- Frank Xia
>
> **Backtesting**: validation/hyper-param tuning through time -- Frank Xia

- How to split data **correctly** (Draw on white board)
- Retrain on train+val is a **must** (when is not a must?)
- Robust backtesting
  - **Rolling backtest**: how to avoid **beginner's luck**?
  - **Model ensemble**: how to reduce variance and seasonality? -- what do ensemble?

> It's a miracle when **loss function** and **evaluation metric** match. -- Frank Xia

- To pick a proper loss function -- an art or a science?