Bayesian Optimisation

Cédric Archambeau
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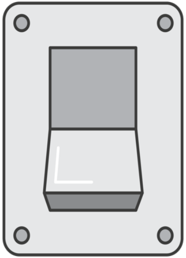
Imperial College, London, 2017

Democratising machine learning



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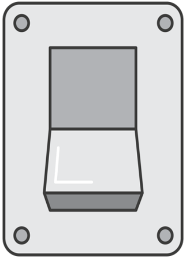

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- Abstract away feature engineering

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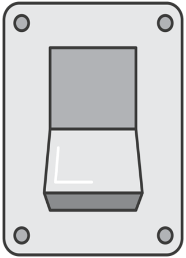

- Abstract away algorithms
- Abstract away feature engineering
- Abstract away memory constraints
- Abstract away network constraints
- Abstract away computing infrastructure

Machine learning aims to estimate (`learn`) a statistical data model to make predictions (`generalise`) about unseen data

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   `Spam detection:`

   - Is this a (binary) classification problem?
   - Shall I use logistic regression or a SVM?
   - How should I represent emails?

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   - Iterative least squares?
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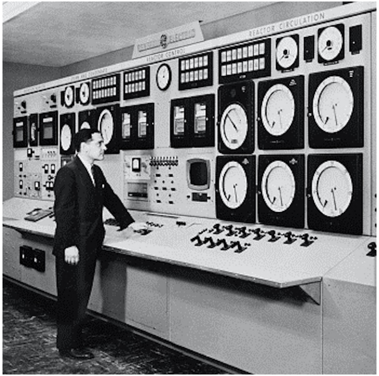
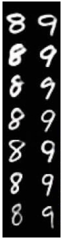
   - Adagrad?
3. Make predictions about new data with the trained model
   `Decide if this new email is spam or not?`
   - Shall I optimise for precision?
   - Shall I optimise for recall?

The performance of machine learning depends on meta-parameters that have to be tuned with care...

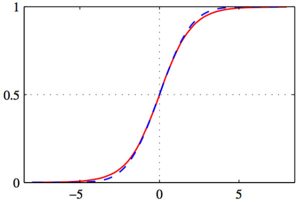


- Regularisation and (hyper)priors
- Optimisation and sampling
- Feature extraction
- Model complexity
- Decision

A toy example: digit classification with (binary) logistic regression



MNIST



Sigmoid: $\sigma(z) = \frac{1}{1+\exp(-z)}$.

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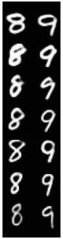

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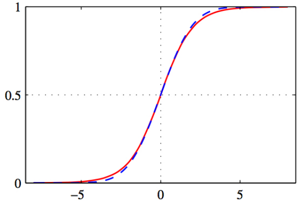

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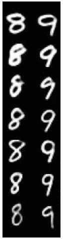

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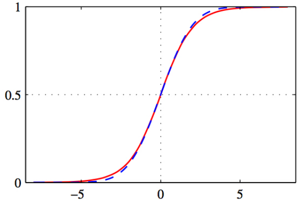

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- Logistic link: $P(t = \text{“8”}) = \sigma(y(\boldsymbol{x}))$.
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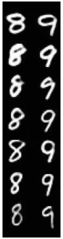

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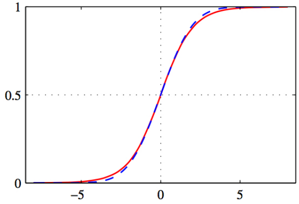

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- Likelihood: $P(t_1, \dots, t_n) = \prod_{i=1}^{n} \mathrm{Bernoulli}\,(P(t_n))$.
- Prior: $P(\boldsymbol{w}) = \mathrm{Gaussian}(\boldsymbol{0}, \lambda \boldsymbol{I})$.

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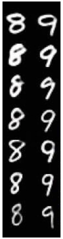

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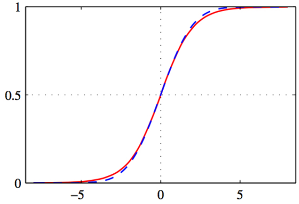

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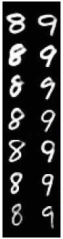

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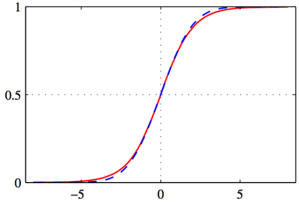

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$$f : \boldsymbol{x} = (\#\text{epochs, learning rate, amount of regularisation}) \mapsto f(\boldsymbol{x}) = \text{AUC}$$

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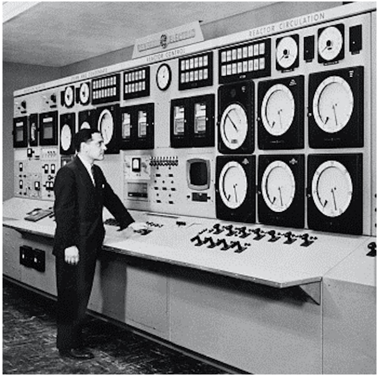

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These parameters are known as hyperparameters or system parameters and are tuned by human experts.

A second example: Is a product review `positive` or `negative`?

A Knight of the Seven Kingdoms (A Song of Ice and Fire)

$20.43 | In Stock. Ships from and sold by Amazon.com. Gift-wrap available.

★★★★★ **I quickly became absorbed in the tales of "Dunk and Egg" and the ancestors of the great houses of Westeros**

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Comment | 3 people found this helpful. Was this review helpful to you? Yes No Report abuse

★★★☆☆ **A taste of game of thrones before 6th book!**

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- That's a binary classification problem!
- Logistic regression model with standard text features.

Revisiting sentiment analysis [YS15]

Hyperparameter	Values
n_{min}	$\{1, 2, 3\}$
n_{max}	$\{n_{min}, \ldots, 3\}$
weighting scheme	{tf, tf-idf, binary}
remove stop words?	{True, False}
regularization	$\{\ell_1, \ell_2\}$
regularization strength	$[10^{-5}, 10^{5}]$
convergence tolerance	$[10^{-5}, 10^{-3}]$

Revisiting sentiment analysis [YS15]

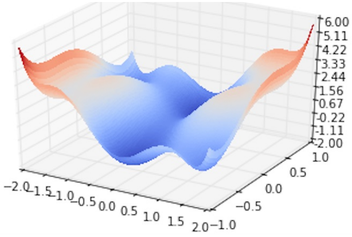
Method	Acc.
SVM-unigrams	88.62
SVM-$\{1,2\}$-grams	90.70
SVM-$\{1,2,3\}$-grams	90.68
NN-unigrams	88.94
NN-$\{1,2\}$-grams	91.10
NN-$\{1,2,3\}$-grams	91.24
LR (this work)	91.56
Bag of words CNN	91.58
Sequential CNN	92.22

Table 5: Comparisons on the Amazon electronics dataset. Scores are as reported by Johnson and Zhang (2014).

Acc.: accuracy

SVM: support vector machine
NN: neural network
LR: logistic regresion
CNN: convolutional neural network

Black-box optimisation



- The function f we wish to optimise can be non-concave.
- The number of hyperparameters p is moderate (typically < 20).

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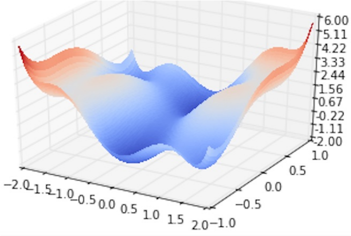

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- The number of hyperparameters p is moderate (typically < 20).

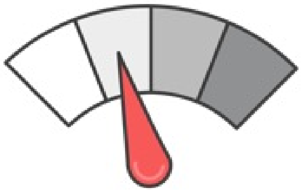
Our goal is to solve the following optimisation problem:

$$\boldsymbol{x}_\star = \operatorname*{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}).$$

- Evaluating $f(\boldsymbol{x})$ is expensive.
- No analytical form or gradient.
- Evaluations may be noisy.

Global optimisation for hyperparameter optimisation

1. Define an objective or metric to optimise
   E.g.: generalisation error
2. Identify the knobs that impact this objective
   E.g.: hyperparameters
3. Measure the quality of configurations
   E.g.: cross-validation



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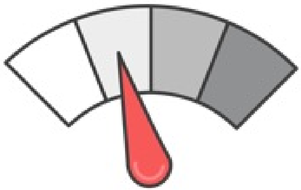
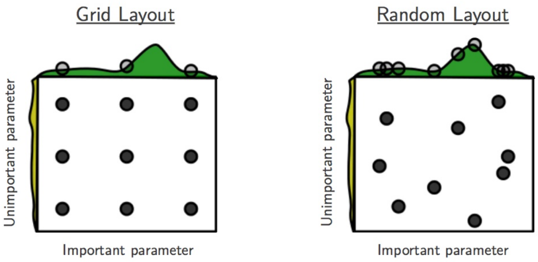


This requires iterating over hyperparameter configurations.

Two straightforward approaches



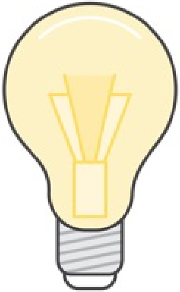
(Figure by Bergstra and Bengio, 2012)

- Exhaustive search on a regular or random grid
- Complexity is exponential in p
- Wasteful of resources, but easy to parallelise

Can we do better?

(Banksy, London)

Bayesian optimisation



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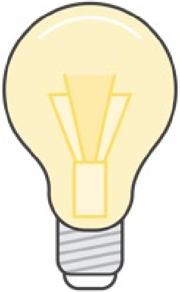
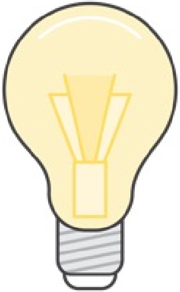


Global optimisation technique that adopts a probabilistic approach:

Bayesian optimisation



Global optimisation technique that adopts a probabilistic approach:

1. Builds a probabilistic model of the objective:
   - Optimises a proxy instead of the objective
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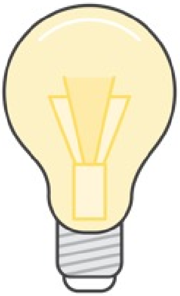

Global optimisation technique that adopts a probabilistic approach:

1. Builds a probabilistic model of the objective:
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   - Models the uncertainty
2. Performs an efficient grid search by balancing exploration against exploitation!

Questions?

Bayesian (black-box) optimisation [MTZ78, SSW+16]

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Bayesian (black-box) optimisation [MTZ78, SSW+16]

$$x_\star = \operatorname*{argmin}_{x \in \mathcal{X}} f(x)$$

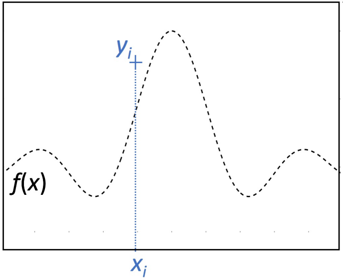
Canonical algorithm:

- Surrogate model $\mathcal{M}$ of f `#cheaper to evaluate`
- Set of evaluated candidates $\mathcal{C} = \{\}$
- While some `BUDGET` available:
  - Select candidate $\mathbf{x}_{\text{new}} \in \mathcal{X}$ using $\mathcal{M}$ and $\mathcal{C}$ `#exploration/exploitation`
  - Collect evaluation y_{new} of f at $\mathbf{x}_{\text{new}}$ `#time-consuming`
  - Update $\mathcal{C} = \mathcal{C} \cup \{(\mathbf{x}_{\text{new}}, y_{\text{new}})\}$
  - Update $\mathcal{M}$ with $\mathcal{C}$ `#Update surrogate model`
  - Update `BUDGET`

Bayesian (black-box) optimisation with Gaussian processes [JSW98]

1. Learn a probabilistic model of f, which is cheap to evaluate:

$$y_i | f(\boldsymbol{x}_i) \sim \mathrm{Gaussian}\left(f(\boldsymbol{x}_i), \varsigma^2\right), \qquad\qquad f(\boldsymbol{x}) \sim \mathcal{GP}(0, \mathcal{K}).$$



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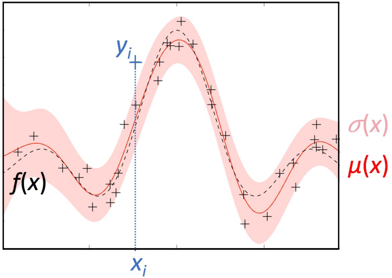

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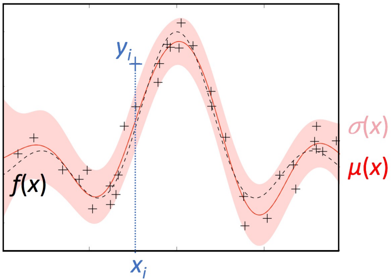

3. Repeatedly query f by balancing **exploitation** against **exploration**!

Ingredient 1: Gaussian processes for regression [RW06]

- A **multivariate Gaussian** is density over D random variables based on correlations:

$$\boldsymbol{f} \equiv (f_1, \ldots, f_D)^\top \sim \mathrm{Gaussian}\left(\boldsymbol{m}, \boldsymbol{K}\right).$$

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- A **Gaussian process** generalises the a multivariate Gaussian to infinitely many variables:

$$f(\boldsymbol{x}) \sim \mathcal{GP}\left(m(\boldsymbol{x}), k(\boldsymbol{x}, \cdot)\right).$$

  - It defines a probability measure over random functions.
  - The joint density of any finite subset is a consistent Gaussian density.

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- The **posterior process** is again a Gaussian process (if Gaussian likelihood):

$$f(\boldsymbol{x})|\boldsymbol{y} \sim \mathcal{GP}\left(\mu(\boldsymbol{x}), \Sigma(\boldsymbol{x}, \cdot)\right),$$

  where

$$\mu(\boldsymbol{x}) = \boldsymbol{k}_N^\top(\boldsymbol{x})(\boldsymbol{K}_N + \sigma^2 \boldsymbol{I}_N)^{-1}\boldsymbol{y},$$
$$\sigma(\boldsymbol{x})^2 = k(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{k}_N^\top(\boldsymbol{x})(\boldsymbol{K}_N + \sigma^2 \boldsymbol{I}_N)^{-1}\boldsymbol{k}_N(\boldsymbol{x}).$$

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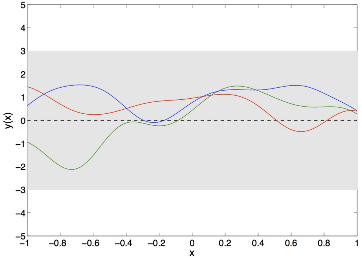
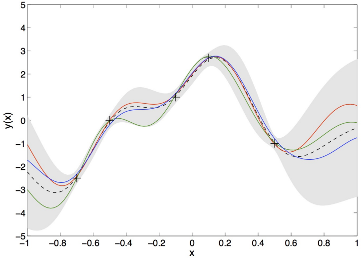


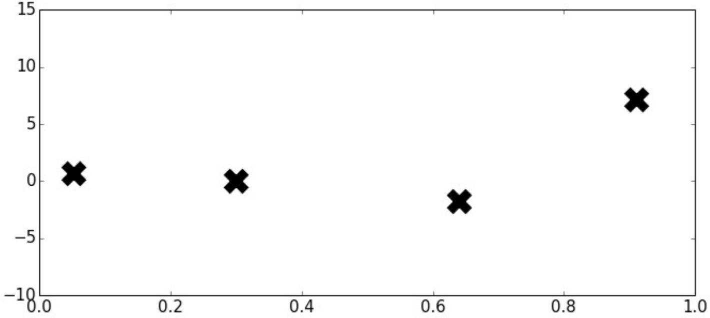
Prior.



Posterior.

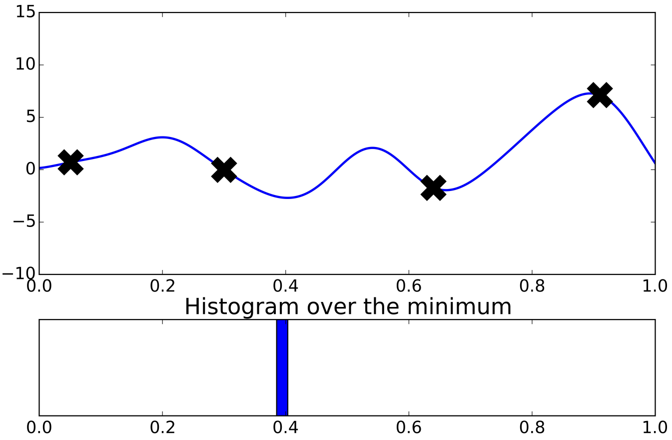
Three random functions generated from (a) the prior GP and (b) the posterior GP. An observation is indicated by a $+$, the mean function by a dashed line and the 3 standard deviation error bars by the shaded regions. We used a squared exponential covariance function.

Where is the minimum of f?



(Image credit: Javier González)

Intuitive solution



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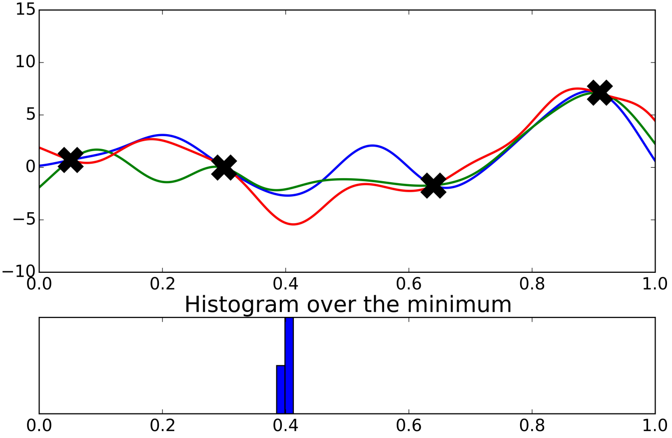

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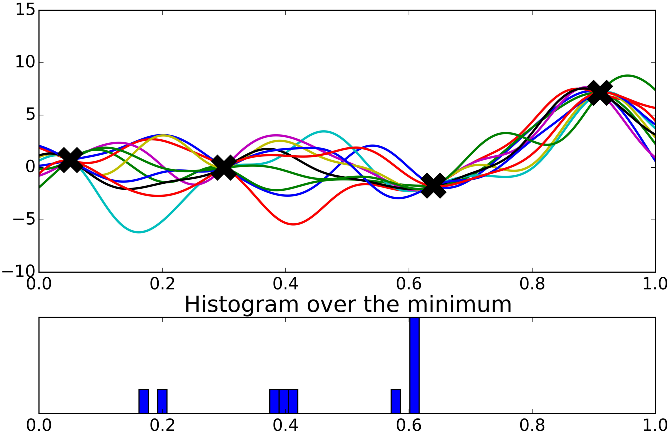

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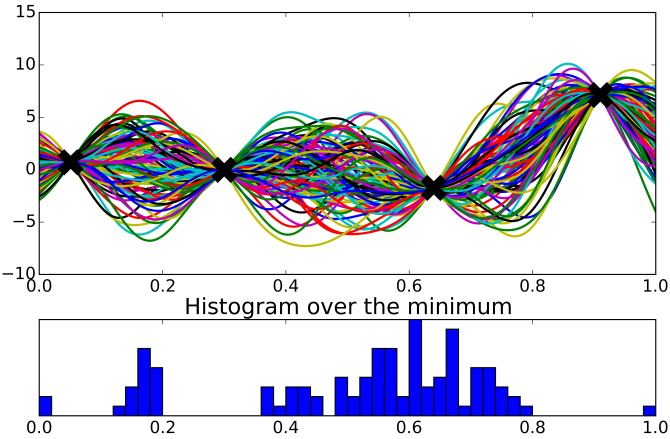

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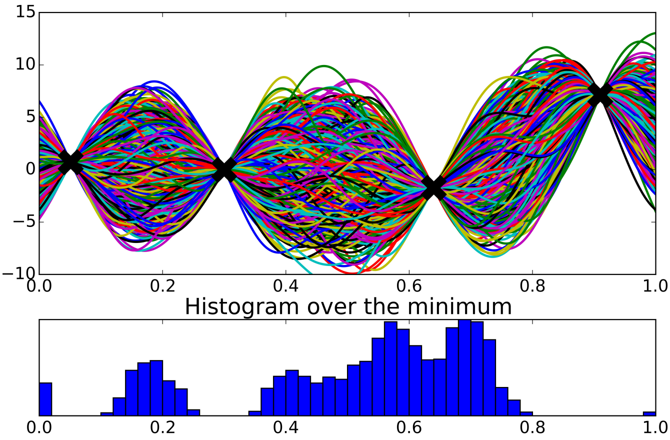

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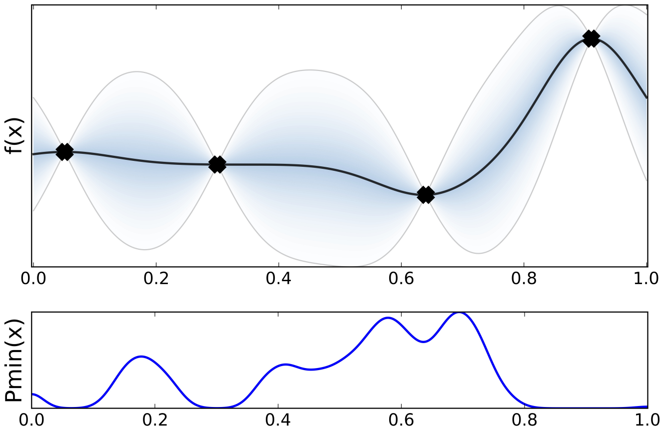

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Ingredient 2: Acquisition function

Let $\mathcal{C} = \{\boldsymbol{x}_c, y_c\}$ denote a set of observed parameter-value pairs. The acquisition function is defined as follows:

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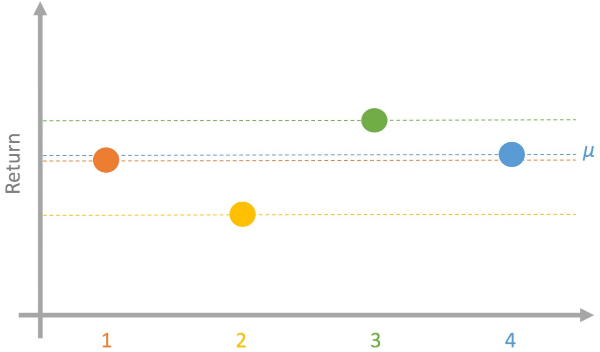
Exploration-exploitation trade-off

Which slot machine should I pick?

Exploration-exploitation trade-off



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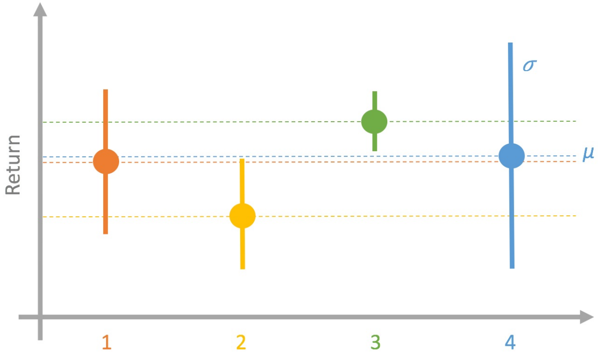

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Ingredient 2: Acquisition function

- Evaluate all candidates according to an **acquisition function** $a(\boldsymbol{x})$.
- Rank them and pick the best one.

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  - Lower confidence bound (GP-LCB) [SKKS09]:

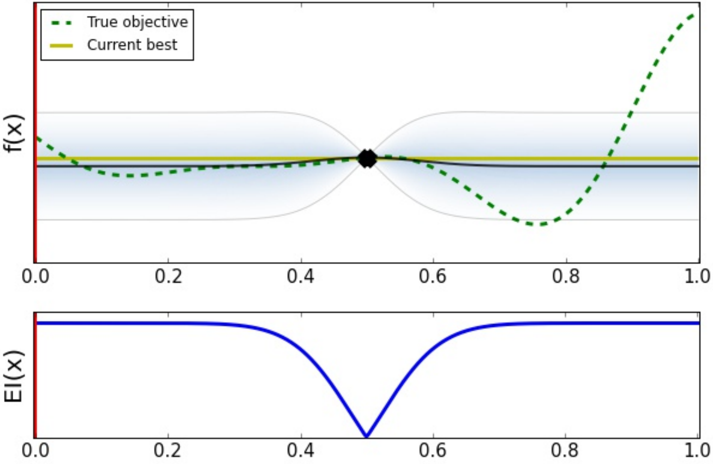
  $$a(\boldsymbol{x}) = -\mu(\boldsymbol{x}) + \alpha\sigma(\boldsymbol{x}) \quad (\alpha \geqslant 0).$$

  - **Expected improvement** (EI):

  $$a(\boldsymbol{x}) = \mathbb{E}\left(\max\{0, y_\star - f(\boldsymbol{x})\}\right).$$

  - Probability of improvement, Thompson sampling, entropy search, etc.

Bayesian optimisation in action



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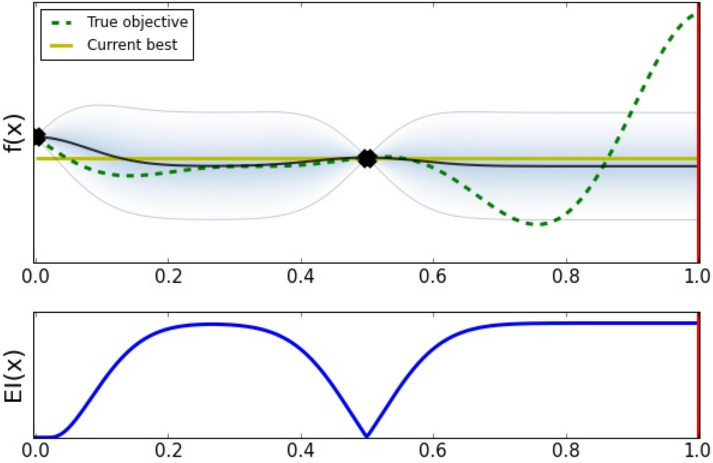

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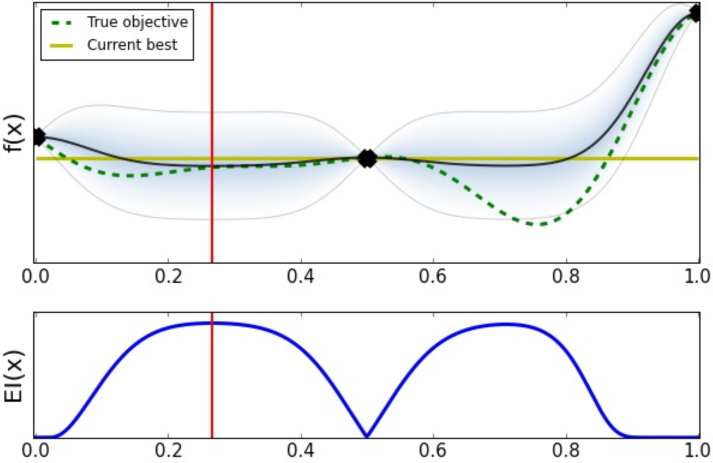

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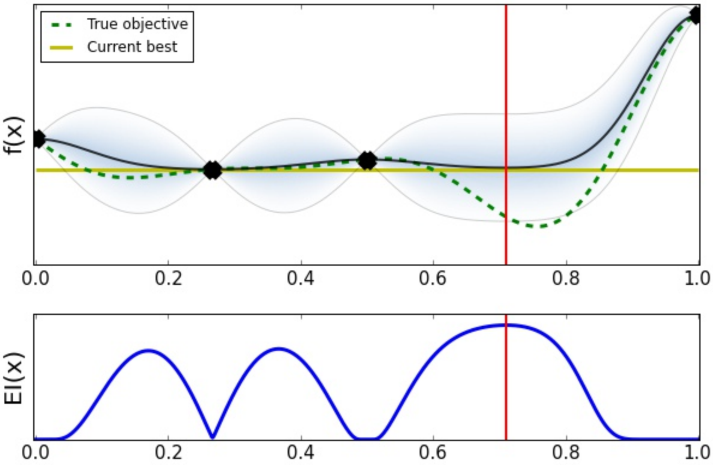

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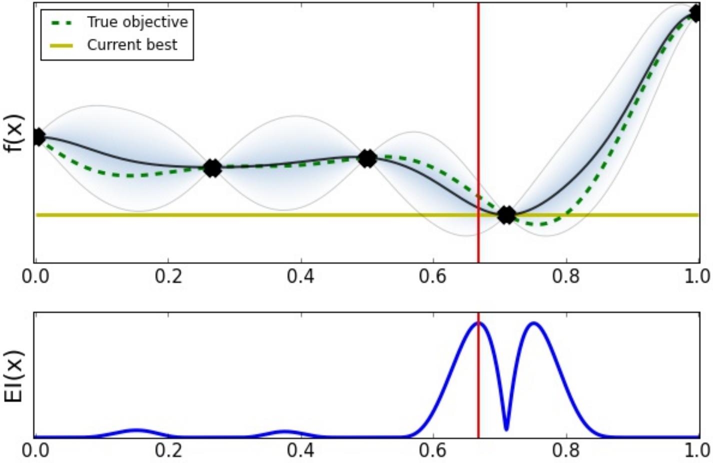

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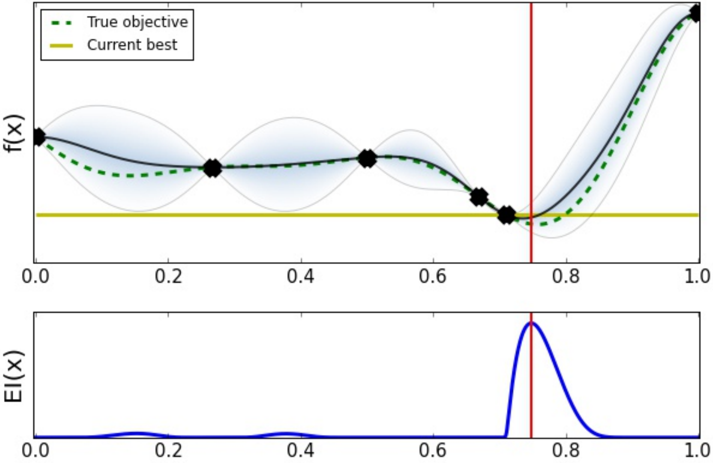

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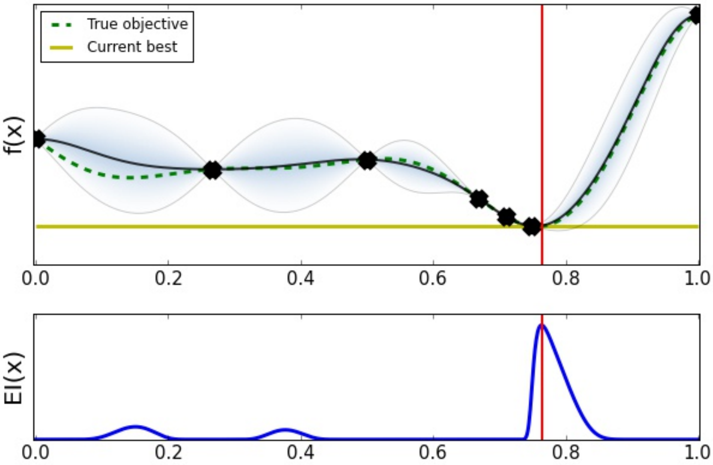

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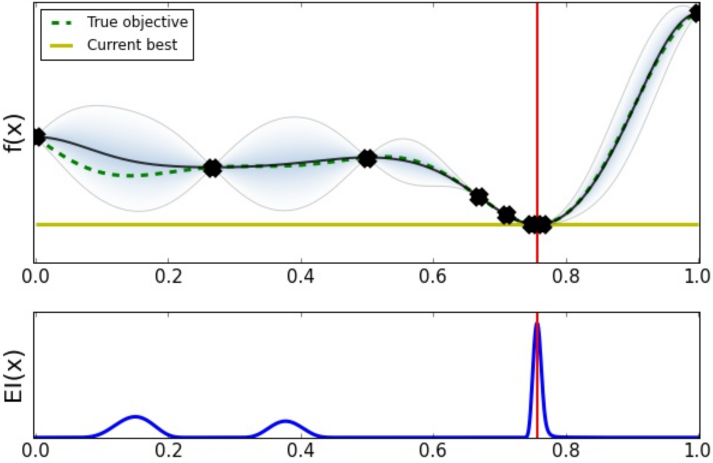

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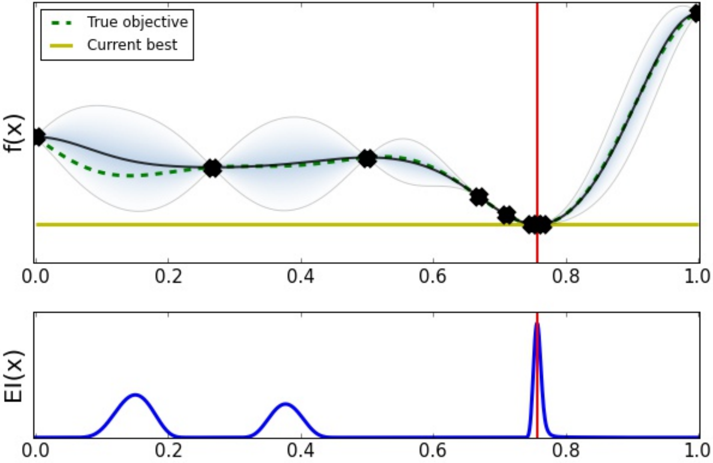

(Image credit: Javier González)

Summary

$$\boldsymbol{x}_\star = \underset{\boldsymbol{x} \in \mathcal{X}}{\operatorname{argmin}} \; f(\boldsymbol{x})$$

Bayesian optimisation algorithm:

- Surrogate model $\mathcal{M}$ of f `#cheaper to evaluate`
- Set of evaluated candidates $\mathcal{C} = \{\}$
- While some `BUDGET` available:
  - Select candidate $\mathbf{x}_{\text{new}} \in \mathcal{X}$ using $\mathcal{M}$ and $\mathcal{C}$ `#acquisition`
  - Collect evaluation y_{new} of f at $\mathbf{x}_{\text{new}}$ `#time-consuming`
  - Update $\mathcal{C} = \mathcal{C} \cup \{(\mathbf{x}_{\text{new}}, y_{\text{new}})\}$
  - Update $\mathcal{M}$ with $\mathcal{C}$ `#GP posterior`
  - Update `BUDGET`

Questions?

How do we handle the hyperparameters of the surrogate model?

How do we handle the hyperparameters of the surrogate model?

Let us denote the kernel parameters by $\boldsymbol{\theta}$. We view the latent functions as nuisance parameters and maximise the log-marginal wrt ς^2 and $\boldsymbol{\theta}$.

The **log-marginal likelihood** is given by

$$\ln p(\boldsymbol{y}|\varsigma, \boldsymbol{\theta}) = -\frac{n}{2}\ln 2\pi \underbrace{-\frac{1}{2}\ln|\boldsymbol{K}(\boldsymbol{\theta}) + \varsigma^2 \boldsymbol{I}_n|}_{\text{complexity penality}} \underbrace{-\frac{1}{2}\boldsymbol{y}^\top(\boldsymbol{K}(\boldsymbol{\theta}) + \varsigma^2 \boldsymbol{I}_n)^{-1}\boldsymbol{y}}_{\text{data fit}}.$$

The negative log-marginal surface is non-convex and the computational complexity for its evaluation is $\mathcal{O}(n^3)$.

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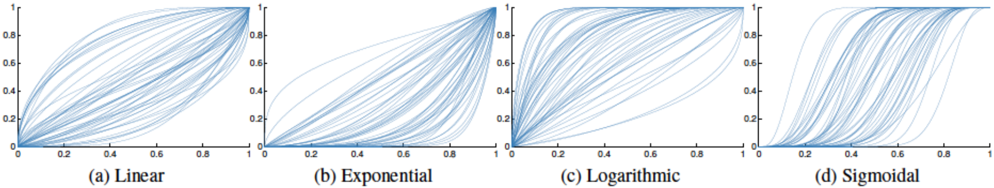

(Image credit: Snoek, et al., 2014)

- Automatic input **warping** [SSZA14]:

$$\omega : x \mapsto \omega(x) = \mathrm{BetaCDF}(x; \alpha, \beta).$$

- Learn α and β as the hyperparameters of the Gaussian process.
- Many alternatives, such as Kumaraswamy distribution: $\omega(x) = 1 - (1 - x^{\alpha})^{\beta}$.

How do we fill the hyperparameter space $\mathcal{X}$?

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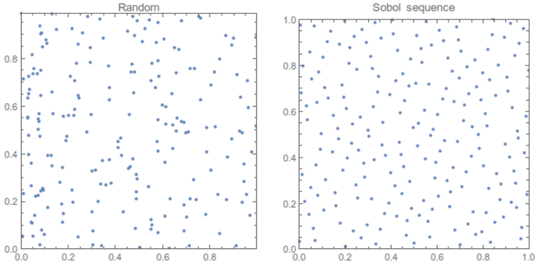

(Image credit: Wikipedia)

- Populate hypercube $[0,1]^D$ as densely as possible (as well as it's lower dimensional faces):

$$\text{Find sequence } \{\boldsymbol{x}_i\} \text{ such that } \lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i) = \int_{[0,1]^D} f(\boldsymbol{x}).$$

- Quasi random sequence generators, such as **Sobol sequences**, are better than random.

Are there other choices for the surrogate model?

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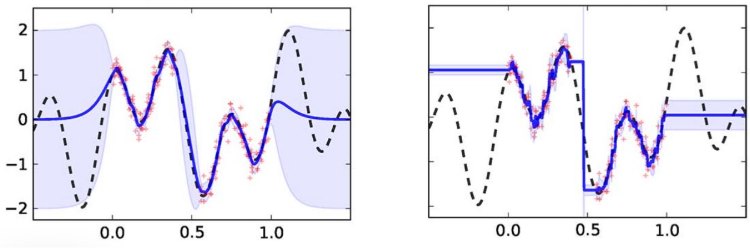

(Image credit: [SSW+16])

- Bayesian (black-box) optimisation with **Random Forests** [HHLB11]:

$$y(\boldsymbol{x}) = \mathrm{RF}, \qquad\qquad f(\boldsymbol{x})|\boldsymbol{y} \sim \mathrm{Gaussian}\left(\mu(\boldsymbol{x}), \Sigma(\mu(\boldsymbol{x}))\right).$$

  where $\mu(\boldsymbol{x}) \approx \frac{1}{B}\sum_i y_i(\boldsymbol{x})$ and $\Sigma(\boldsymbol{x}) \approx \frac{1}{B-1}\sum_i (y_i(\boldsymbol{x}) - \mu(\boldsymbol{x}))^2$.
- But very competitive baseline!

Reference material

Review paper by Shahriari, et al. (2016): Taking the Human Out of the Loop: A Review of Bayesian Optimization. *Proceedings of the IEEE 104(1):148–175*.

Slides by Ryan Adams (2014): A Tutorial on Bayesian Optimization for Machine Learning. *CIFAR NCAP Summer School*.

Slides by Peter Frazier (2010): Tutorial: Bayesian Methods for Global and Simulation Optimization. *INFORMS Annual Meeting*.

Very brief historical overview

- Closely related to optimal design of experiments, dating back to *Kirstine Smith* (1918).
- As Bayesian optimisation, studied first by *Kushner* (1964), then by *Mockus* (1978), and more recently by *Jones, et al.* (1998).

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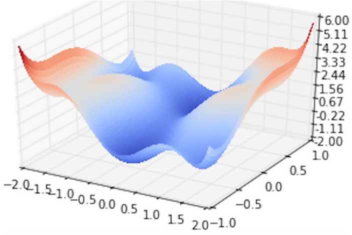
- Multiple workshops at NIPS (`bayesopt.com`) and ICML (`www.automl.org`)
- Open source software:
  SMAC (`http://www.cs.ubc.ca/labs/beta/Projects/SMAC/`) – RF,
  HyperOpt (`http://jaberg.github.io/hyperopt/`) – TPE,
  Spearmint (`https://github.com/JasperSnoek/spearmint`) – GP,
  GPyOpt (`https://github.com/SheffieldML/GPyOpt`) – GP,
  BayesOpt (`http://rmcantin.bitbucket.org/`) – GP,
- Challenges and benchmarks (HPOLib: `www.automl.org/hpolib.html`)!

Questions?

Black-box optimisation with (tree-structured) dependencies [JAGS17]



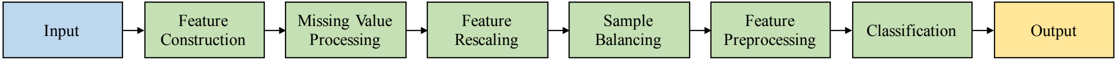
- The function f we wish to optimise can be non-concave.
- The number of hyperparameters p is moderate (typically < 20).

Our goal is to solve the following optimisation problem:

$$\boldsymbol{x}_\star = \operatorname*{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}).$$

- Evaluating $f(\boldsymbol{x})$ is expensive.
- No analytical form or gradient.
- Evaluations may be noisy.
- The domain $\mathcal{X}$ is structured.

Example 1: Data analytics pipeline [THHLB13, FKE+15, ZBSS16]



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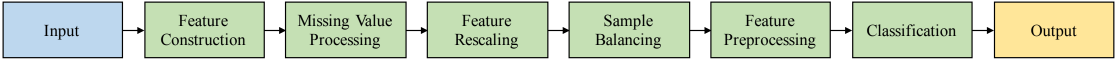

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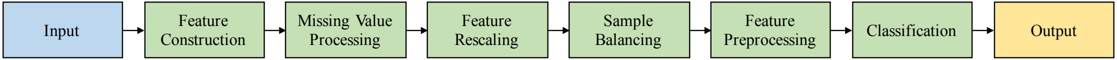

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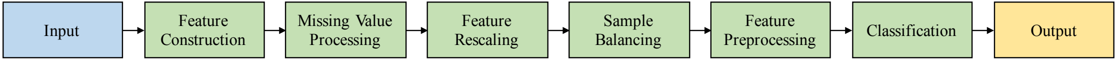
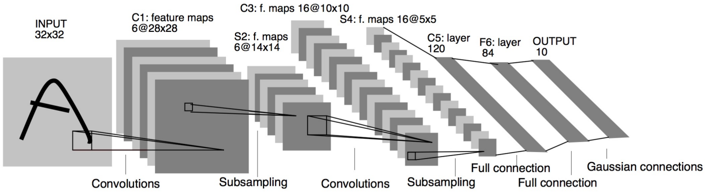


- $f(\mathbf{x})$ measures the quality of entire pipeline with hyperparameter(s) $\mathbf{x}$
- Evaluating $f(\mathbf{x})$ is possibly **costly**
- The search space $\mathcal{X}$ can be large:
  - Feature processing parameters
  - Dimensionality reduction method
  - Dimensionality reduction parameters
  - Classifier type
  - Classifier hyperparameters
  - ...

Example 2: Deep learning [SLA12, SRS$^+$15, KFB$^+$16]



LeNet5 [LBBH98]

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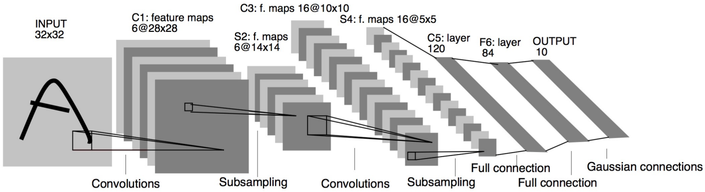

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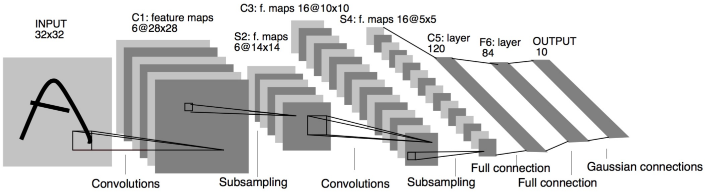

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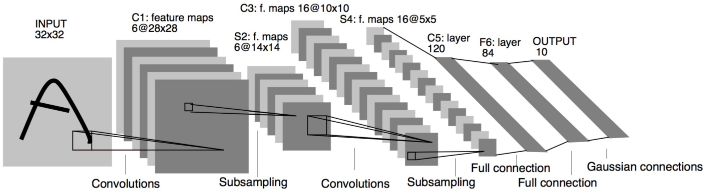

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- Evaluating $f(\mathbf{x})$ is very **costly** $\approx$ up to weeks
- The search space $\mathcal{X}$ can be large:
  - Architecture: # hidden layers, activation functions, ...
  - Model complexity: regularization, dropout, ...
  - Optimisation parameters: learning rates, momentum, batch size, ...

What is a structured search space $\mathcal{X}$?

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- The search space $\mathcal{X}$ exhibits **conditional** relationships, such that

$$\mathcal{X} = \mathcal{X}_0 \times \mathcal{X}_1 \times \cdots \times \mathcal{X}_K.$$

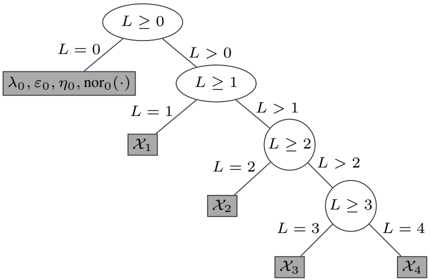
- Depending on some values in $\mathcal{X}_i$, values in $\mathcal{X}_j$ are irrelevant:
  - **Data analytics pipeline:**

$$\mathcal{X} = \underbrace{\mathcal{X}_0}_{\text{classifier type}} \times \overbrace{\mathcal{X}_1}^{\text{hyperparams LR}} \times \underbrace{\mathcal{X}_2}_{\text{hyperparams RF}} \times \cdots \times \mathcal{X}_K$$

  - **Feedforward neural nets:**

$$\mathcal{X} = \underbrace{\mathcal{X}_0}_{\text{\# hidden layers}} \times \overbrace{\mathcal{X}_1}^{\text{hyperparams layer 1}} \times \underbrace{\mathcal{X}_2}_{\text{hyperparams layer 2}} \times \cdots \times \mathcal{X}_K$$

Tuning of feedforward neural nets



$$\mathcal{X}_k \triangleq \left\{ \lambda_k, \{u_j^{(k)}\}_{j=1}^{k}, \varepsilon_k, \eta_k, \mathrm{nor}_k(\cdot), \mathrm{act}_k(\cdot) \right\}$$

- L: Number of hidden layers in $\{0, 1, 2, 3, 4\}$
- λ: Regularization parameter
- u_j: Number of units in j-th layer
- ε, η: Stopping criterion and learning rate of `Adam` [KB14]
- $\mathrm{nor}(\cdot)$: Normalization of the dataset
- $\mathrm{act}(\cdot)$: Activation function

Naive approach: Agnostic to the structure

For $\mathbf{x} \in \mathcal{X}$,

$$
\begin{aligned}
f(\mathbf{x}) &\sim \mathcal{GP}(0, \mathcal{K}) \\
y|f(\mathbf{x}) &\sim \mathcal{N}(f(\mathbf{x}), \varsigma^2)
\end{aligned}
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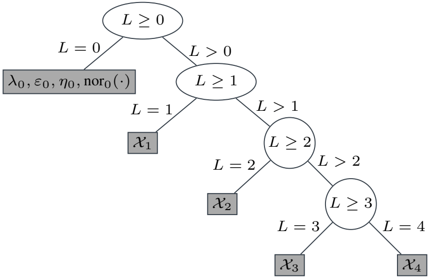

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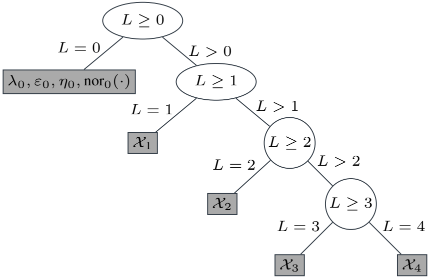

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- Single, joint model
- Ignores conditional dependencies: $\mathcal{X} = \cancel{\mathcal{X}_0 \times \mathcal{X}_1 \times \cdots \times \mathcal{X}_K}$.
- Complexity: $\mathcal{O}\big((\sum_p n_p)^3\big)$.

Baseline: Independent models [BBBK11]

For $\mathbf{x} \in \mathcal{X}_{p_0}$,

$$\begin{aligned} f_{p_0}(\mathbf{x}) &\sim \mathcal{GP}(0, \mathcal{K}_{p_0}) \\ y|f_{p_0}(\mathbf{x}) &\sim \mathcal{N}(f_{p_0}(\mathbf{x}), \varsigma_{p_0}{}^2) \end{aligned}$$

For $\mathbf{x} \in \mathcal{X}_{p_1}$,

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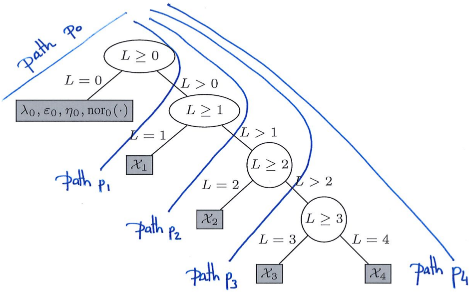
$\vdots$

For $\mathbf{x} \in \mathcal{X}_{p_4}$,

$$\begin{aligned} f_{p_4}(\mathbf{x}) &\sim \mathcal{GP}(0, \mathcal{K}_{p_4}) \\ y|f_{p_4}(\mathbf{x}) &\sim \mathcal{N}(f_{p_4}(\mathbf{x}), \varsigma_{p_4}{}^2) \end{aligned}$$



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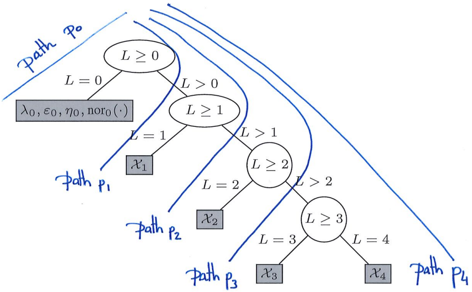
$\vdots$

For $\mathbf{x} \in \mathcal{X}_{p_4}$,

$$\begin{aligned} f_{p_4}(\mathbf{x}) &\sim \mathcal{GP}(0, \mathcal{K}_{p_4}) \\ y|f_{p_4}(\mathbf{x}) &\sim \mathcal{N}(f_{p_4}(\mathbf{x}), \varsigma_{p_4}{}^2) \end{aligned}$$

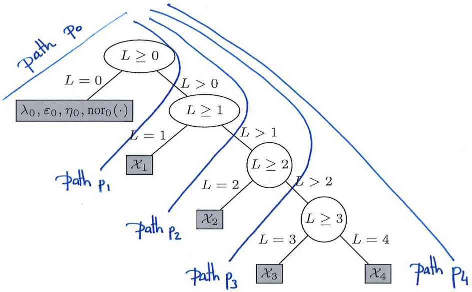


$$\mathcal{X}_k \triangleq \left\{\lambda_k, \{u_j^{(k)}\}_{j=1}^k, \varepsilon_k, \eta_k, \mathrm{nor}_k(\cdot), \mathrm{act}_k(\cdot)\right\}$$

- No sharing of information across leaves
- Compare leaves via utility functions
- $\mathcal{O}\left(\sum_p n_p^3\right)$ vs. $\mathcal{O}\left((\sum_p n_p)^3\right)$.

Tree-structured sharing

Joint prior on the mean:: $\mathbf{c} = [c_1, \ldots, c_V] \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\mathbf{c}})$



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$\vdots$

For $\mathbf{x} \in \mathcal{X}_{p_4}$,

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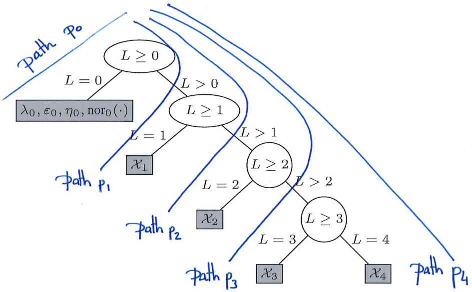

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$\vdots$

For $\mathbf{x} \in \mathcal{X}_{p_4}$,

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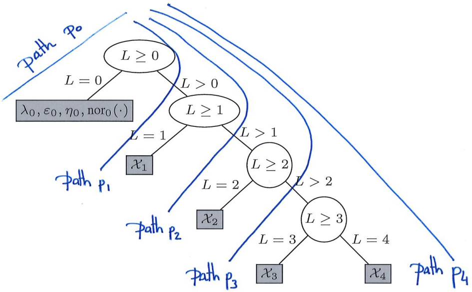

$$\mathcal{X}_k \triangleq \left\{\lambda_k, \{u_j^{(k)}\}_{j=1}^k, \varepsilon_k, \eta_k, \mathrm{nor}_k(\cdot), \mathrm{act}_k(\cdot)\right\}$$

- **Sharing** of information across leaves: if p similar to p', $\sum_{v \in p} c_v \approx \sum_{v \in p'} c_v$.
- $\mathcal{O}\left(\sum_p n_p^3 + V^3\right)$ vs. $\mathcal{O}\left((\sum_p n_p)^3\right)$.

The induced kernel corresponds to the intersection kernel

Let $\mathbf{H} = [\mathbf{H}_p] \in \mathbb{R}^{V \times n}$ be stacked binary masks and $\mathbf{K}^{\text{block}} \in \mathbb{R}^{n \times n}$ be the block-diagonal matrix with blocks $\mathbf{K}_p$.

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The marginal likelihood is given by

$$P(\mathbf{y}) = \int_{\mathbf{f},\mathbf{c}} P(\mathbf{y}, \mathbf{f}, \mathbf{c}) = \mathcal{N}\left(\mathbf{0}, \mathbf{H}^\top \boldsymbol{\Sigma}_c \mathbf{H} + \mathbf{K}^{\text{block}} + \text{diag}\{\varsigma^2\}\right).$$

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If we assume that $\boldsymbol{\Sigma}_c = \sigma_c^2 \mathbf{I}_V$, then

$$\mathbf{H}^\top \boldsymbol{\Sigma}_c \mathbf{H} = \left[\sigma_c^2 (\mathbf{h}_p^\top \mathbf{h}_{p'}) \mathbf{1}_{n_p} \mathbf{1}_{n_{p'}}^\top\right]_{p,p'}.$$

- Diagonal blocks are proportional to the length of path p.
- Off-diagonal blocks are proportional to the path overlap between p and p'.

Two-step acquisition function to reduce complexity

$$(\boldsymbol{x}_\star, p_\star) = \operatorname*{argmax}_{p \in \mathcal{P}, \boldsymbol{x} \in \mathcal{X}_p} a(\boldsymbol{x}, p | \mathcal{D}_n).$$

Two-step acquisition function to reduce complexity

$$(\boldsymbol{x}_\star, p_\star) = \underset{p\in\mathcal{P}, \boldsymbol{x}\in\mathcal{X}_p}{\operatorname{argmax}} \ a(\boldsymbol{x}, p|\mathcal{D}_n).$$

- Exploit the tree structure through a **path acquisition** function:

$$p_\star = \underset{p\in\mathcal{P}}{\operatorname{argmax}} \ a(p|\mathcal{D}_n), \quad \boldsymbol{x}_\star = \underset{\boldsymbol{x}\in\mathcal{X}_{p_\star}}{\operatorname{argmax}} \ a(\boldsymbol{x}, p_\star|\mathcal{D}_n).$$

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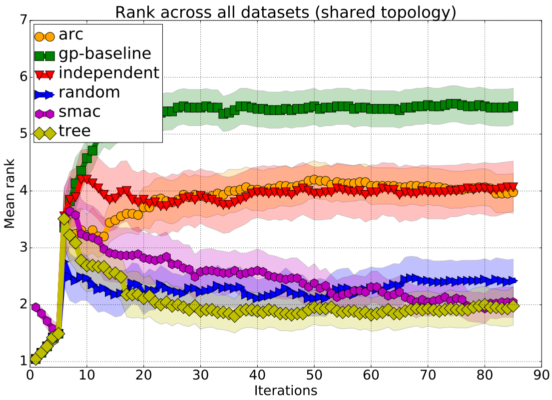
- The path EI is given by

$$a(p | \mathcal{D}_n) = \mathbb{E}\left(\max\{0, y_\star - \mathbf{h}_p^\top \mathbf{c}\} \right).$$

Experiment with feedforward neural network for classification



- Binary classification: 45 datasets from LIBSVM repository
- Mean rank based on mean classification accuracy for each dataset (25 replications)
- `Arc` [SDS+14], `Smac` [HHLB11], `Random` [BB12]

Conclusion

Bayesian optimisation automates machine learning:

- Algorithm tuning
- Model tuning
- Pipeline tuning

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- For example, it can exploit dependency structure
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Conclusion

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https://sheffieldml.github.io/GPyOpt/

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