InfoSeminar

Deep Learning Seminar

Chapter 11 Practical Methodology
Chapter 12 Applications

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  - 11.1 Performance Metrics
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Introduction

- Applying deep learning techniques require more
- A good practitioner needs to know how to monitor it
- Practitioners need to
  - Decide whether to gather more data
  - Increase or decrease model capacity
  - Add or remove regularizing features
  - Improve the optimization of a model
  - Improve approximate inference in a model
  - Debug the software implementation of the model
- It is important to be able to determine the right course

Introduction

- [Andrew Ng] Advice for applying Machine Learning
  - Determine your goals
  - Establish a working end-to-end pipeline as soon as possible
  - Diagnose which components are performing well
  - Repeatedly make incremental changes

Performance Metrics

- Determine your goals
  - What metric to use
  - What level of performance you desire
- Guide all of your future actions
  - With error metric
- Keep in mind that no app achieve zero error
- Keep in mind that data can be limited

Performance Metrics

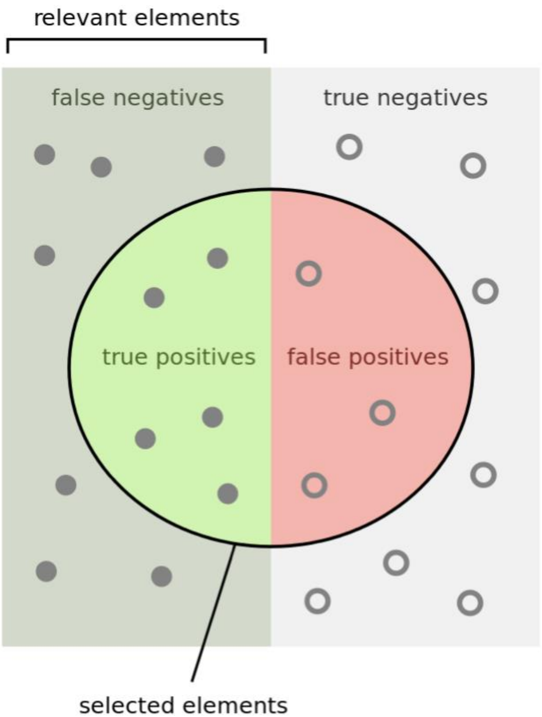
- In the academic setting
  - Attainable error rate based on published benchmark results
- In the real-word setting
  - Safe error rate
  - Cost-effective
  - Appealing to consumers
- One kind of a mistake > another
- E-mail spam detection system
  - incorrectly classifying a legitimate message as spam
  - incorrectly allowing a spam message to appear in the inbox

Performance Metrics

- Training a binary classifier to detect some rare event
- Medical test for a rare disease
- 1%
  - Probability of having disease
- 99%
  - Accuracy by simply hard-coding
- Is that excellent?

Precision and recall

- **Precision**
  - The detections reported by the model that were correct
- **Recall**
  - The true events that were detected



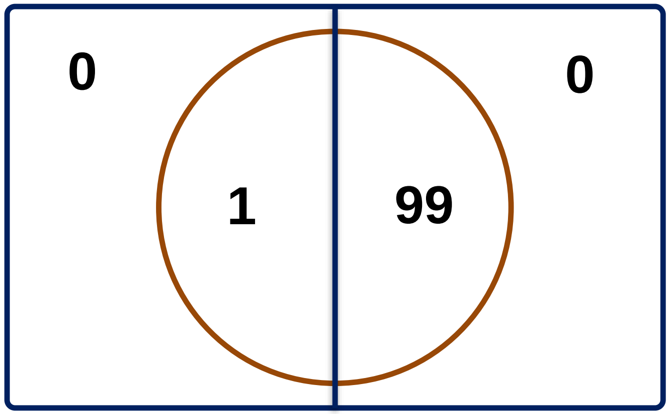
$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

https://en.wikipedia.org/wiki/Precision_and_recall

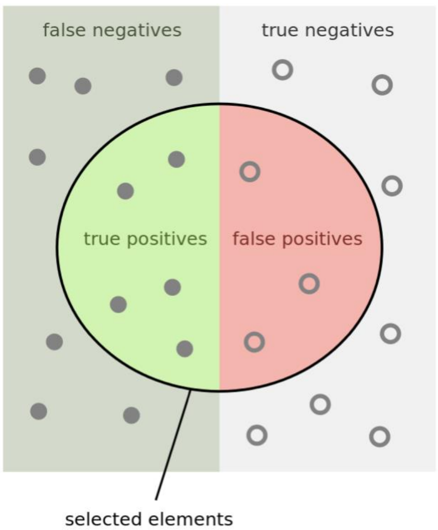
Detecting disease

- **A detector that says everyone has the disease**



Precision: $\frac{1}{99+1} = 0.01$

Recall: $\frac{1}{1+0} = 1$

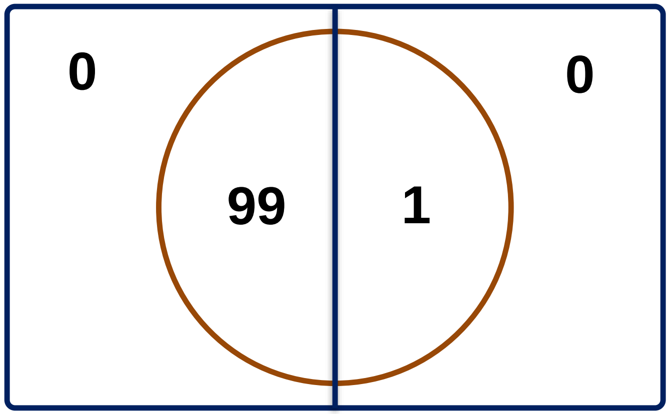


$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

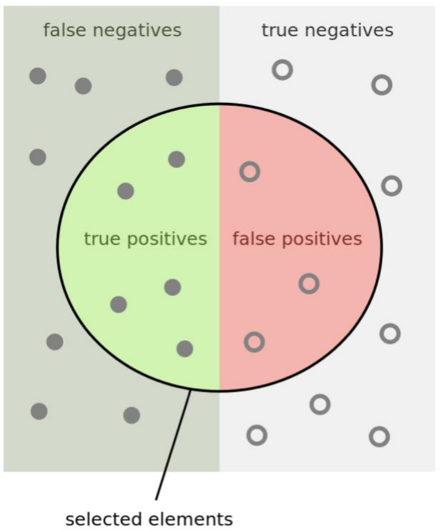
Detecting disease

- **A detector that says no one has the disease**



Precision: Perfect

Recall: 0



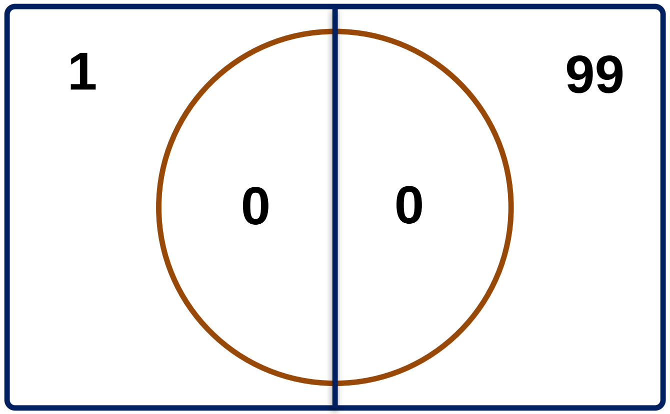
$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

Wrong!

Detecting disease

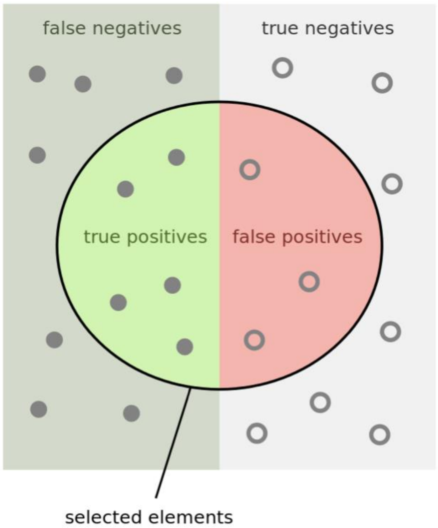
- **A detector that says no one has the disease**



Precision: $\frac{0}{0+0}$

Recall: $\frac{0}{1+0} = 0$

Accuracy: $\frac{99}{1+0+0+99} = 0.99$



$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

Correct!

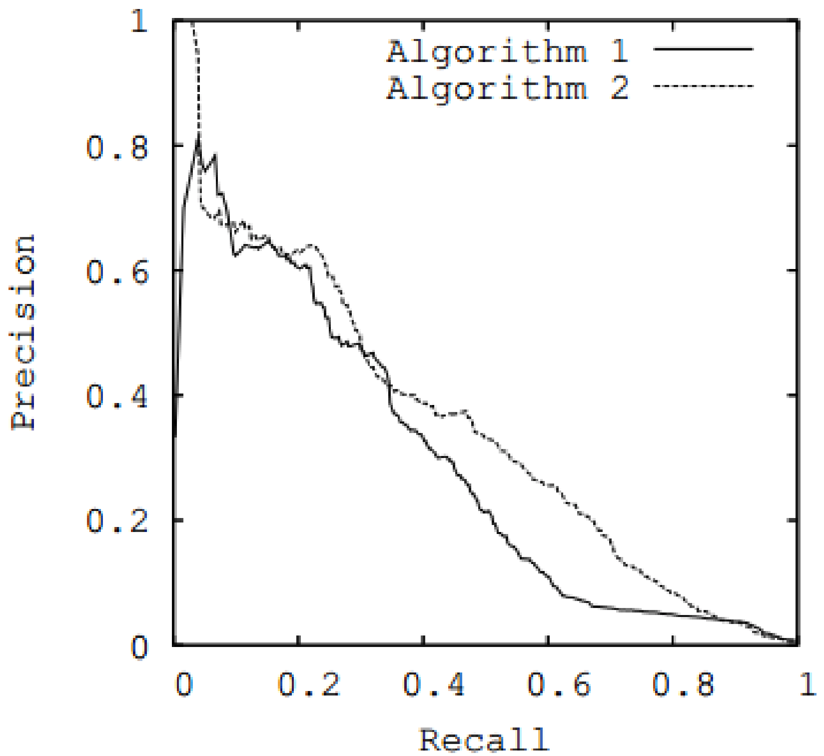
Precision and recall(PR)

- **Summarizing PR with a single number**
- **F-score**
  - $F = \frac{2pr}{p+r}$
  - Harmonic mean

$$\bar{x} = n \times \left(\sum_{i=1}^{n} \frac{1}{x_i}\right)^{-1}$$

Precision and recall

- **Summarizing PR with graph**
- **PR curve**



https://www.quora.com/What-is-Precision-Recall-PR-curve

Performance Metrics

- Refusing to make a decision
  - Reducing the amount of job that the human must process
- Coverage
  - A response range of system
- Coverage V.S. Accuracy

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Default Baseline Models

- Recommendations for which algorithms to use
- Depending on the complexity of your problem
  - Shallow learning model
  - Deep learning model
- Depending on structure of your data
  - Fully connected layer networks
  - Convolutional neural networks
  - Recurrent neural networks

Default Baseline Models - Optimization

- SGD with a decaying learning rate
  - Decaying linearly until reaching minimum learning rate
  - Decaying exponentially
  - Decreasing the learning rate by a factor of 2-10 each time
  - Momentum, Nesterov, Adagrad, RMSprop, Adam
- Batch normalization (BN)
  - Dramatic effect on optimization performance
  - Especially for convolutional networks and networks with sigmoidal nonlinearities

Default Baseline Models - Optimization

- **BN V.S. Whitening**
- **Definition of BN**

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

https://kratzert.github.io/2016/02/12/understanding-the-gradient-flow-through-the-batch-normalization-layer.html

Default Baseline Models

- **If your training set is limited**
  - You should include regularization from the start
  - Early stopping should be used almost universally
  - Dropout is an excellent regularizer
  - BN sometimes reduces generalization error

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Determining Whether to Gather More Data

- How does one decide whether to gather more data?
  - Determine whether the performance on the training set is acceptable.
- If performance on the training set is poor
  - Try increasing the size of the model
  - Try improving the learning algorithm
- If large models and algorithms do not work well
  - The problem might be the of the training data.
  - Try collecting cleaner data or collecting a richer set of features.

Determining Whether to Gather More Data

- If the performance on the test set is acceptable
  - There is nothing left to be done
- If test set performance is worse than training
  - Gathering more data is one of the most effective solutions
- The key considerations
  - The cost and feasibility of gathering more data
  - The cost and feasibility of reducing test error by other means
  - The amount of data that is expected to be necessary

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Selecting Hyperparameters

- **Characters of hyperparameter**
  - Affecting **the time and memory cost** of running the algorithm
  - Affecting the **quality** of the model recovered by the training
  - Affecting its **ability** to **infer** correct results
- **Various hyperparameters**
  - Convolution kernel width
  - Implicit zero padding
  - Dropout rate
  - **Learning rate**
  - Weight decay coefficient(Regularization parameter)
  - Number of hidden units

Selecting Hyperparameters - manual

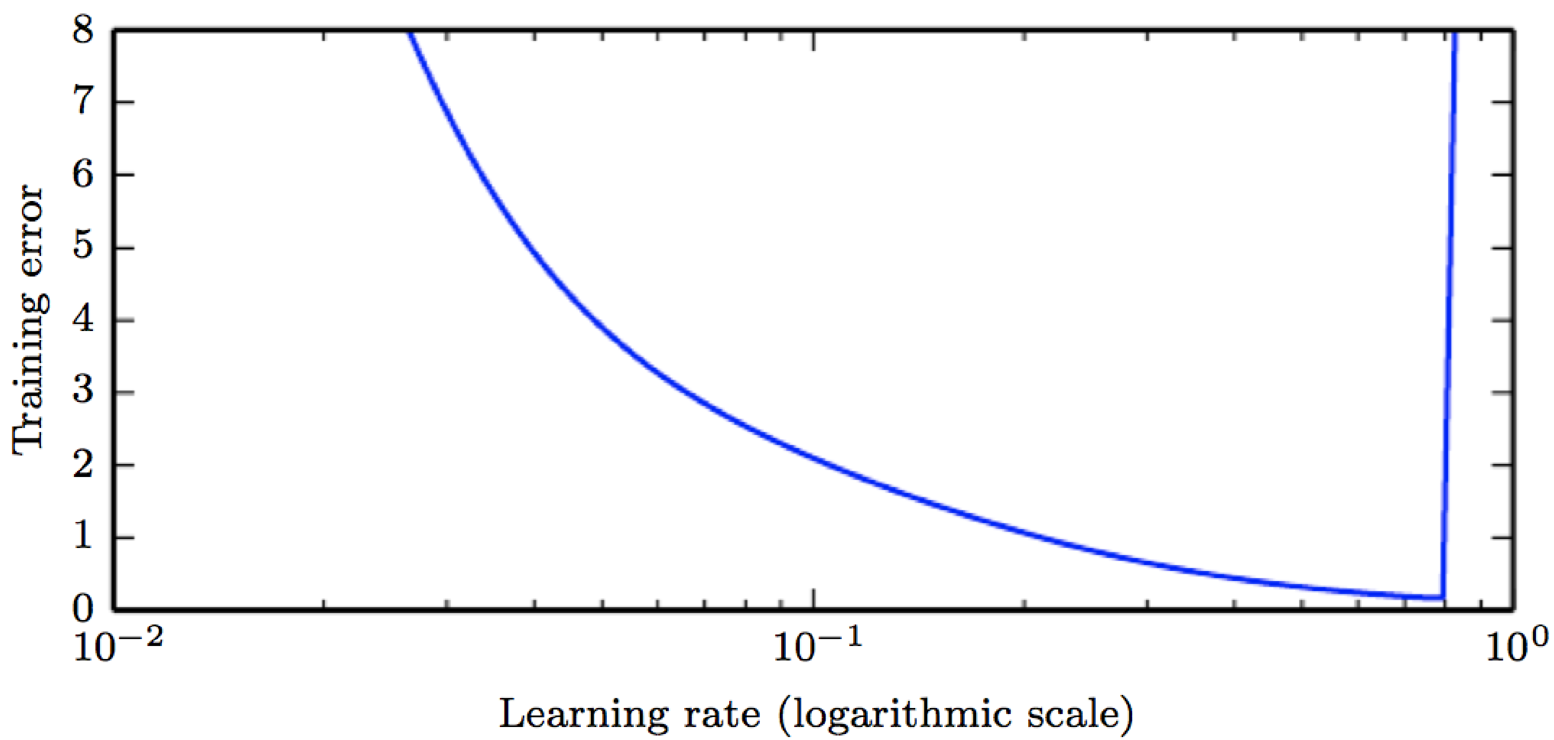
- Understanding the relationship between
  - Hyperparameters
  - Training error
  - Generalization error
  - Computational resources (memory and runtime)
- The goal of manual hyperparameter search
  - To find the **lowest generalization error**
- Three factors
  - The representational **capacity** of the model
  - The ability to minimize **the cost function** used to train the model
  - The degree to which training procedure **regularize** the model

Selecting Hyperparameters - manual

- The hyperparameter value corresponds to low capacity
  - Generalization error is high, training error is high
  - Underfitting regime
- The hyperparameter value corresponds to high capacity
  - Generalization error is high, training error is low
  - Overfitting regime
- Somewhere in the middle lies the optimal capacity

Selecting Hyperparameters - manual

- **Learning rate**



Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased

Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased
Learning rate	**tuned optimally**

Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased
Learning rate	tuned optimally
Convolution kernel width	**increased**

Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased
Learning rate	tuned optimally
Convolution kernel width	increased
Implicit zero padding	**increased**

Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased
Learning rate	tuned optimally
Convolution kernel width	increased
Implicit zero padding	increased
Weight decay coefficient	**decreased**

Selecting Hyperparameters - manual

- **The effect of various hyperparameters on capacity**

Hyperparameter	Increase capacity when..
Number of hidden units	increased
Learning rate	tuned optimally
Convolution kernel width	increased
Implicit zero padding	increased
Weight decay coefficient	decreased
Dropout rate	**decreased**

Selecting Hyperparameters – automatic

- Manual hyperparameter tuning can work very well
  - When the user has a good starting point
  - When the user has months or years of experience
- However, for many applications,
  - These starting points are not available
  - In these cases, automated algorithms can be useful
- Grid search, random search, model-based optimization

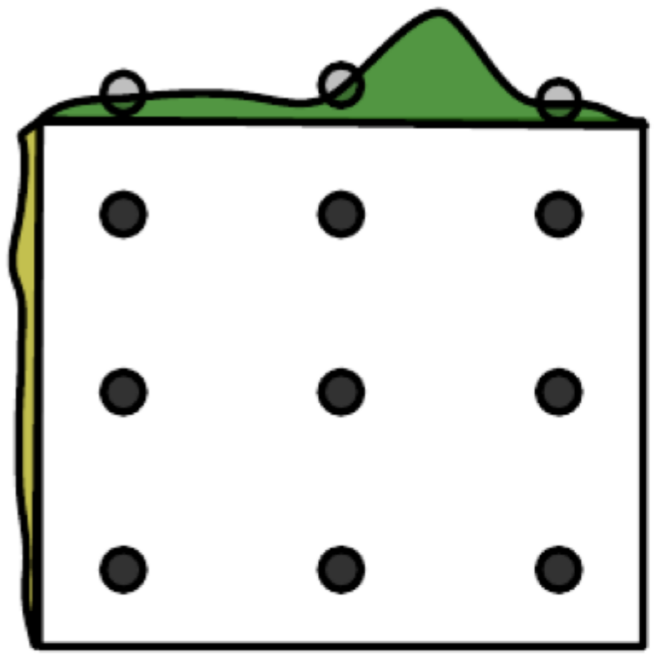
Grid search(parameter sweep)

- **Best value**
- **Shifting the grid**
- **Zooming in**

Large computation cost $O(n^m)$

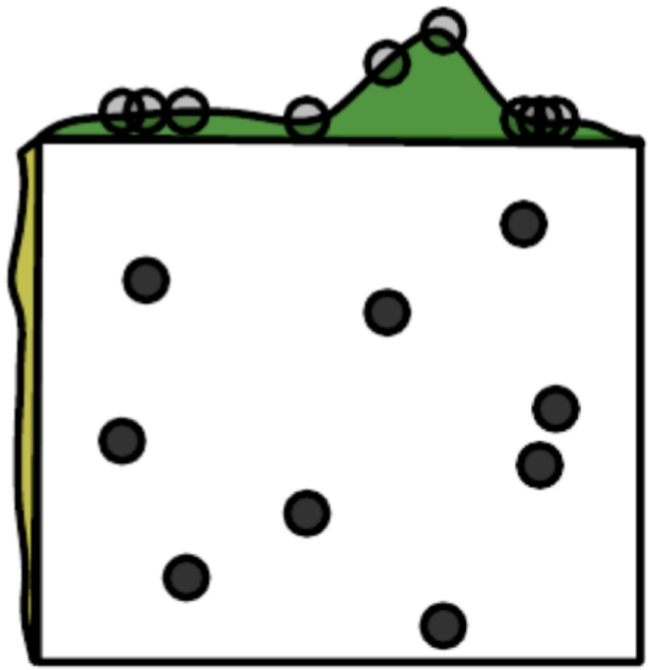
m : # of hyperparameters

n : # of values



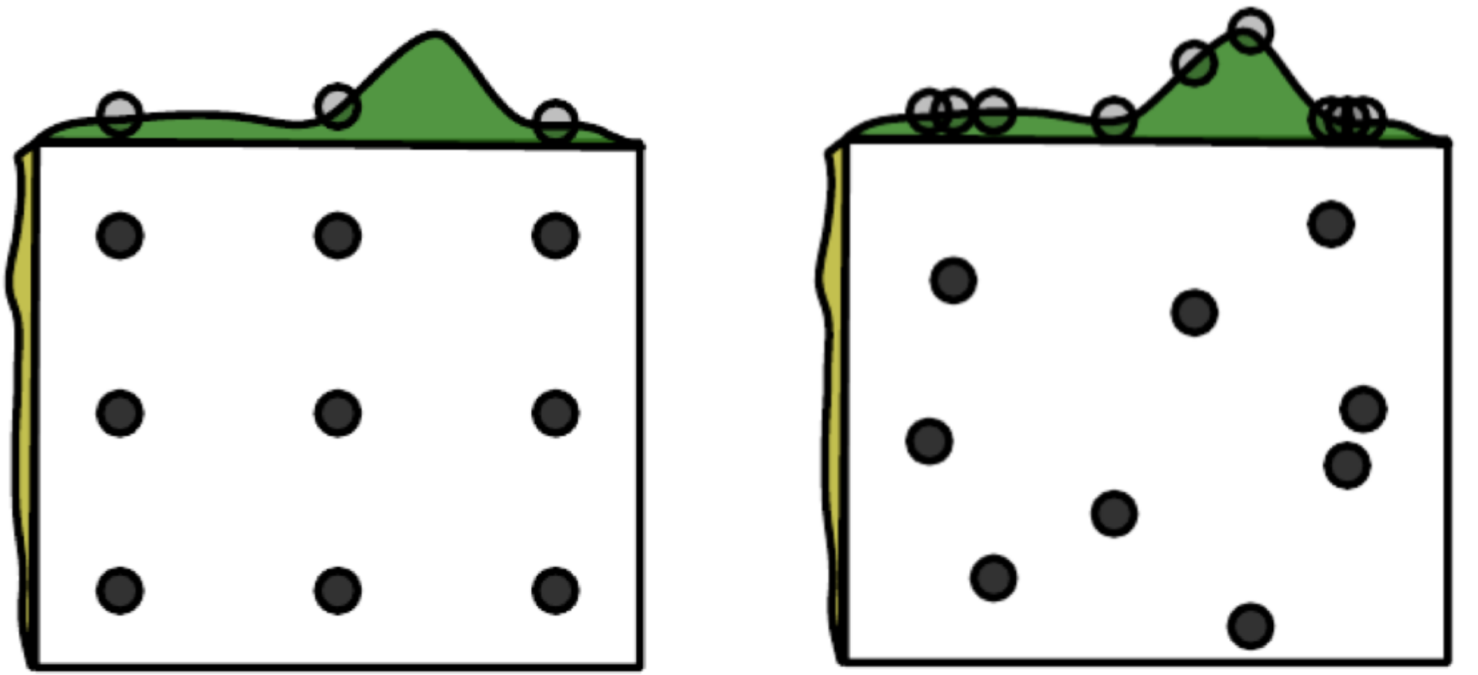
Random search(parameter sweep)

- **Probability distribution**



Grid and random search

- All the trials are independent
- Parallelization is pros



Bayesian inference

- Set of data samples $\{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(m)}\}$
- Parameter $\boldsymbol{\theta}$ is represented as random variable
- Combine the data likelihood with the prior via Bayes' rule:

likelihood prior

$$\boxed{p\left(\boldsymbol{\theta} \middle| \boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(m)}\right)} = \frac{p\left(\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(m)} \middle| \boldsymbol{\theta}\right) p(\boldsymbol{\theta})}{p\left(\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(m)}\right)}$$

Bayesian inference

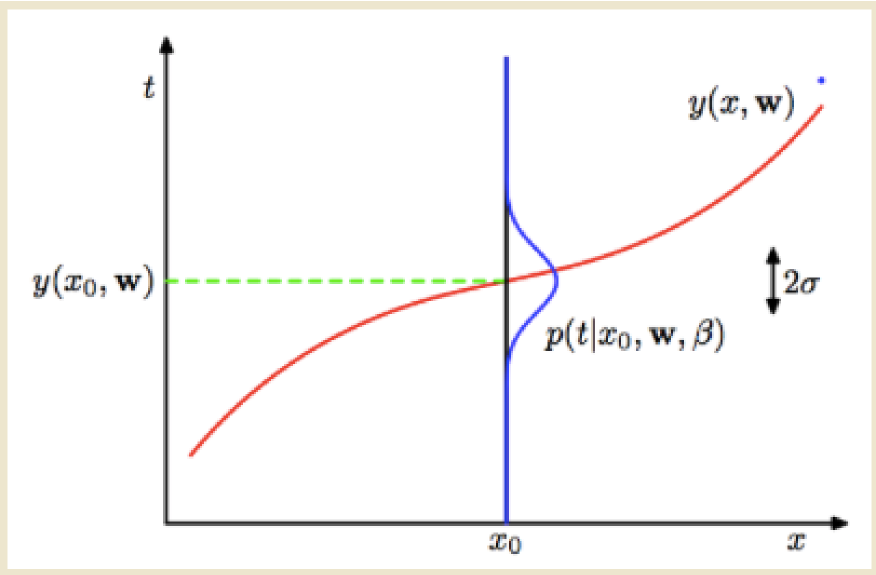
Maximum A Posterior (MAP) Estimation

- **Chose the point of maximal posterior probability**

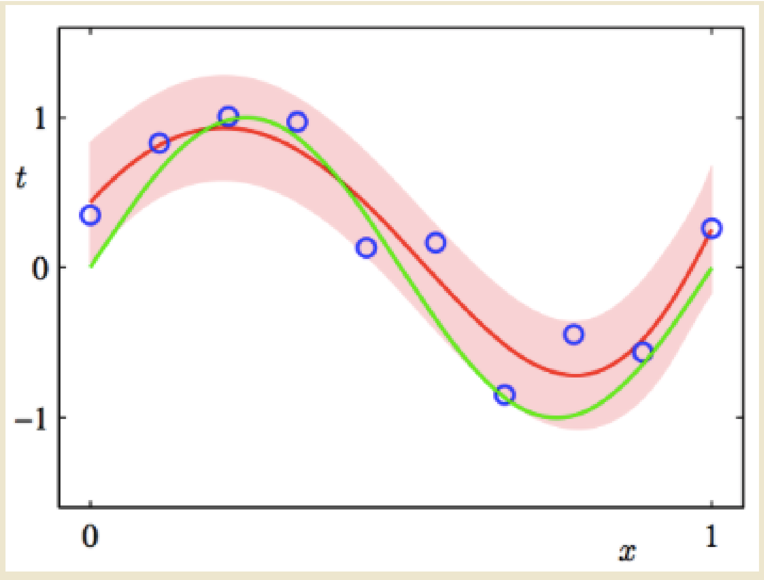
$$\theta_{MAP} = \underbrace{\arg\max_{\theta} p(\theta|x)}_{\text{posterior}} = \underbrace{\arg\max_{\theta} \log p(x|\theta)}_{\text{likelihood}} + \boxed{\underbrace{\log p(\theta)}_{\text{prior}}}$$

Similar with weight decay term

MLE vs MAP



<MLE>



<MAP>

Model-based Hyperparameter Optimization

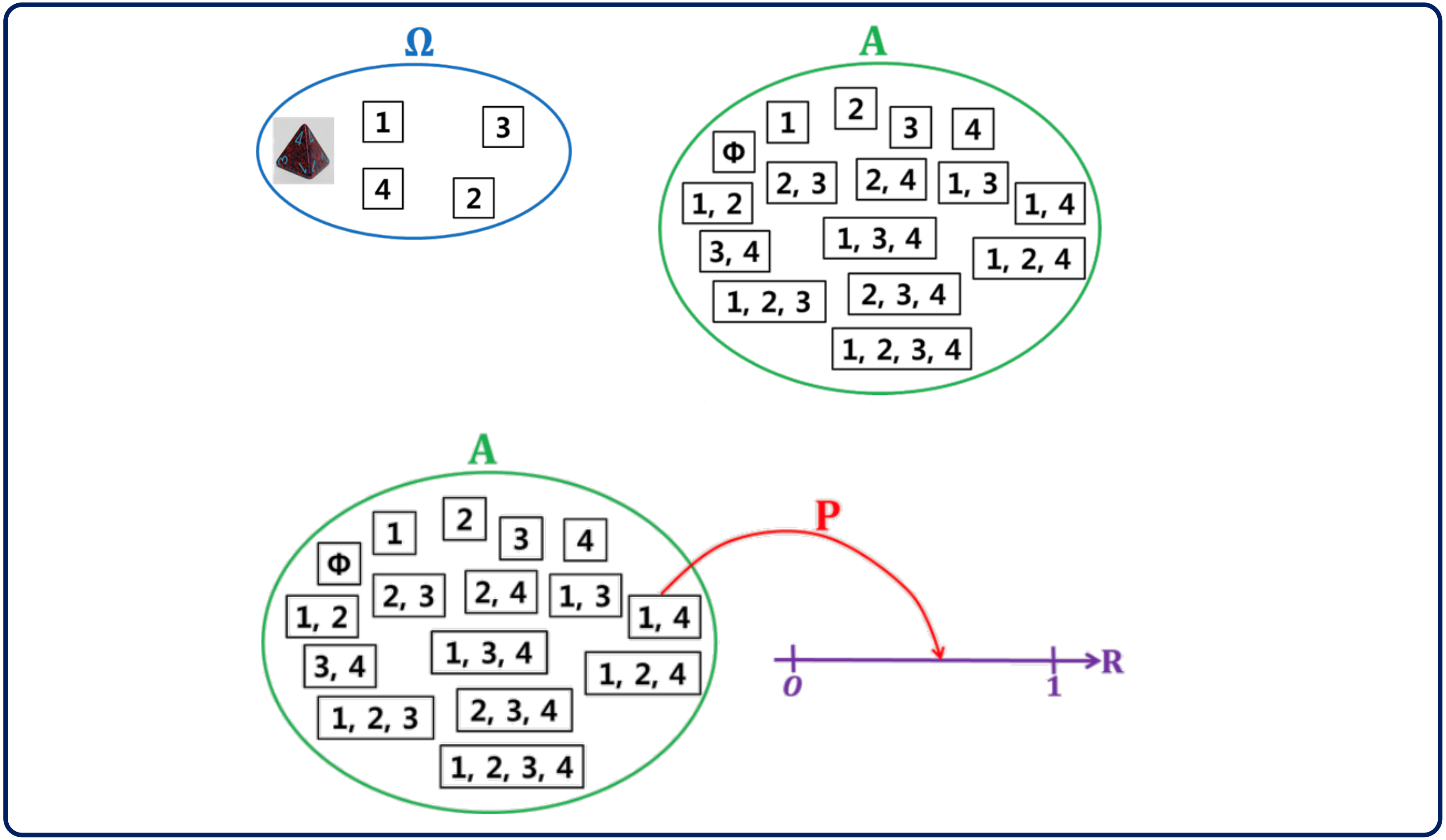
- **Measure space**
  - (U, B, μ)
  - U: data set
  - B: sub sets of U
  - μ: measure. function from B to real space

Model-based Hyperparameter Optimization

- **Probability space**
  - (Ω, A, P)
  - Ω: a sample space
  - A: a set of events
  - P: the assignment of probability to the events

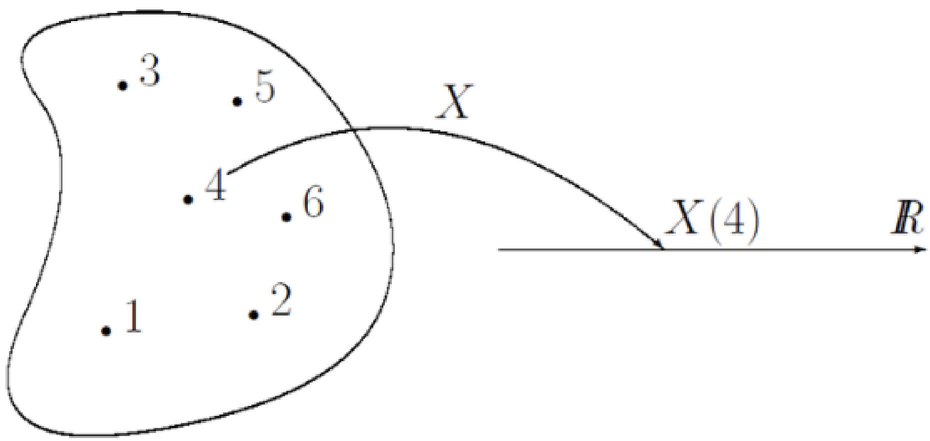
Model-based Hyperparameter Optimization

- **Probability space** (Ω, A, P)



Model-based Hyperparameter Optimization

- **Random variable**
  - Function from probability space to real space

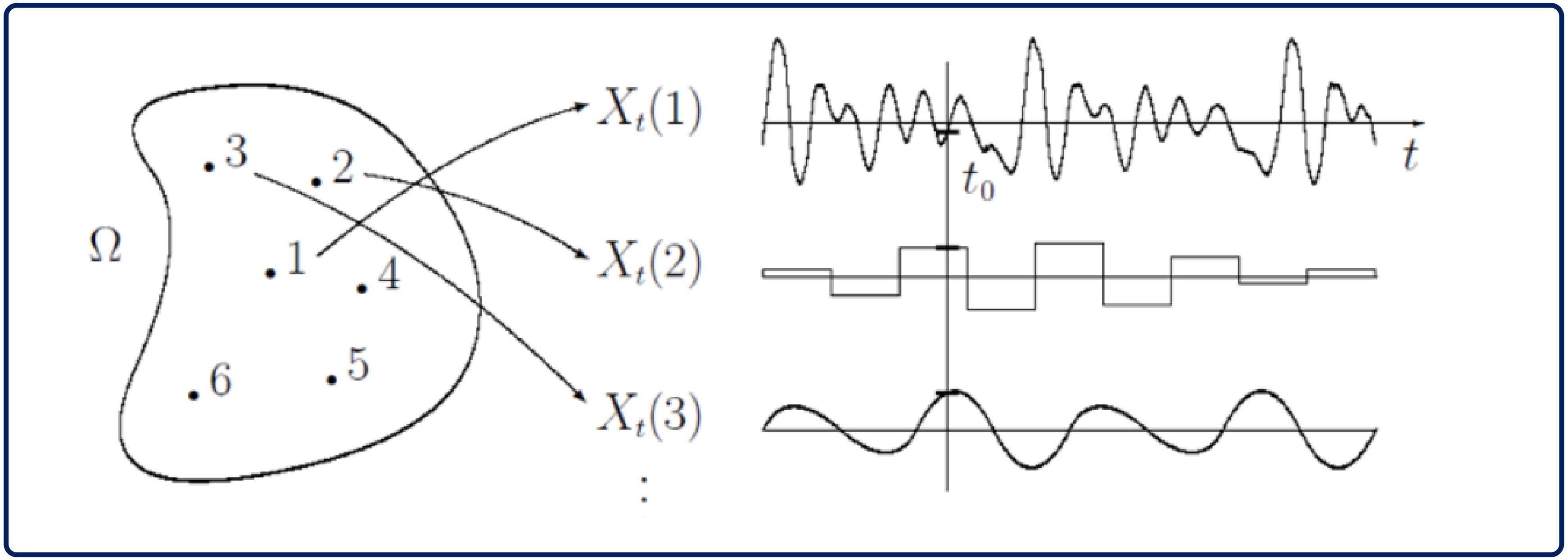


$$X = \begin{cases} 1 \text{ with probability } 1/6, \\ 2 \text{ with probability } 1/6, \\ 3 \text{ with probability } 1/6, \\ 4 \text{ with probability } 1/6, \\ 5 \text{ with probability } 1/6, \\ 6 \text{ with probability } 1/6 \end{cases}$$

http://sanghyukchun.github.io/99/

Model-based Hyperparameter Optimization

- **Stochastic process(random process)**
  - Function from probability space to function space
  - $X_t(w), t \in I$



http://sanghyukchun.github.io/99/

Model-based Hyperparameter Optimization

- **Gaussian process(GP)**
  - Random process
    finite sample → multivariate normal distribution
  - Mean function: $\boldsymbol{m}(\boldsymbol{x})$
  - $\{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\}$, random variable $\{\boldsymbol{h}(\boldsymbol{x}_1), \cdots, \boldsymbol{h}(\boldsymbol{x}_n)\}$

$$\begin{bmatrix} h(x_1) \\ \vdots \\ h(x_n) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{bmatrix} \right)$$

$$f(x) \sim GP(m(x), k(x, x'))$$

$$f_i = f(x_i)$$

x_i: i-th data of data set

Model-based Hyperparameter Optimization

- **Covariance matrix**

$$k_{sqe}(x, x') = \alpha \exp\left\{ -\frac{1}{2} \sum_{d=1}^{D} \left(\frac{x_d - x'_d}{\theta_d} \right) \right\}$$

$$K = \begin{pmatrix} k_{1,1} & k_{1,2} & \cdots & k_{1,n} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ k_{n,1} & k_{n,2} & \cdots & k_{n,n} \end{pmatrix}$$

k_{sqe}: squared-exponential kernel function

(covariance function)

x: one point

x': onother point

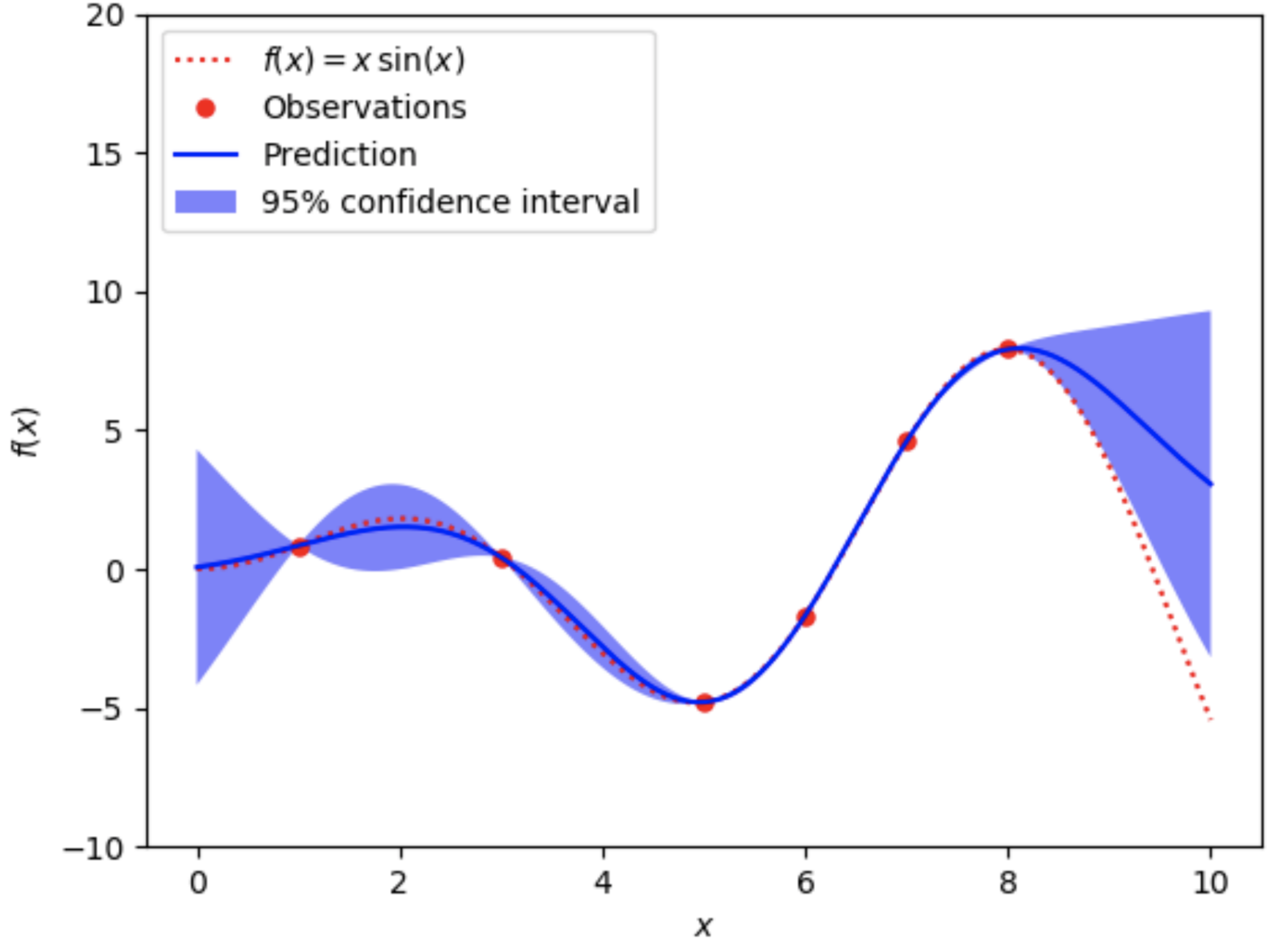
x_d: d dimension value of x

α, θ_d: hyperparameter

K: covariance matrix

Model-based Hyperparameter Optimization

- **Gaussian Process Regression(GPR)**



http://sanghyukchun.github.io/99/

Model-based Hyperparameter Optimization

- **Bayesian Optimization for "Black-box" function**

$$\boxed{x^* = \arg\min_{x \in X} f(x).}$$

  - Estimate $f(x)$ by using data
  - Choice point by using decision rule
  - Adding the point to data and repeat this until achieve criteria

- **Acquisition function $EI(x)$**
  - Balancing between explore and exploit

Model-based Hyperparameter Optimization

Acquisition function(AF) - Probability of Improvement

$$\gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{\text{best}}) - \mu(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}{\sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}$$

$$a_{\text{PI}}(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) = \Phi(\gamma(\mathbf{x}))$$

$a(x;\{x_n, y_n\}, \theta)$: dependence(AF and previous observations)

$\{x_n,\ y_n\}_{n=1}^{N}$: observations form

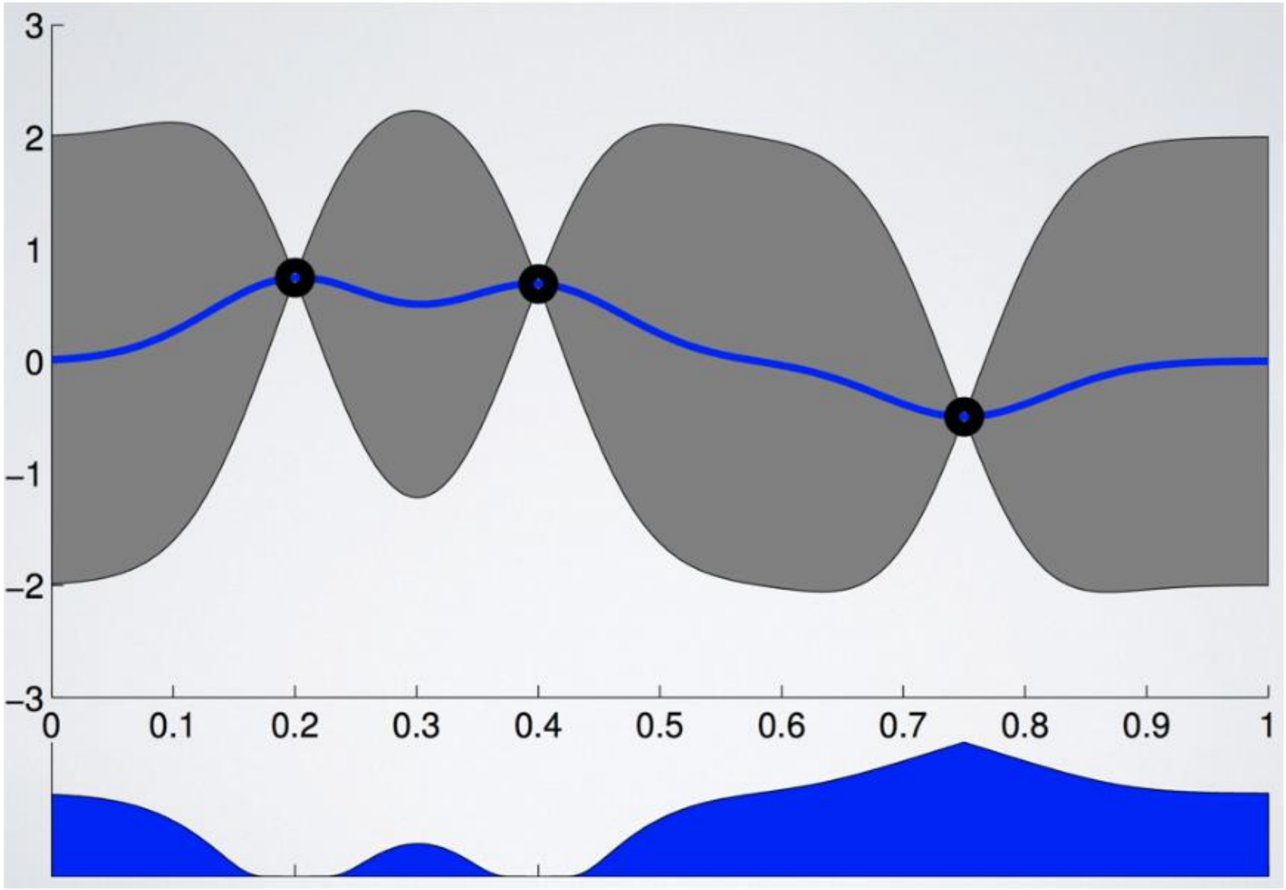
x_{best}: best current value as $x_{best} = argmin_{x_n} f(x_n)$

$\phi(\cdot)$: cumulative distribution function

[NIPS 12]Practical Bayesian Optimization of Machine Learning Algorithms

Model-based Hyperparameter Optimization

- **Acquisition function(AF) - Probability of Improvement**



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Model-based Hyperparameter Optimization

- **Acquisition function - Expected Improvement**

$$\gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{\mathsf{best}}) - \mu(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}{\sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}$$

$$a_{\mathsf{EI}}(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) = \sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)\,(\gamma(\mathbf{x})\,\Phi(\gamma(\mathbf{x})) + \mathcal{N}(\gamma(\mathbf{x})\,;\,0, 1))$$

$a(x;\{x_n, y_n\}, \theta)$: dependence(AF and previous obserbations)

$\{x_n,\ y_n\}_{n=1}^{N}$: observations form

x_{best}: best current value as $x_{best} = argmin_{x_n} f(x_n)$

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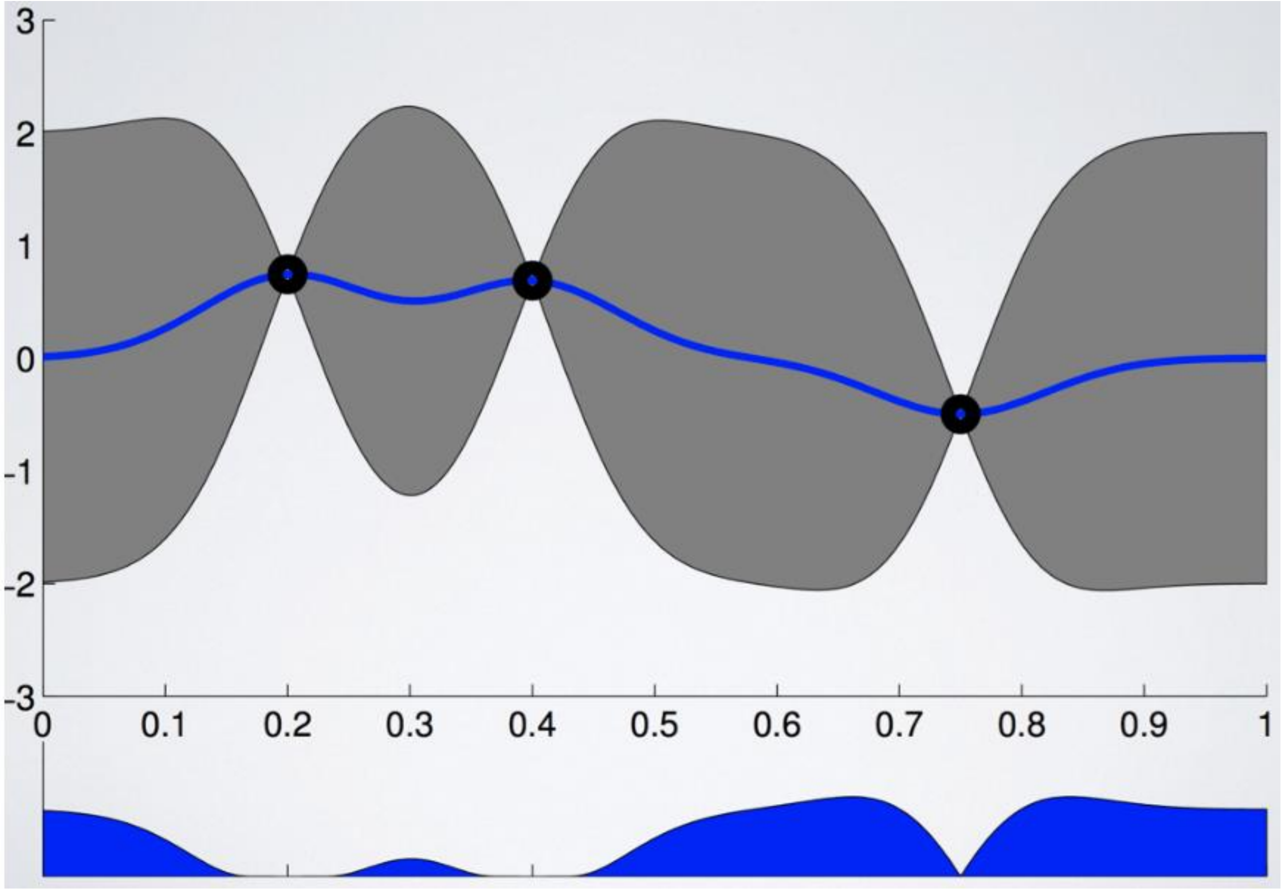
[NIPS 12]Practical Bayesian Optimization of Machine Learning Algorithms

Model-based Hyperparameter Optimization

- **Acquisition function - Expected Improvement**



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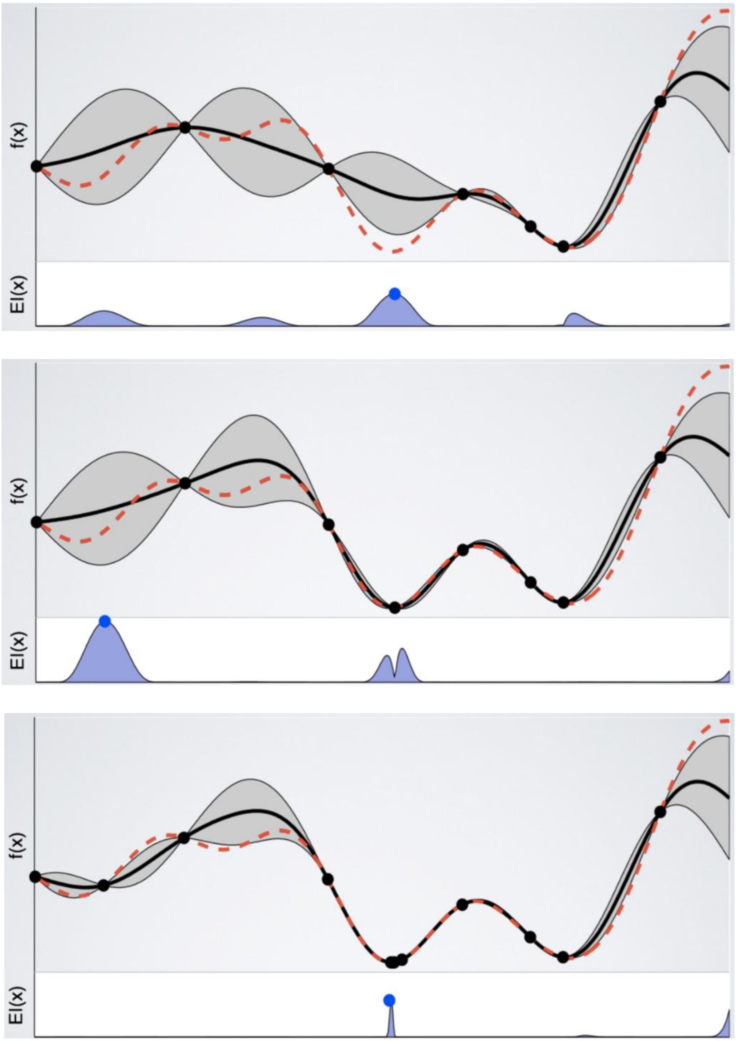
Practical Bayesian Optimization of Machine Learning Algorithms



Red line: unknown black box function $f(x)$

Black line: estimation

$EI(x)$: acquisition function

http://sanghyukchun.github.io/99/

Model-based Hyperparameter Optimization

- Limitation of Bayesian Optimization
  - Tuning the second hyper parameters(e.g. kernel function)
  - No guide about stochastic assumption
  - Impossible parallelization
  - Difficult to implement software
- To solve this, refer to this paper
  - [NIPS 12] Practical Bayesian Optimization of Machine Learning Algorithms
  - Jasper Snoek, Hugo Larochelle, Ryan P. Adams
  - Citation: 1031

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Debugging

- **Deep learning systems are difficult to debug**
- **Bias update error example**
  - $b \leftarrow b - \alpha$ 　$\boldsymbol{b}$: biases, $\boldsymbol{\alpha}$: learning rate
  - **It is so difficult to find this error**
- **Debugging tests**
  - **Visualize the model in action**
  - **Reasoning about software using train and test error**
  - **Fit a tiny dataset**
  - **Compare back-propagated derivatives to numerical derivatives**
  - **Monitor histograms of activations and gradient**

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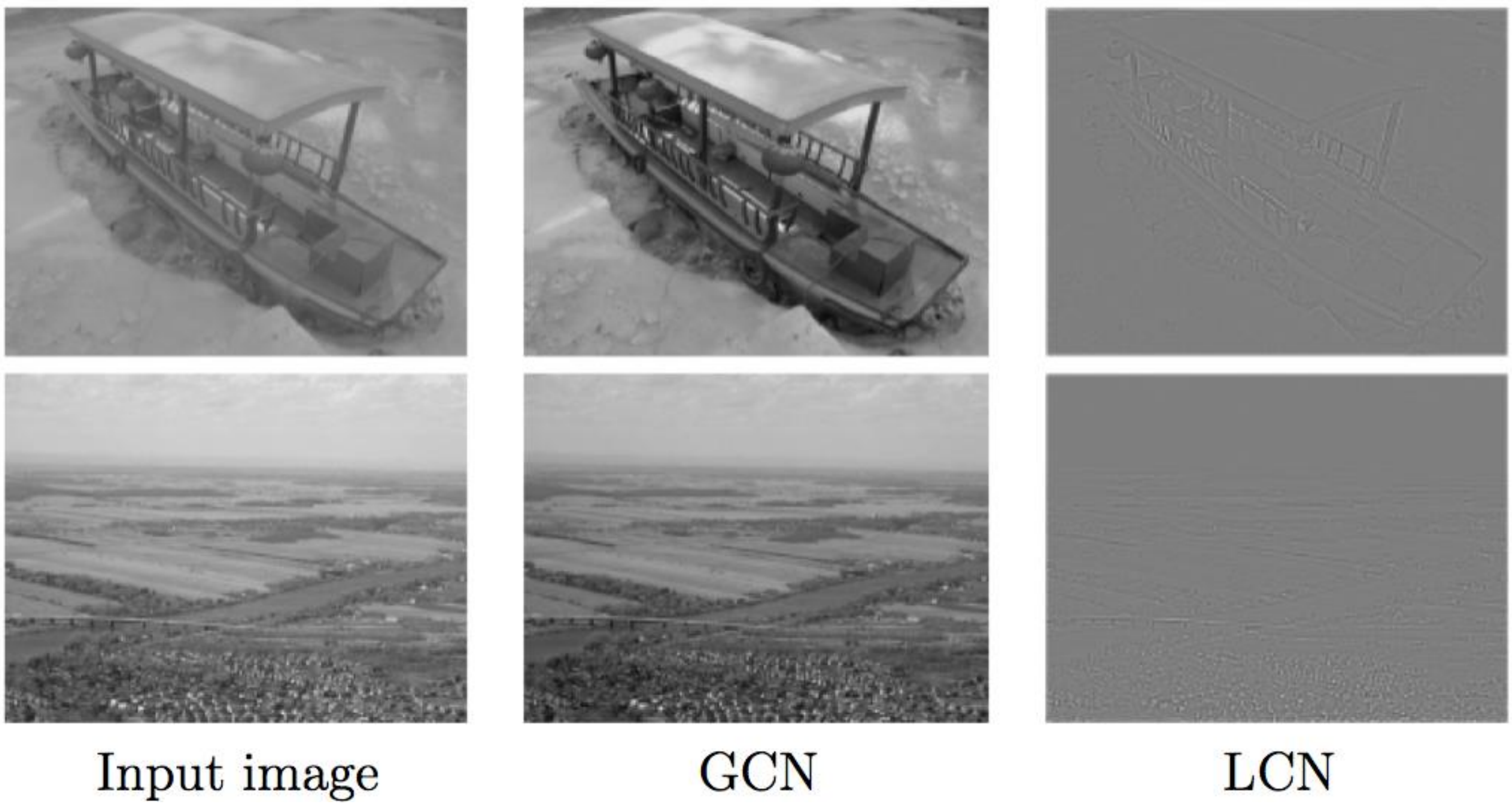
Computer Vision – Contrast Normalization

- **A comparison of global and local contrast normalization**



Computer Vision – Contrast Normalization

- **Contrast Normalization**
- **Contrast formula**
  - One of the sources of variation that can be safely removed

$$\bar{\mathsf{X}} = \frac{1}{3rc}\sum_{i=1}^{r}\sum_{j=1}^{c}\sum_{k=1}^{3}\mathsf{X}_{i,j,k}$$

$$\sqrt{\frac{1}{3rc}\sum_{i=1}^{r}\sum_{j=1}^{c}\sum_{k=1}^{3}\left(\mathsf{X}_{i,j,k}-\bar{\mathsf{X}}\right)^2}$$

$X \in \mathbb{R}^{r\times c\times 3}$: image tensor

$X_{i,j,1}$: red intensity

$X_{i,j,1}$: green intensity

$X_{i,j,1}$: blue intensity

Computer Vision – Contrast Normalization

- **Global contrast normalization(GCN)**
  - Preventing images from having varying amounts of contrast

$$X'_{i,j,k} = s\frac{X_{i,j,k} - \bar{X}}{\max\left\{\epsilon, \sqrt{\lambda + \frac{1}{3rc}\sum_{i=1}^{r}\sum_{j=1}^{c}\sum_{k=1}^{3}\left(X_{i,j,k} - \bar{X}\right)^2}\right\}}$$

$X_{i,j,1}$: red intensity

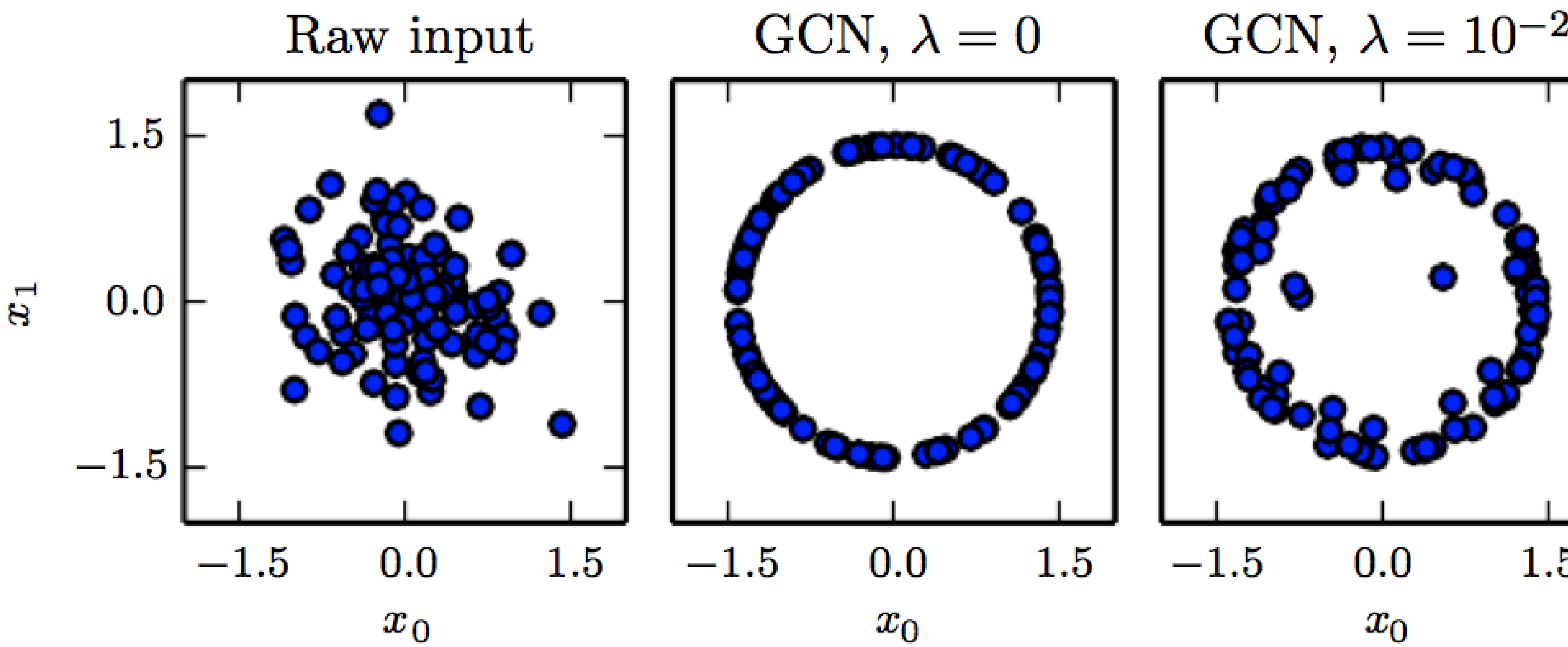
$X_{i,j,1}$: green intensity

$X_{i,j,1}$: blue intensity

s, ϵ, λ: hyper parameters

Computer Vision – Contrast Normalization

- **GCN maps examples onto a sphere**



Thank you