# Statistical Models & Computing Methods

## Lecture 1: Introduction


**Cheng Zhang**

School of Mathematical Sciences, Peking University

September 24, 2020

# General Information

- Class times:
  - Thursday 6:40-9:30pm
  - Classroom Building No.2, Room 401
- Instructor:
  - Cheng Zhang: `chengzhang@math.pku.edu.cn`
- Teaching assistants:
  - Dequan Ye: `1801213981@pku.edu.cn`
  - Zihao Shao: `zh.s@pku.edu.cn`
- Tentative office hours:
  - 1279 Science Building No.1
  - Thursday 3:00-5:00pm or by appointment
- Website:

  `https://zcrabbit.github.io/courses/smcm-f20.html`

- A branch of mathematical sciences focusing on efficient numerical methods for statistically formulated problems
- The focus lies on computer intensive statistical methods and efficient modern statistical models.
- Developing rapidly, leading to a broader concept of computing that combines the theories and techniques from many fields within the context of statistics, mathematics and computer sciences.

# Goals



- Become familiar with a variety of modern computational statistical techniques and knows more about the role of computation as a tool of discovery
- Develop a deeper understanding of the mathematical theory of computational statistical approaches and statistical modeling.
- Understand what makes a good model for data.
- Be able to analyze datasets using a modern programming language (e.g., python).

# Textbook



- No specific textbook required for this course
- Recommended textbooks:
  - Givens, G. H. and Hoeting, J. A. (2005) Computational Statistics, 2nd Edition, Wiley-Interscience.
  - Gelman, A., Carlin, J., Stern, H., and Rubin, D. (2003). Bayesian Data Analysis, 2nd Edition, Chapman & Hall.
  - Liu, J. (2001). Monte Carlo Strategies in Scientific Computing, Springer-Verlag.
  - Lange, K. (2002). Numerical Analysis for Statisticians, Springer-Verlag, 2nd Edition.
  - Hastie, T., Tibshirani, R. and Friedman, J. (2009). The Elements of Statistical Learning, 2nd Edition, Springer.
  - Goodfellow, I., Bengio, Y. and Courville, A. (2016). Deep Learning, MIT Press.

# Tentative Topics



- Optimization Methods
  - Gradient Methods
  - Expectation Maximization
- Approximate Bayesian Inference Methods
  - Markov chain Monte Carlo
  - Variational Inference
  - Scalable Approaches
- Applications in Machine Learning & Related Fields
  - Variational Autoencoder
  - Generative Adversarial Networks
  - Flow-based Generative Models
  - Bayesian Phylogenetic Inference

Familiar with at least one programming language (with python preferred!).

- All class assignments will be in python (and use numpy).
- You can find a good Python tutorial at

  `http://www.scipy-lectures.org/`

  You may find a shorter python+numpy tutorial useful at

  `http://cs231n.github.io/python-numpy-tutorial/`

Familiar with the following subjects

- Probability and Statistical Inference
- Stochastic Processes

# Grading Policy



- 4 Problem Sets: $4 \times 15\% = 60\%$
- Final Course Project: $40\%$
  - up to 4 people for each team
  - Teams should be formed by the end of week 4
  - Midterm proposal: $5\%$
  - Oral presentation: $10\%$
  - Final write-up: $25\%$
- Late policy
  - 7 free late days, use them in your ways
  - Afterward, 25% off per late day
  - Not accepted after 3 late days per PS
  - Does not apply to Final Course Project
- Collaboration policy
  - Finish your work independently, verbal discussion allowed

# Final Project



- Structure your project exploration around a general problem type, algorithm, or data set, but should explore around your problem, testing thoroughly or comparing to alternatives.
- Present a project proposal that briefly describe your teams' project concept and goals in one slide in class on 11/12.
- There will be in class project presentation at the end of the term. Not presenting your projects will be taken as voluntarily giving up the opportunity for the final write-ups.
- Turn in a write-up ($< 10$ pages) describing your project and its outcomes, similar to a research-level publication.

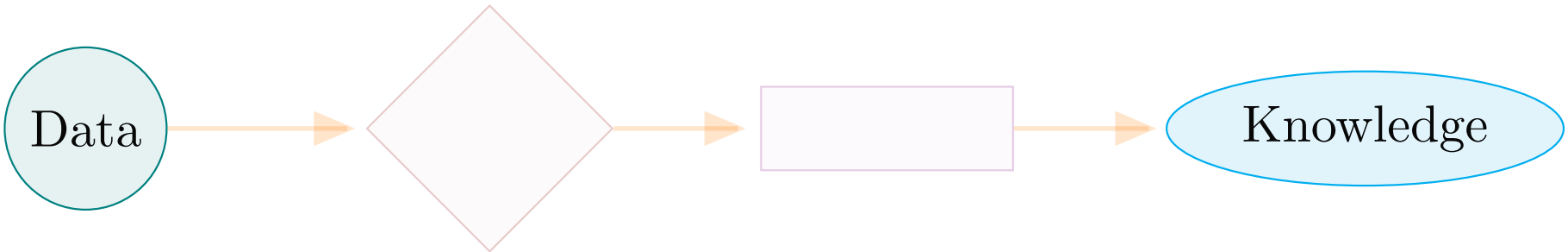
# Today's Agenda



- A brief overview of statistical approaches
- Basic concepts in statistical computing
- Convex optimization

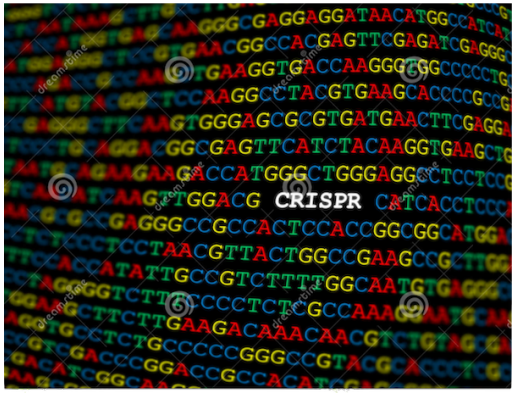
# Statistical Pipeline

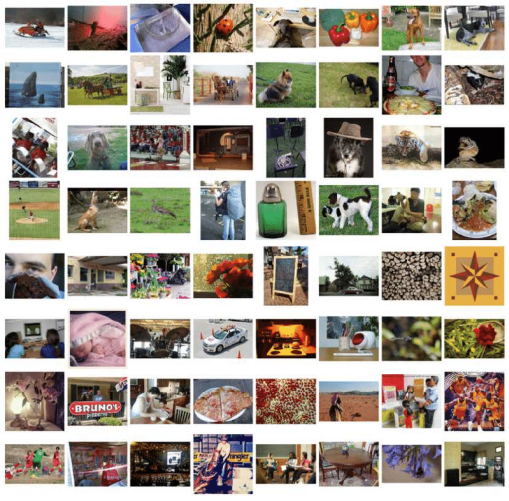




# Statistical Pipeline



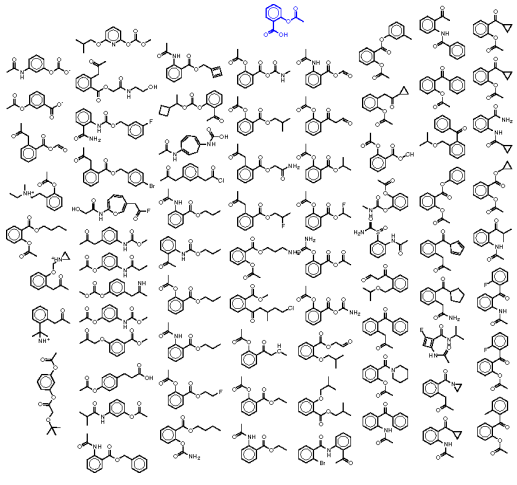



Data

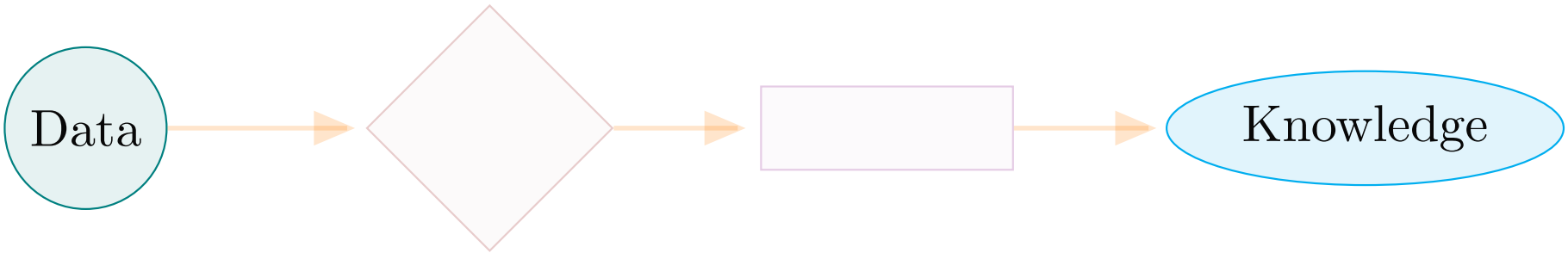
In fact, the Chinese NORP market has the three CARDINAL most influential names of the retail and tech space – Alibaba GPE , Baidu ORG , and Tencent PERSON (collectively touted as BAT ORG ), and is betting big in the global AI GPE in retail industry space . The three CARDINAL giants which are claimed to have a cut-throat competition with the U.S. GPE (in terms of resources and capital) are positioning themselves to become the 'future AI PERSON platforms'. The trio is also expanding in other Asian NORP countries and investing heavily in the U.S. GPE based AI GPE startups to leverage the power of AI GPE . Backed by such powerful initiatives and presence of these conglomerates, the market in APAC AI is forecast to be the fastest-growing one CARDINAL , with an anticipated CAGR PERSON of 45% PERCENT over 2018 - 2024 DATE .

To further elaborate on the geographical trends, North America LOC has procured more than 50% PERCENT of the global share in 2017 DATE and has been leading the regional landscape of AI GPE in the retail market. The U.S. GPE has a significant credit in the regional trends with over 65% PERCENT of investments (including M&As, private equity, and venture capital) in artificial intelligence technology. Additionally, the region is a huge hub for startups in tandem with the presence of tech titans, such as Google ORG , IBM ORG , and Microsoft ORG .



# Statistical Pipeline






$\mathcal{D}$

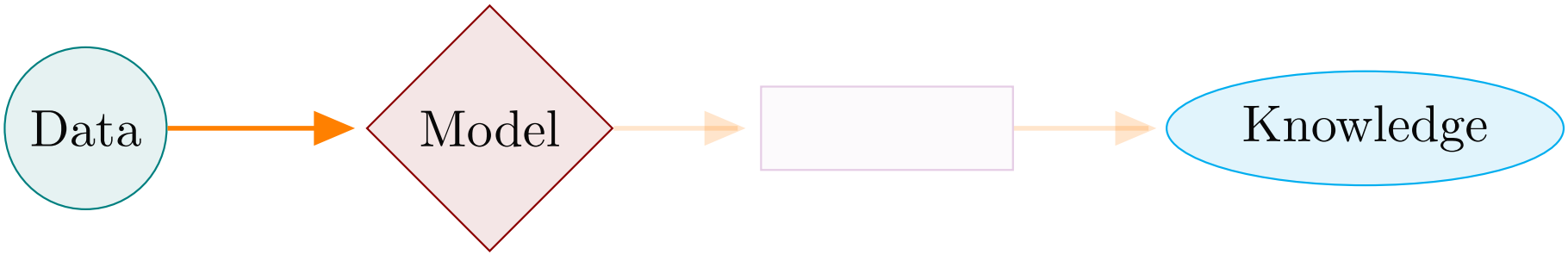
# Statistical Pipeline



Linear Models  Latent Variable Models  Neural Networks

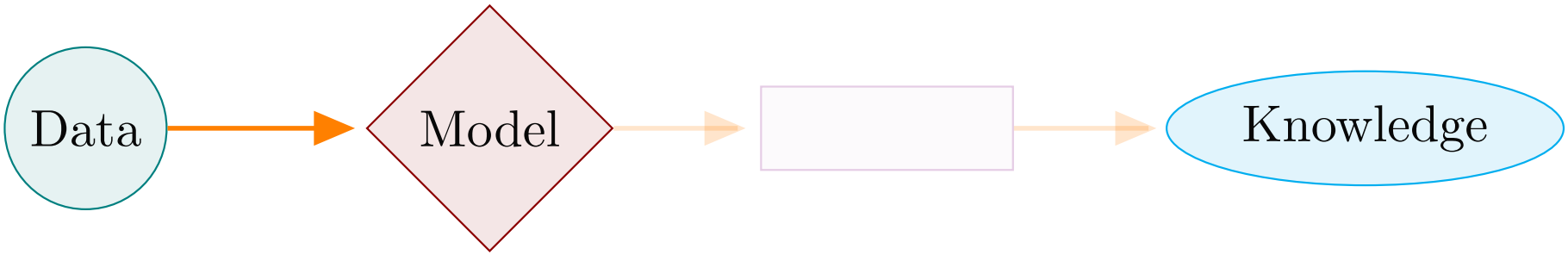
Bayesian Nonparametric Models

Generalized Linear Models



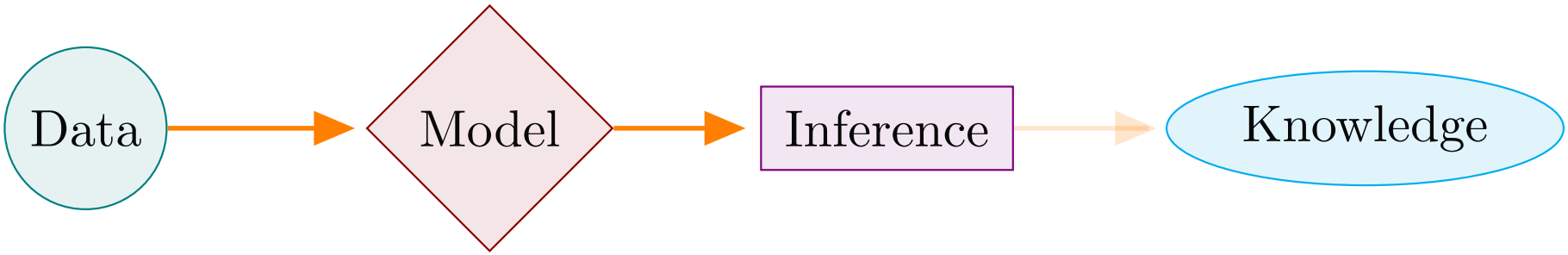

$\mathcal{D}$

# Statistical Pipeline




$\mathcal{D}$ $p(\mathcal{D}|\theta)$

# Statistical Pipeline




$\mathcal{D}$ $p(\mathcal{D}|\theta)$

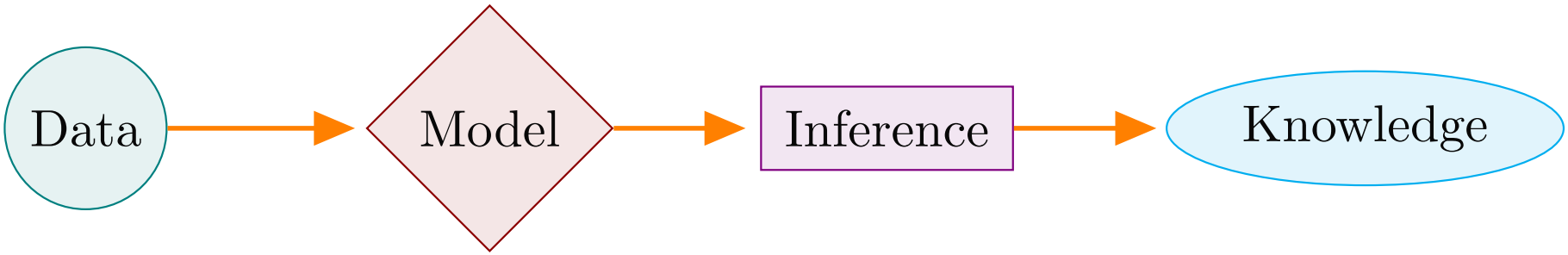
Gradient Descent

EM

MCMC

Variational Methods

# Statistical Pipeline

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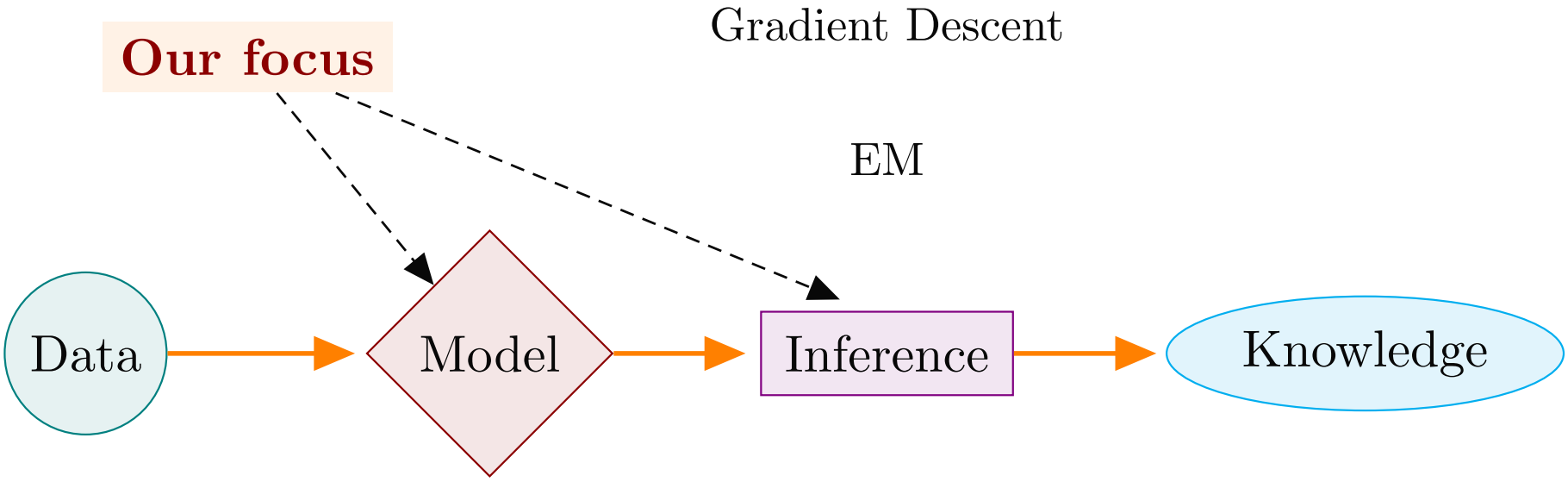
$\mathcal{D}$

$p(\mathcal{D}|\theta)$

# Statistical Pipeline



"All models are wrong, but some are useful."

George E. P. Box

Models are used to describe the data generating process, hence prescribe the probabilities of the observed data $\mathcal{D}$

$$p(\mathcal{D}|\theta)$$

also known as the **likelihood**.

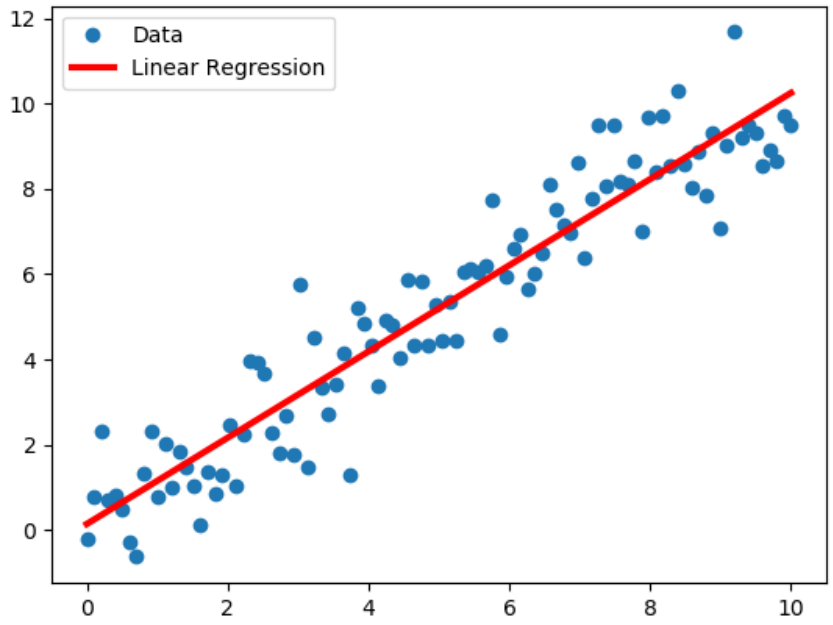
# Examples: Linear Models

**Data**: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$

**Model**:

$$Y = X\theta + \epsilon,\ \epsilon \sim \mathcal{N}(0, \sigma^2 I_n)$$

$$\Rightarrow Y \sim \mathcal{N}(X\theta, \sigma^2 I_n)$$




$$p(Y|X,\theta) = (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{\|Y - X\theta\|_2^2}{2\sigma^2}\right)$$

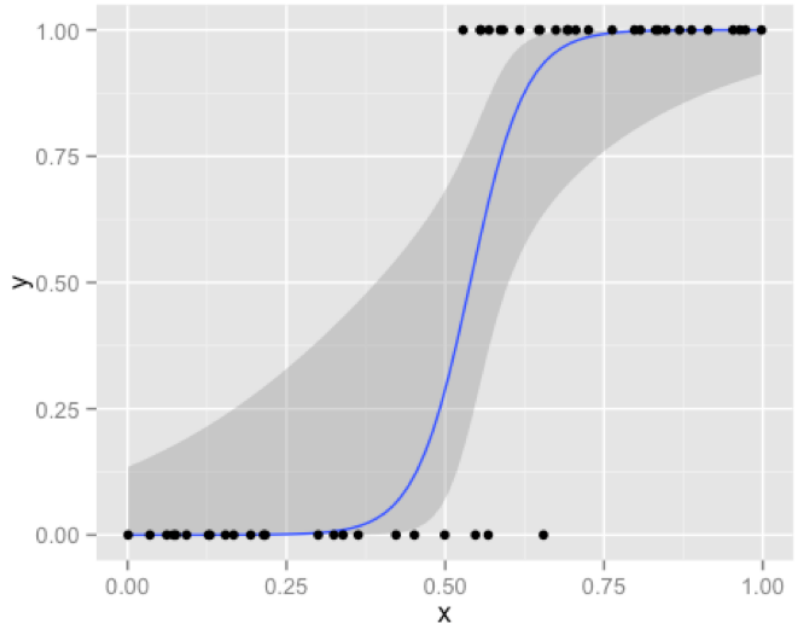
**Data**:

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n, \ y_i \in \{0, 1\}$$

**Model**:

$$Y \sim \text{Bernoulli}(p)$$

$$p = \frac{1}{1 + \exp(-X\theta)}$$




$$p(Y|X, \theta) = \prod_{i=1}^n p_i^{y_i}(1 - p_i)^{1-y_i}$$

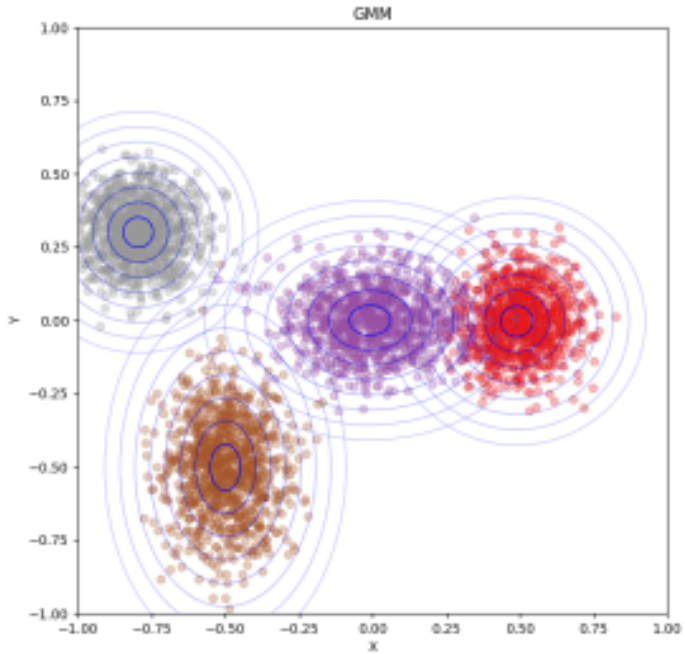
# Examples: Gaussian Mixture Model

**Data**: $\mathcal{D} = \{y_i\}_{i=1}^n,\ y_i \in \mathbb{R}^d$

**Model**:

$$y|Z = z \ \sim \ \mathcal{N}(\mu_z, \sigma_z^2 I_d)$$

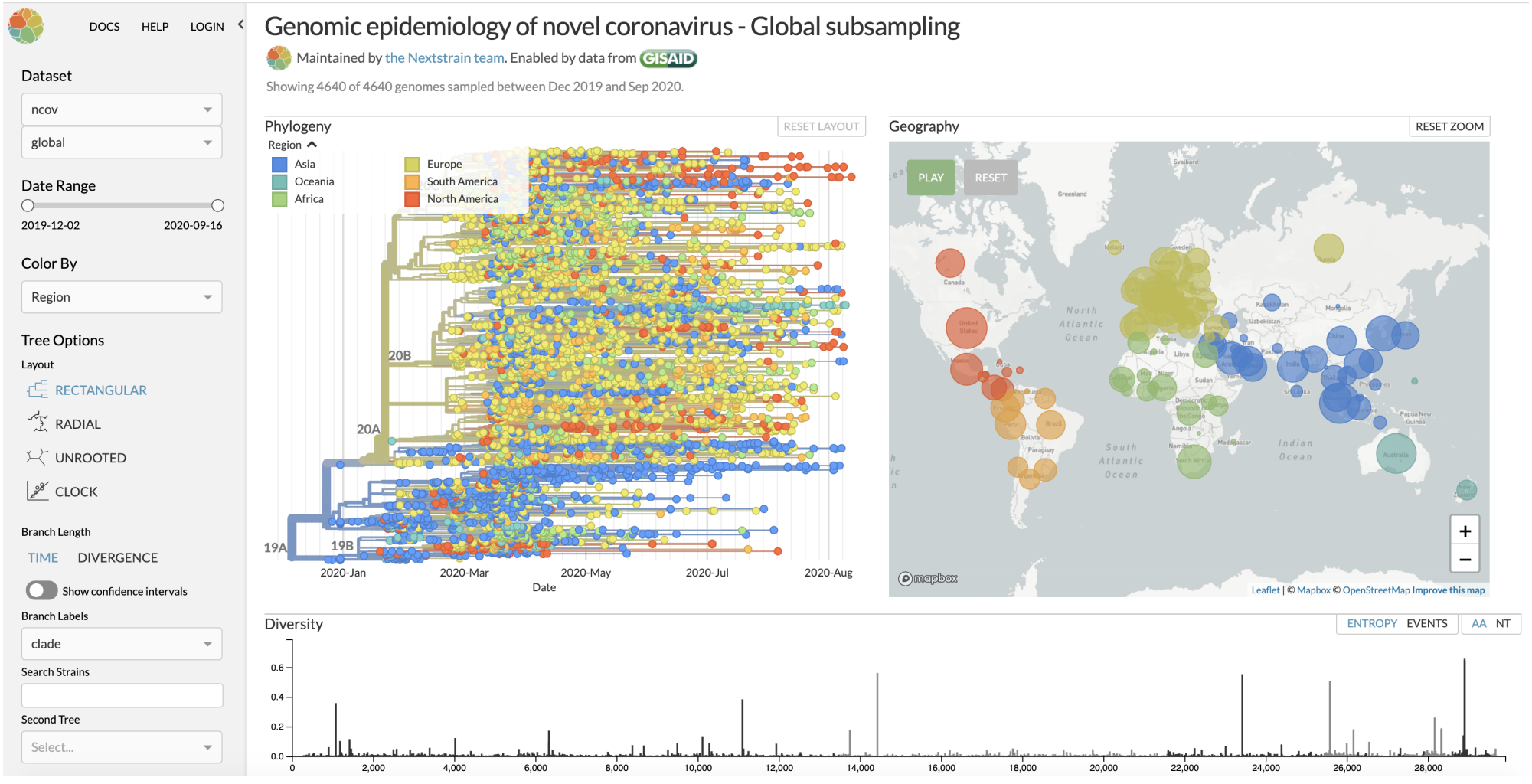
$$Z \sim \text{Categorical}(\alpha)$$




$$p(Y|\mu, \sigma, \alpha) = \prod_{i=1}^{n} \sum_{k=1}^{K} \alpha_k \, (2\pi\sigma_k^2)^{(-d/2)} \exp\left(-\frac{\|y_i - \mu_k\|_2^2}{2\sigma_k^2}\right)$$

# Examples: Phylogenetic Model





# Examples: Phylogenetic Model

**Data**: DNA sequences $\mathcal{D} = \{y_i\}_{i=1}^n$

```
CTTTTCAAGG AGTATTTCCT ATGAACGAGT TAGACGGCAT
CATTGCAAAG GGAATAATCT ATGAACGCAA TAATTATTGA
CATTTTCAGG ATAACTTTCT ATGAAAGTAA ACTTAATACT
GAAAAGAAAT CGAGGCAAAA ATGAGCAAAG TCAGACTCGC
TGCAAAAAAA GGAAGACCAT ATGCTTGACG CTCAAACCAT
TTTTTGTGGA GAAGACGCGT GTGATTGTTA AACGACCCGT
GTTATTAAGG ATATGTTCAT ATGTTTTTCA AAAAGAACCT
TACCCACCGG ATTTTTTACCC ATGCTCACCG TTAAGCAGAT
AATCAAAATG GAATAAAATC ATGCTACCAT CTATTTCAAT
ATCACAGGGG AAGGTGAGAT ATGCACTCTC AAATCTGGGT
ACATCCAGTG AGAGAGACCG ATGCATCCGA TGCTGAACAT
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TTTTTGTGGA GAAGACGCGT GTGATTGTTA AACGACCCGT
GTTATTAAGG ATATGTTCAT ATGTTTTTCA AAAAGAACCT
TACCCACCGG ATTTTTTACCC ATGCTCACCG TTAAGCAGAT
AATCAAAATG GAATAAAATC ATGCTACCAT CTATTTCAAT
ATCACAGGGG AAGGTGAGAT ATGCACTCTC AAATCTGGGT
ACATCCAGTG AGAGAGACCG ATGCATCCGA TGCTGAACAT
```
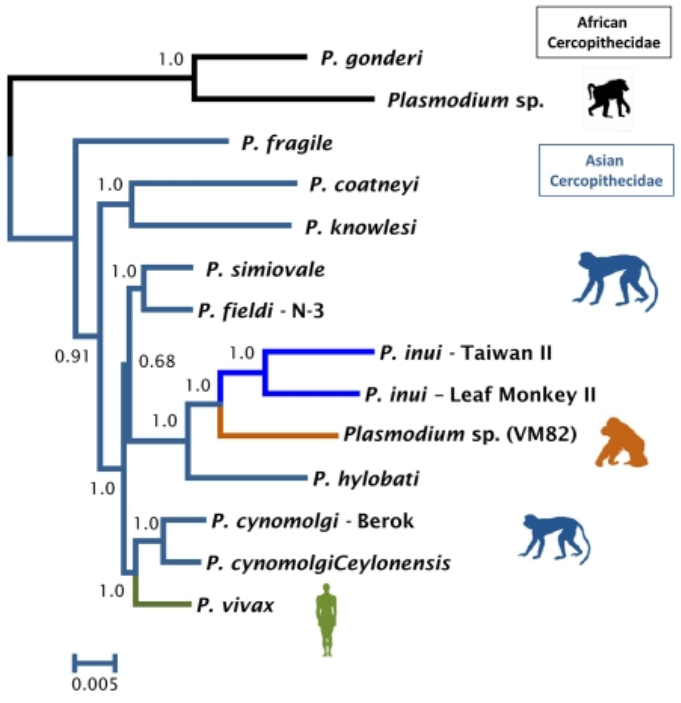



# Examples: Phylogenetic Model

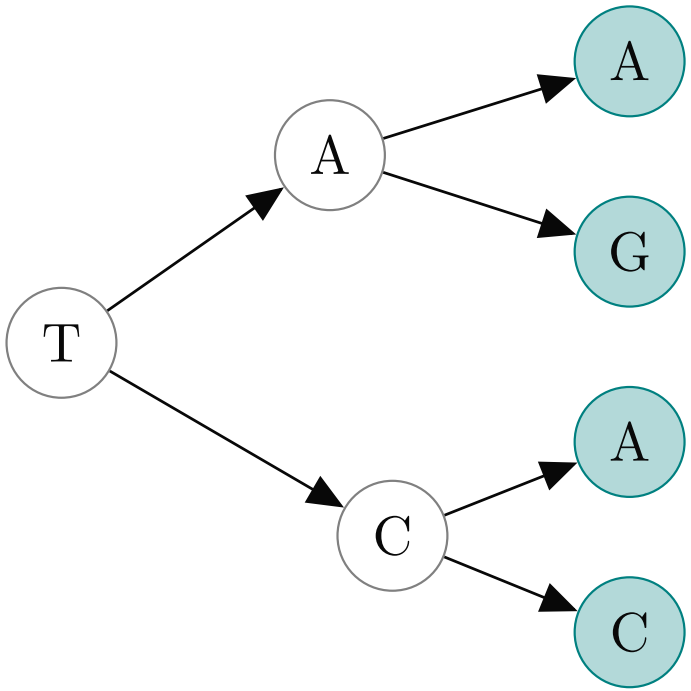


**Data**: DNA sequences $\mathcal{D} = \{y_i\}_{i=1}^n$

**Model**: Phylogenetic tree: $(\tau, q)$.
Substitution model:

- stationary distribution: $\eta(a_\rho)$.
- transition probability:

$$p(a_u \to a_v | q_{uv}) = P_{a_u a_v}(q_{uv})$$



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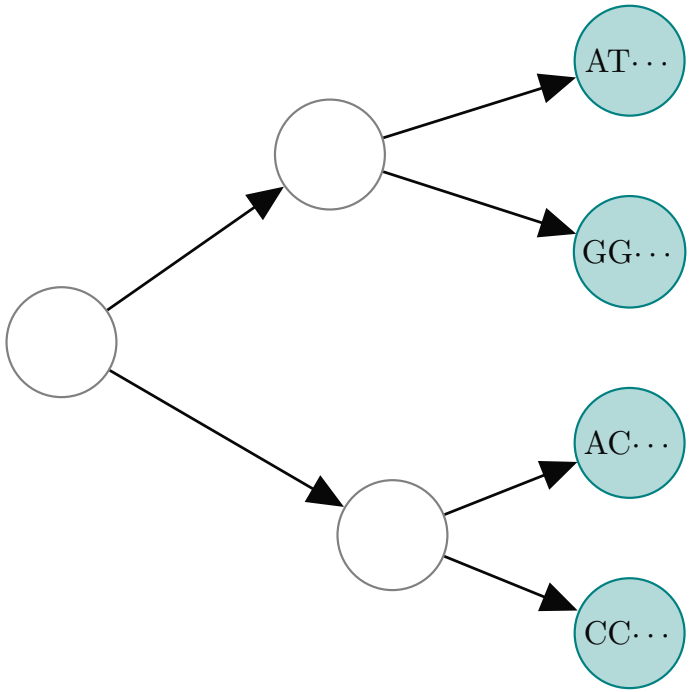


$$p(Y|\tau, q) = \prod_{i=1}^{n} \sum_{a^i} \eta(a_\rho^i) \prod_{(u,v)\in E(\tau)} P_{a_u^i a_v^i}(q_{uv})$$

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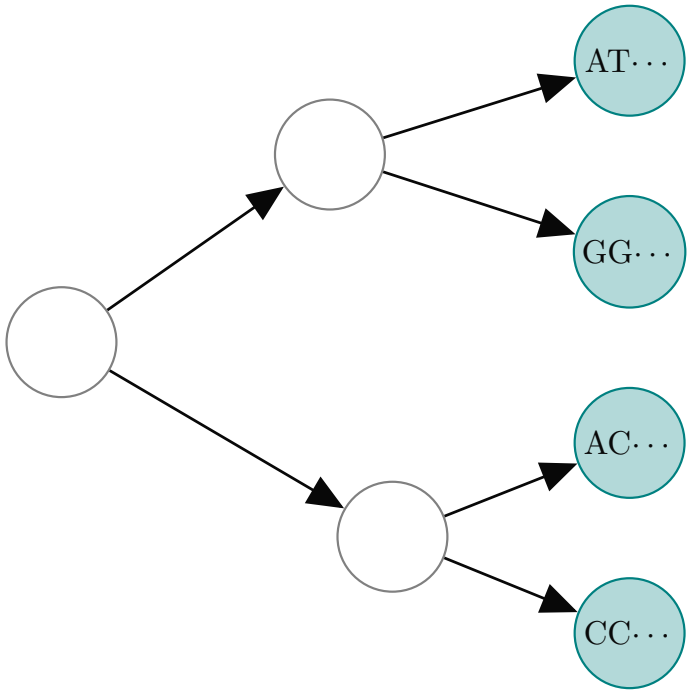


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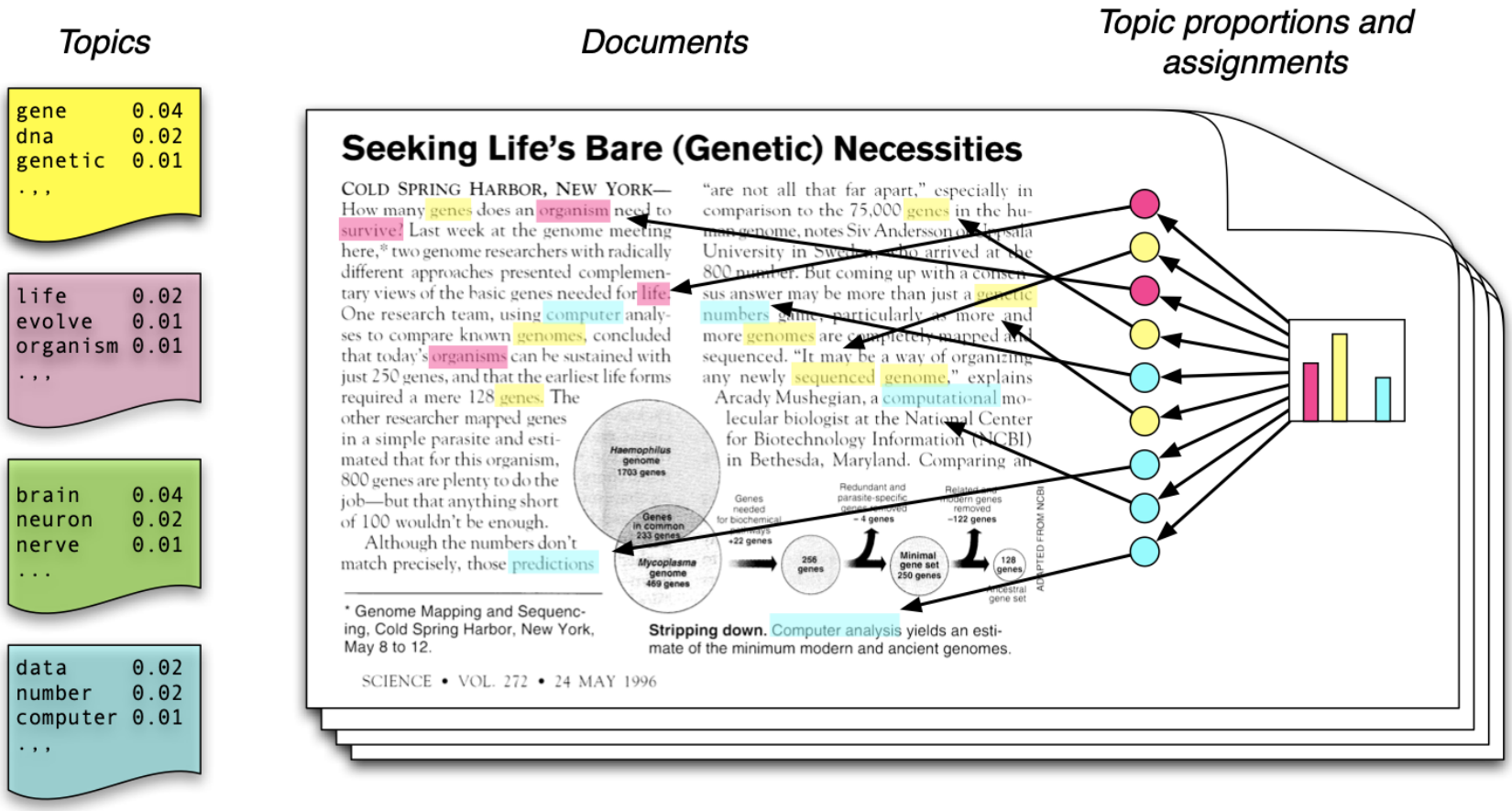
where $a^i$ agree with $y_i$ at the tips

# Examples: Latent Dirichlet Allocation



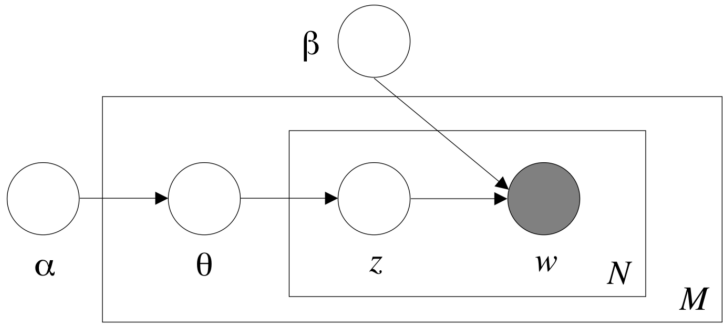



- Each topic is a distribution over words
- Documents exhibit multiple topics

# Examples: Latent Dirichlet Allocation



**Data**: a corpus $\mathcal{D} = \{\boldsymbol{w}_i\}_{i=1}^{M}$

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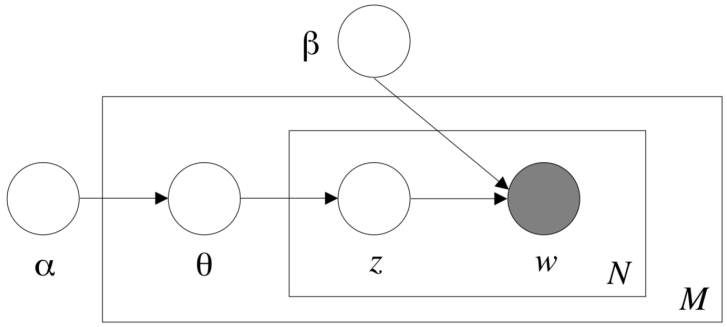


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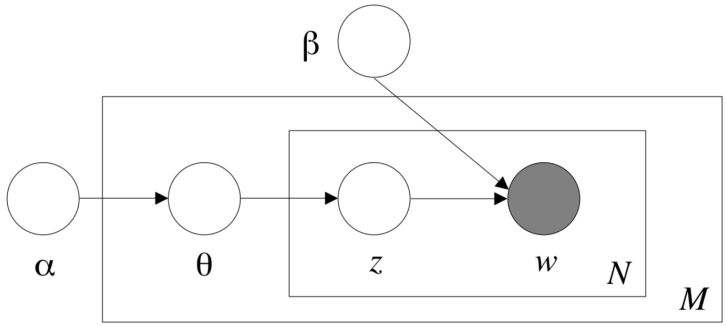


**Model**: for each document $\boldsymbol{w}$ in $\mathcal{D}$,

- choose a mixture of topics $\theta \sim \mathrm{Dir}(\alpha)$
- for each of the $N$ words $w_n$,

$$z_n \sim \mathrm{Multinomial}(\theta), \quad w_n|z_n, \beta \sim p(w_n|z_n, \beta)$$

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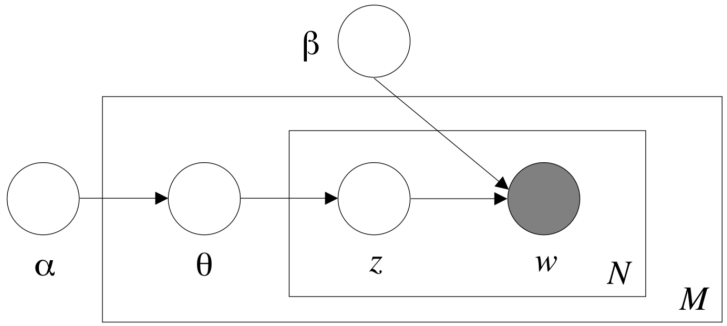


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$$z_n \sim \text{Multinomial}(\theta), \quad w_n|z_n, \beta \sim p(w_n|z_n, \beta)$$

$$p(\mathcal{D}|\alpha, \beta) = \prod_{d=1}^{M} \int p(\theta_d|\alpha) \prod_{n=1}^{N_d} \sum_{z_{dn}} p(z_{dn}|\theta_d) p(w_{dn}|z_{dn}, \beta) \, d\theta_d$$

Many well-known distributions take the following form

$$p(y|\theta) = h(y) \exp\left(\phi(\theta) \cdot T(y) - A(\theta)\right)$$

- $\phi(\theta)$: natural/canonical parameters
- $T(y)$: sufficient statistics
- $A(\theta)$: log-partition function

$$A(\theta) = \log\left(\int_y h(y) \exp(\phi(\theta) \cdot T(y))\, dy\right)$$

# Examples: Bernoulli Distribution

$Y \sim \text{Bernoulli}(\theta)$:

$$\begin{aligned} p(y|\theta) &= \theta^y (1-\theta)^{1-y} \\ &= \exp\left(\log\left(\frac{\theta}{1-\theta}\right) y + \log(1-\theta)\right) \end{aligned}$$

- $\phi(\theta) = \log\left(\frac{\theta}{1-\theta}\right)$
- $T(y) = y$
- $A(\theta) = -\log(1-\theta) = \log(1+e^{\phi(\theta)})$
- $h(y) = 1$

# Examples: Gaussian Distribution

$Y \sim \mathcal{N}(\mu, \sigma^2)$:

$$
\begin{aligned}
p(y|\mu, \sigma^2) &= \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2\right) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left(\frac{\mu}{\sigma^2}y - \frac{1}{2\sigma^2}y^2 - \frac{\mu^2}{2\sigma^2} - \log\sigma\right)
\end{aligned}
$$

- $\phi(\theta) = [\frac{\mu}{\sigma^2}, -\frac{1}{2\sigma^2}]^T$
- $T(y) = [y, y^2]^T$
- $A(\theta) = \frac{\mu^2}{2\sigma^2} + \log\sigma$
- $h(y) = \frac{1}{\sqrt{2\pi}}$

$Y = \{y_i\}_{i=1}^n$, $y_i \sim p(y_i|\theta)$, the Log-likelihood

$$L(\theta; Y) = \sum_{i=1}^{n} \log p(y_i|\theta)$$

The gradient of $L$ with respect to $\theta$ is called the **score**

$$s(\theta) = \frac{\partial L}{\partial \theta}$$

The expected value of the score is zero

$$\mathbb{E}(s) = \sum_{i=1}^{n} \int \frac{\partial \log p(y_i|\theta)}{\partial \theta} p(y_i|\theta)\, dy_i = \sum_{i=1}^{n} \frac{\partial}{\partial \theta} \int p(y_i|\theta)\, dy_i = 0$$

**Fisher information** is the variance of the score.

$$\mathcal{I}(\theta) = \mathbb{E}(ss^T)$$

Under mild assumptions (e.g., exponential families),

$$\mathcal{I}(\theta) = -\mathbb{E}\left(\frac{\partial^2 L}{\partial\theta\partial\theta^T}\right)$$

Intuitively, Fisher information is a measure of the curvature of the Log-likelihood function. Therefore, it reflects the sensitivity of model about the parameter at its current value.

- Kullback-Leibler divergence or KL divergence is a measure of statistical distance between two distributions $p(x)$ and $q(x)$

$$D_{KL}(q\|p) = \int q(x) \log \frac{q(x)}{p(x)}\, dx$$

- KL divergence is non-negative

$$D_{KL}(q\|p) = -\int q(x) \log \frac{p(x)}{q(x)} \geq -\log \int p(x)\, dx = 0$$

- Consider a family of distributions $p(x|\theta)$, Fisher information is Hessian of KL-divergence between two distributions $p(x|\theta)$ and $p(x|\theta')$ with respect to $\theta'$ at $\theta' = \theta$

$$\nabla^2_{\theta'} D_{KL}\left(p(x|\theta)\|p(x|\theta')\right)|_{\theta'=\theta} = \mathcal{I}(\theta)$$

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg\max_{\theta} L(\theta) \approx \arg\max_{\theta} \mathbb{E}_{y\sim p_{data}} \log \frac{p(y|\theta)}{p_{data}(y)} \\ &= \arg\min_{\theta} D_{KL}(p_{data}(y)||p(y|\theta))\end{aligned}$$

- **Consistency**. Under weak regularity condition, $\hat{\theta}_{MLE}$ is consistent: $\hat{\theta}_{MLE} \to \theta_0$ in probability as $n \to \infty$, where $\theta_0$ is the "true" parameter
- **Asymptotical Normality**.

$$\hat{\theta}_{MLE} - \theta_0 \to \mathcal{N}(0, \mathcal{I}^{-1}(\theta_0))$$

See Rao 1973 for more details.

# Example: Poisson Distribution



$$L(\theta; y_1, \ldots, y_n) = \sum_{i=1}^{n} y_i \log \theta - n\theta - \sum_{i=1}^{n} \log y_i!$$

$$s(\theta) = \frac{\sum_{i=1}^{n} y_i}{\theta} - n, \quad \mathcal{I}(\theta) = \frac{n}{\theta}$$

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} y_i \log \theta - n\theta = \frac{\sum_{i=1}^{n} y_i}{n}$$

By the **Law of large numbers**

$$\hat{\theta}_{MLE} \xrightarrow{p} \theta_0$$

By **central limit theorem**

$$\hat{\theta}_{MLE} - \theta_0 \xrightarrow{d} \mathcal{N}\left(0, \frac{\theta_0}{n}\right)$$

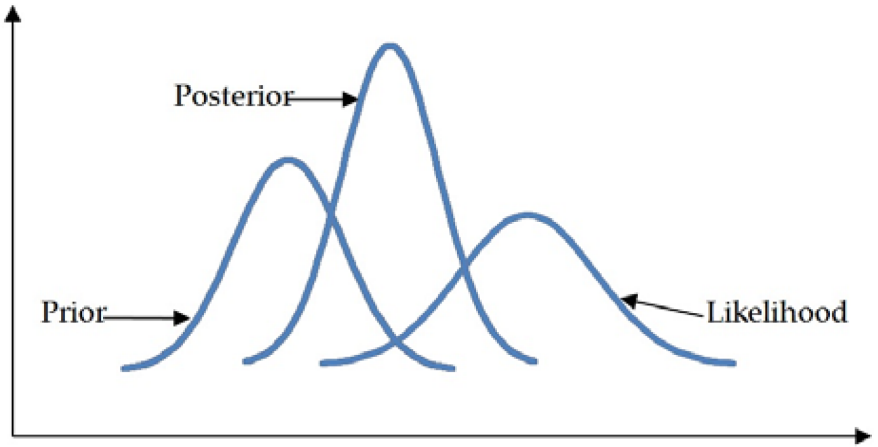
- Can we find an unbiased estimator with smaller variance than $\mathcal{I}^{-1}(\theta_0)$?
- **Cramér-Rao Lower Bound**: For any unbiased estimator $\hat{\theta}$ of $\theta_0$ based on independent observations following the true distribution, the variance of the estimator is bounded by the reciprocal of the Fisher information

$$\mathbb{V}\mathrm{ar}(\hat{\theta}) \geq \frac{1}{\mathcal{I}(\theta_0)}$$

- Sketch of proof: Consider a general estimator $T = t(X)$ with $\mathbb{E}(T) = \psi(\theta_0)$. Let $s$ be the score function,

$$\mathbb{C}\mathrm{ov}(T, s) = \mathbb{E}(Ts) = \psi'(\theta_0) \Rightarrow \mathbb{V}\mathrm{ar}(T) \geq \frac{[\psi'(\theta_0)]^2}{\mathbb{V}\mathrm{ar}(s)} = \frac{[\psi'(\theta_0)]^2}{\mathcal{I}(\theta_0)}$$

In Bayesian statistics, besides specifying a model $p(y|\theta)$ for the observed data, we also specify our **prior** $p(\theta)$ for the model parameters.




**Bayes rule** for inverse probability

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta) \cdot p(\theta)}{p(\mathcal{D})} \propto p(\mathcal{D}|\theta) \cdot p(\theta)$$

known as the **posterior**.

- uncertainty quantification, provides more useful information
- reducing overfitting. Regularization $\Longleftrightarrow$ Prior.

**Prediction**

$$p(x|\mathcal{D}) = \int p(x|\theta, \mathcal{D}) p(\theta|\mathcal{D}) d\theta$$

**Model Comparison**

$$p(m|\mathcal{D}) = \frac{p(\mathcal{D}|m)p(m)}{p(\mathcal{D})}$$

$$p(\mathcal{D}|m) = \int p(\mathcal{D}|\theta, m) p(\theta|m) \, d\theta$$

- **Subjective Priors**. Priors should reflect our beliefs as well as possible. They are subjective, but not arbitrary.
- **Hierarchical Priors**. Priors of multiple levels.

$$\begin{aligned} p(\theta) &= \int p(\theta|\alpha)p(\alpha)\, d\alpha \\ &= \int p(\theta|\alpha)\, d\alpha \int p(\alpha|\beta)p(\beta)\, d\beta \end{aligned}$$

- **Conjugate Priors**. Priors that ease computation, often used to facilitate the development of inference and parameter estimation algorithms.

- **Conjugacy**: prior $p(\theta)$ and posterior $p(\theta|Y)$ belong to the same family of distribution
- Exponential family

$$p(Y|\theta) \propto \exp\left(\phi(\theta) \cdot \sum_i T(y_i) - nA(\theta)\right)$$

- Conjugate prior

$$p(\theta) \propto \exp\left(\phi(\theta) \cdot \nu - \eta A(\theta)\right)$$

- Posterior

$$p(\theta|Y) \propto \exp\left(\phi(\theta) \cdot (\nu + \sum_i T(y_i)) - (n+\eta)A(\theta)\right)$$

# Example: Multinomial Distribution

**Data**: $\mathcal{D} = \{\boldsymbol{x}_i\}_{i=1}^m$. For each $\boldsymbol{x}$ in $\mathcal{D}$

$$p(\boldsymbol{x}|\theta) \propto \exp\left(\sum_{k=1}^K x_k \log \theta_k\right)$$

Use $\mathrm{Dir}(\alpha)$ as the conjugate prior

$$p(\theta) \propto \exp\left(\sum_{k=1}^K (\alpha_k - 1) \log \theta_k\right)$$

$$p(\theta|\mathcal{D}) \propto \exp\left(\sum_{k=1}^K \left(\alpha_k - 1 + \sum_{i=1}^M x_{ik}\right) \log \theta_k\right)$$

Consider random variables $\{X_t\}, t = 0, 1, \ldots$ with state space $\mathcal{S}$

**Markov Property**

$$p(X_{n+1} = x | X_0 = x_0, \ldots, X_n = x_n) = p(X_{n+1} = x | X_n = x_n)$$

*Transition Probability*

$$P_{ij}^n = p(X_{n+1} = j | X_n = i), \quad i, j \in \mathcal{S}.$$

A Markov chain is called *time homogeneous* if $P_{ij}^n = P_{ij}, \forall n$.

A Markov chain is governed by its transition probability matrix.

- Stationary Distribution.

$$\pi^T P = \pi^T.$$

- Ergodic Theorem. If the Markov chain is irreducible and aperiodic, with stationary distribution $\pi$, then

$$X_n \xrightarrow{d} \pi$$

and for any function $h$

$$\frac{1}{n}\sum_{t=1}^{n} h(X_t) \to \mathbb{E}_\pi h(X), \quad n \to \infty$$

given $\mathbb{E}_\pi |h(X)|$ exists.

# What's Next?



- In general, finding MLE and posterior analytically is difficult. We almost always have to resort to computational methods.
- In this course, we'll discuss a variety of computational techniques for numerical optimization and integration, approximate Bayesian inference methods, with applications in statistical machine learning, computational biology and other related field.

- Consider the following least square problem

$$\text{minimize} \quad L(\beta) = \frac{1}{2}\|Y - X\beta\|^2$$

- Note that this is a quadratic problem, which can be solved by setting the gradient to zero

$$\nabla_\beta L(\beta) = -X^T(Y - X\hat{\beta}) = 0$$
$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

given that the Hessian is positive definite:

$$\nabla^2 L(\beta) = X^T X \succ 0$$

which is true iff $X$ has independent columns.

- In practice, we would like to solve the least square problems with some constraints on the parameters to control the complexity of the resulting model
- One common approach is to use Bridge regression models (Frank and Friedman, 1993)

$$\begin{aligned} \text{minimize} \quad & L(\beta) = \frac{1}{2}\|Y - X\beta\|^2 \\ \text{subject to} \quad & \sum_{j=1}^{p} |\beta_j|^\gamma \leq s \end{aligned}$$

- Two important special cases are ridge regression (Hoerl and Kennard, 1970) $\gamma = 2$ and Lasso (Tibshirani, 1996) $\gamma = 1$

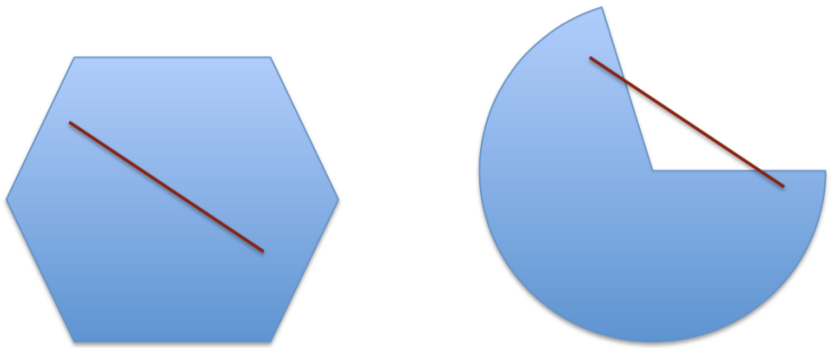
- In general, optimization problems take the following form:

$$\begin{array}{rll} \text{minimize} & f_0(x) & \\ \text{subject to} & f_i(x) \leq 0, & i = 1, \ldots, m \\ & h_j(x) = 0, & j = 1, \ldots, p \end{array}$$

- We are mostly interested in **convex** optimization problems, where the objective function $f_0(x)$, the inequality constraints $f_i(x)$ and the equality constraints $h_j(x)$ are all convex functions.

- A set $C$ is *convex* if the line segment between any two points in $C$ also lies in $C$, i.e.,

$$\theta x_1 + (1-\theta)x_2 \in C, \quad \forall x_1, x_2 \in C,\ 0 \le \theta \le 1$$

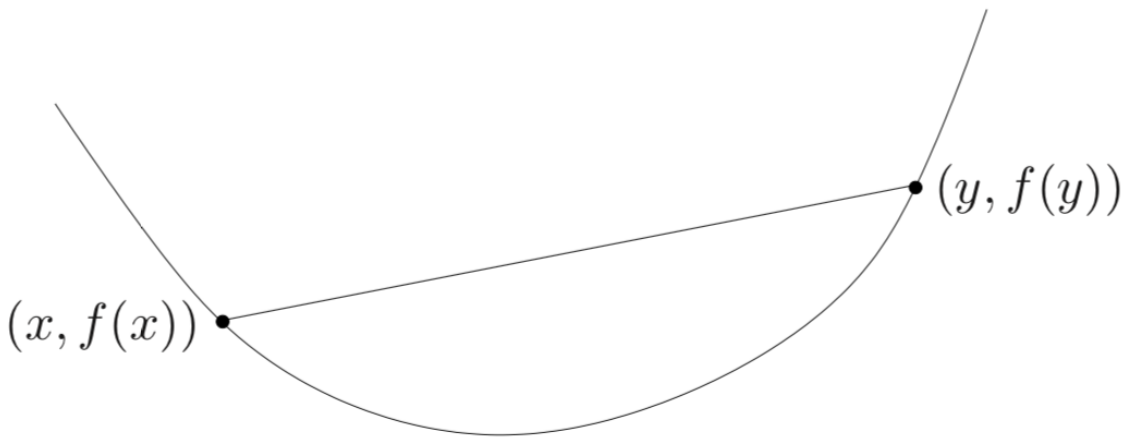


Convex Set Non-convex Set

- If $C$ is a convex set in $\mathbb{R}^n$ and $f(x) : \mathbb{R}^n \to \mathbb{R}^n$ is an affine function, then $f(C)$, i.e., the image of $C$ is also a convex set.

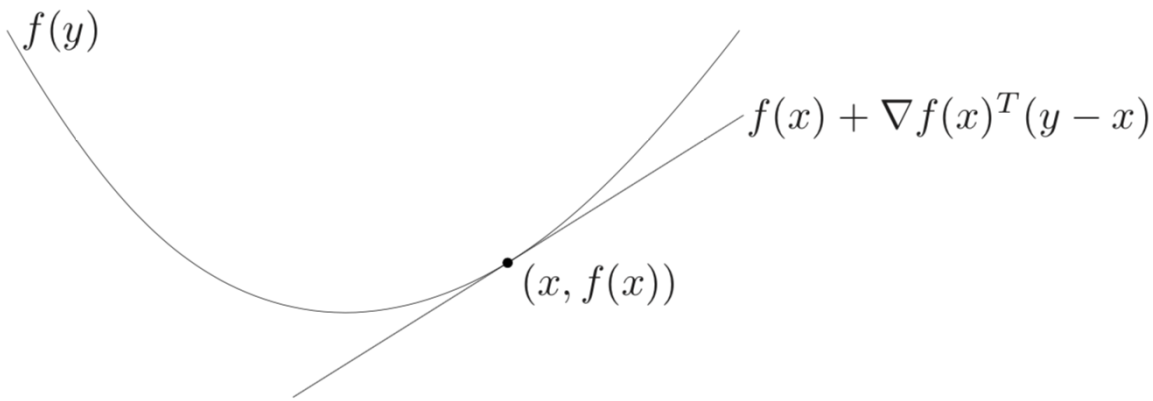
- A function $f : \mathbb{R}^n \to \mathbb{R}$ is *convex* if its domain $D_f$ is a convex set, and $\forall x, y \in D_f$ and $0 \leq \theta \leq 1$

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y)$$




- For example, many norms are convex functions

$$\|x\|_p = (\sum_i |x_i|^p)^{1/p}, \quad p \geq 1$$




- First order conditions. Suppose $f$ is differentiable, then $f$ is convex iff $D_f$ is convex and

$$f(y) \geq f(x) + \nabla f(x)^T(y - x), \quad \forall x, y \in D_f$$

**Corollary**: For convex function $f$,

$$f(\mathbb{E}(X)) \leq \mathbb{E}(f(X))$$

- Second order conditions. $\nabla^2 f(x) \succeq 0$, $\forall x \in D_f$

- Optimial value $p^* = \inf\{f_0(x) | f_i(x) \leq 0,\ h_j(x) = 0\}$
- $x$ is feasible if $x \in D = \bigcap_{i=0}^{m} D_{f_i} \cap \bigcap_{j=1}^{p} D_{h_j}$ and satisfies the constraints.
- A feasible $x^*$ is optimal if $f(x^*) = p^*$
- Optimality criterion. Assuming $f_0$ is convex and differentiable, $x$ is optimal iff

$$\nabla f_0(x)^T (y - x) \geq 0, \quad \forall \text{ feasible y}$$

Remark: for unconstrained problems, $x$ is optimial iff

$$\nabla f_0(x) = 0$$

- Consider a general optimization problem

$$\begin{array}{rll} \text{minimize} & f_0(x) & \\ \text{subject to} & f_i(x) \leq 0, & i = 1, \ldots, m \\ & h_j(x) = 0, & j = 1, \ldots, p \end{array}$$

- To take the constraints into account, we augment the objective function with a weighted sum of the constraints and define the **Lagrangian** $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ as

$$L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{j=1}^{p} \nu_j h_j(x)$$

where $\lambda$ and $\nu$ are dual variables or *Lagrangian multipliers*.

- We define the Lagrangian dual function as follows

$$g(\lambda, \nu) = \inf_{x \in D} L(x, \lambda, \nu)$$

- The dual function is the pointwise infimum of a family of affine functions of $(\lambda, \nu)$, it is concave, even when the original problem is not convex.
- If $\lambda \geq 0$, for each feasible point $\tilde{x}$

$$g(\lambda, \nu) = \inf_{x \in D} L(x, \lambda, \nu) \leq L(\tilde{x}, \lambda, \nu) \leq f_0(\tilde{x})$$

- Therefore, $g(\lambda, \nu)$ is a lower bound for the optimial value

$$g(\lambda, \nu) \leq p^*, \quad \forall \lambda \geq 0, \nu \in \mathbb{R}^p$$

- Finding the best lower bound leads to the Lagrangian dual problem

$$\text{maximize} \;\; g(\lambda, \nu), \quad \text{subject to} \;\; \lambda \geq 0$$

- The above problem is a convex optimization problem.
- We denote the optimal value as $d^*$, and call the corresponding solution $(\lambda^*, \nu^*)$ the dual optimal
- In contrast, the original problem is called the primal problem, whose solution $x^*$ is called primal optimal

- $d^*$ is the best lower bound for $p^*$ that can be obtained from the Lagrangian dual function.
- Weak Duality

$$d^* \leq p^*$$

- The difference $p^* - d^*$ is called the *optimal dual gap*
- Strong Duality

$$d^* = p^*$$

- Strong duality doesn't hold in general, but if the primal is convex, it usually holds under some conditions called *constraint qualifications*
- A simple and well-known constraint qualification is Slater's condition: there exist an $x$ in the relative interior of $D$ such that

$$f_i(x) < 0, \quad i = 1, \ldots, m, \qquad Ax = b$$

# Complementary Slackness

- Consider primal optmial $x^*$ and dual optimal $(\lambda^*, \nu^*)$
- If strong duality holds

$$\begin{aligned} f_0(x^*) &= g(\lambda^*, \nu^*) \\ &= \inf_x \left( f_0(x) + \sum_{i=1}^m \lambda_i^* f_i(x) + \sum_{i=1}^p v_j^* h_i(x) \right) \\ &\leq f_0(x^*) + \sum_{i=1}^m \lambda_i^* f_i(x^*) + \sum_{i=1}^p v_j^* h_i(x^*) \\ &\leq f_0(x^*). \end{aligned}$$

- Therefore, these are all equalities

- Important conclusions:
  - $x^*$ minimize $L(x, \lambda^*, \nu^*)$
  - $\lambda_i^* f_i(x^*) = 0, \quad i = 1, \ldots, m$
- The latter is called complementary slackness, which indicates

$$\begin{aligned} \lambda_i^* > 0 \quad &\Rightarrow \quad f_i(x^*) = 0 \\ f_i(x^*) < 0 \quad &\Rightarrow \quad \lambda_i^* = 0 \end{aligned}$$

- When the dual problem is easier to solve, we can find $(\lambda^*, \nu^*)$ and then minimize $L(x, \lambda^*, \nu^*)$. If the resulting solution is primal feasible, then it is primal optimal.

- Consider the entropy maximization problem

$$\begin{aligned} \text{minimize} \quad & f_0(x) = \sum_{i=1}^n x_i \log x_i \\ \text{subject to} \quad & -x_i \leq 0, \quad i = 1, \ldots, n \\ & \sum_{i=1}^n x_i = 1 \end{aligned}$$

- Lagrangian

$$L(x, \lambda, \nu) = \sum_{i=1}^n x_i \log x_i - \sum_{i=1}^n \lambda_i x_i + \nu(\sum_{i=1}^n x_i - 1)$$

- We minimize $L(x, \lambda, \mu)$ by setting $\frac{\partial L}{\partial x}$ to zero

$$\log \hat{x}_i + 1 - \lambda_i + \nu = 0 \Rightarrow \hat{x}_i = \exp(\lambda_i - \nu - 1)$$

- The dual function is

$$g(\lambda, \nu) = -\sum_{i=1}^{n} \exp(\lambda_i - \nu - 1) - \nu$$

- Dual:

$$\text{maximize} \;\; g(\lambda, \nu) = -\exp(-\nu - 1) \sum_{i=1}^{n} \exp(\lambda_i) - \nu, \quad \lambda \geq 0$$

- We find the dual optimal

$$\lambda_i^* = 0, \;\; i = 0, \ldots, n, \quad \nu^* = -1 + \log n$$

- We now minimize $L(x, \lambda^*, \nu^*)$

$$\log x_i^* + 1 - \lambda_i^* + \nu^* = 0 \quad \Rightarrow \quad x_i^* = \frac{1}{n}$$

- Therefore, the discrete probability distribution that has maximum entropy is the uniform distribution

Exercise

Show that $X \sim \mathcal{N}(\mu, \sigma^2)$ is the maximum entropy distribution such that $EX = \mu$ and $EX^2 = \mu^2 + \sigma^2$. How about fixing the first $k$ moments at $EX^i = m_i,\ i = 1, \ldots, k$?

# Karush-Kun-Tucker (KKT) conditions

- Suppose the functions $f_0, f_1, \ldots, f_m, h_1, \ldots, h_p$ are all differentiable; $x^*$ and $(\lambda^*, \nu^*)$ are primal and dual optimal points with zero duality gap
- Since $x^*$ minimize $L(x, \lambda^*, \nu^*)$, the gradient vanishes at $x^*$

$$\nabla f_0(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla f_i(x^*) + \sum_{j=1}^{p} \nu_i^* \nabla h_j(x^*) = 0$$

- Additionally

$$\begin{aligned} f_i(x^*) &\leq 0, \quad i = 1, \ldots, m \\ h_j(x^*) &= 0, \quad j = 1, \ldots, p \\ \lambda_i^* &\geq 0, \quad i = 1, \ldots, m \\ \lambda_i^* f_i(x^*) &= 0, \quad i = 1, \ldots, m \end{aligned}$$

- These are called Karush-Kuhn-Tucker (KKT) conditions

- When the primal problem is convex, the KKT conditions are also sufficient for the points to be primal and dual optimal with zero duality gap.
- Let $\tilde{x}, \tilde{\lambda}, \tilde{\nu}$ be any points that satisfy the KKT conditions, $\tilde{x}$ is primal feasible and minimizes $L(\tilde{x}, \tilde{\lambda}, \tilde{\nu})$

$$\begin{aligned} g(\tilde{\lambda}, \tilde{\nu}) &= L(\tilde{x}, \tilde{\lambda}, \tilde{\nu}) \\ &= f_0(\tilde{x}) + \sum_{i=1}^{m} \tilde{\lambda}_i f_i(\tilde{x}) + \sum_{j=1}^{p} \tilde{\nu}_j h_j(\tilde{x}) \\ &= f_0(\tilde{x}) \end{aligned}$$

- Therefore, for convex optimization problems with differentiable functions that satisfy Slater's condition, the KKT condtions are necessary and sufficient

- Consider the following problem:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}x^T P x + q^T x + r, \quad P \succeq 0 \\ \text{subject to} \quad & Ax = b \end{aligned}$$

- KKT conditions:

$$\begin{aligned} Px^* + q + A^T \nu^* &= 0 \\ Ax^* &= b \end{aligned}$$

- To find $x^*, v^*$, we can solve the above system of linear equations

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