

Statistical Models & Computing Methods

Lecture 1: Introduction



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School of Mathematical Sciences, Peking University

September 09, 2024

- ▶ Class times:
 - ▶ Monday 3:10-5:00pm, Even Friday 1:00-2:50pm
 - ▶ Classroom Building No.3, Room 505
- ▶ Instructor:
 - ▶ Cheng Zhang: chengzhang@math.pku.edu.cn
- ▶ Teaching assistants:
 - ▶ Shiyue Zhang: zhangshiyue@stu.pku.edu.cn
 - ▶ Zhekun Shi: 2100010658@stu.pku.edu.cn
- ▶ Tentative office hours:
 - ▶ 315 Building No.20
 - ▶ Thursday 3:00-5:00pm or by appointment
- ▶ Website:

<https://zcrabbit.github.io/courses/smcm-f24.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.

- ▶ 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).

- ▶ 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.

- ▶ 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

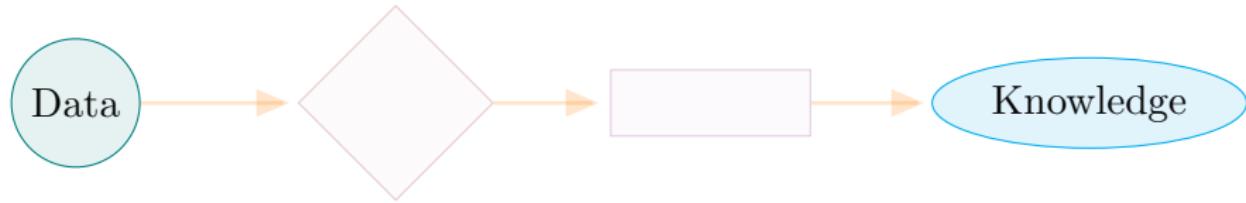
- ▶ Probability and Statistical Inference
- ▶ Stochastic Processes

- ▶ 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
 - ▶ No more than 3 late days per PS
 - ▶ Does not apply to Final Course Project
- ▶ Collaboration policy
 - ▶ Finish your work independently, verbal discussion allowed

- ▶ 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 11/10.
- ▶ 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.

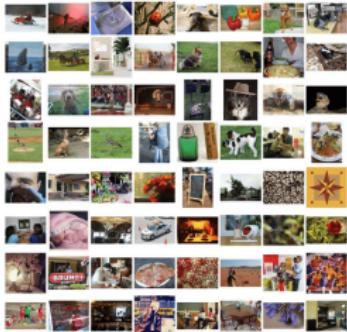
- ▶ A brief overview of statistical approaches

- ▶ Basic concepts in statistical computing



Statistical Pipeline

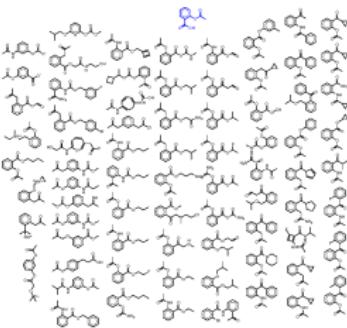
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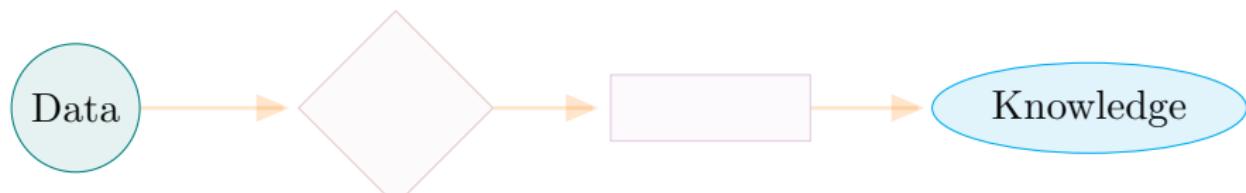
Data

In fact, **China** market has **China** most influential names of the retail and tech space: **Alibaba**, **Baidu**, and **Tencent** (collectively ranked as **Asia's** and is betting big in the global **AI** retail industry space). The **China** government also seems to have a focus on the development of **AI** on series of **workshops** and **conferences** to become the **new** **China**. The Chinese government is also **investing heavily** in **AI** research and **developing** **new** **AI** **technologies** to leverage the power of **AI**. Backed by such powerful initiatives and presence of these companies, the market in APAC is forecast to be the fastest growing **market** with an anticipated **growth** of **over** **10%**.

To further elaborate on the geographical theme, **South Korea** has promoted **more than \$50 billion** of the global there is **AI** and is also setting the **regulatory landscape** of **AI** in the retail market. The **AI** has a significant impact on the retail and needs with **AI** **driven** **systems** **including** **AI** **driven** **private** **label** and **various** **retail** **in** **artificial** **intelligence** **retail**. The region is a huge hub for startups in tandem with the presence of tech firms, such as **Doosan**, **SK**, and **Meguro**.



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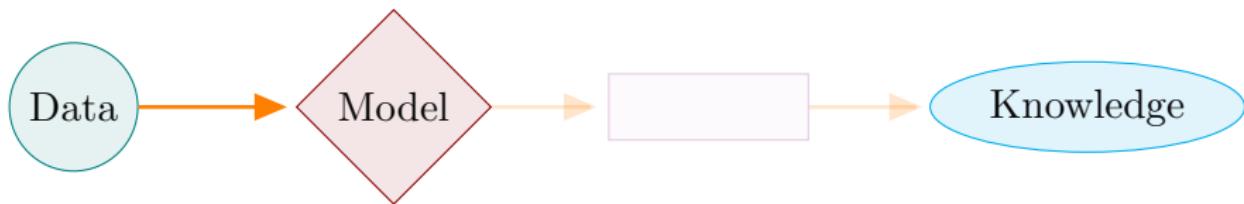
\mathcal{D}

Linear Models

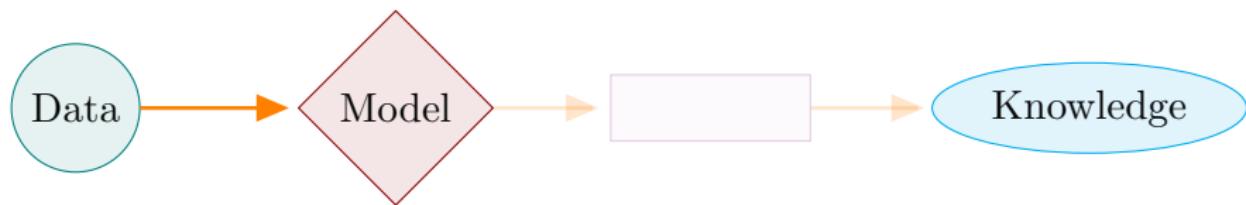
Neural Networks

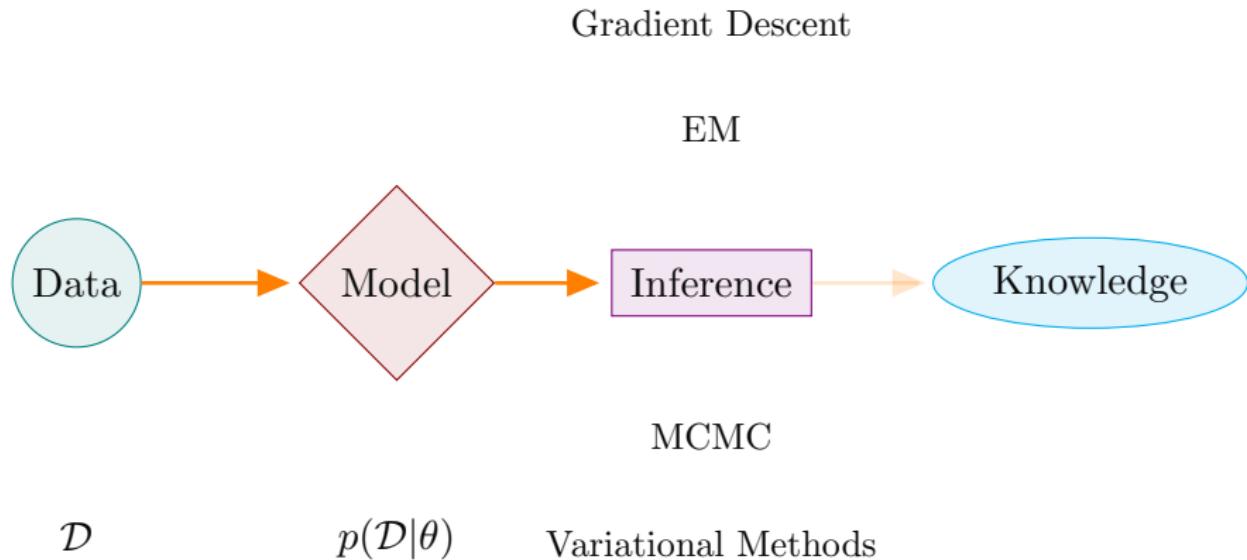
Bayesian Nonparametric Models

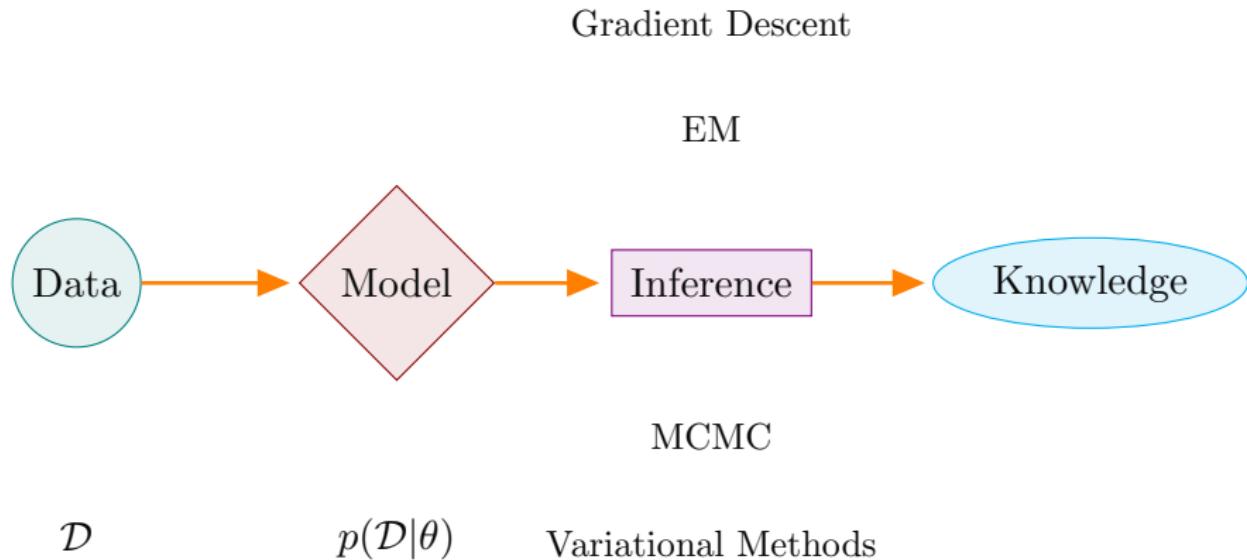
Generalized Linear Models

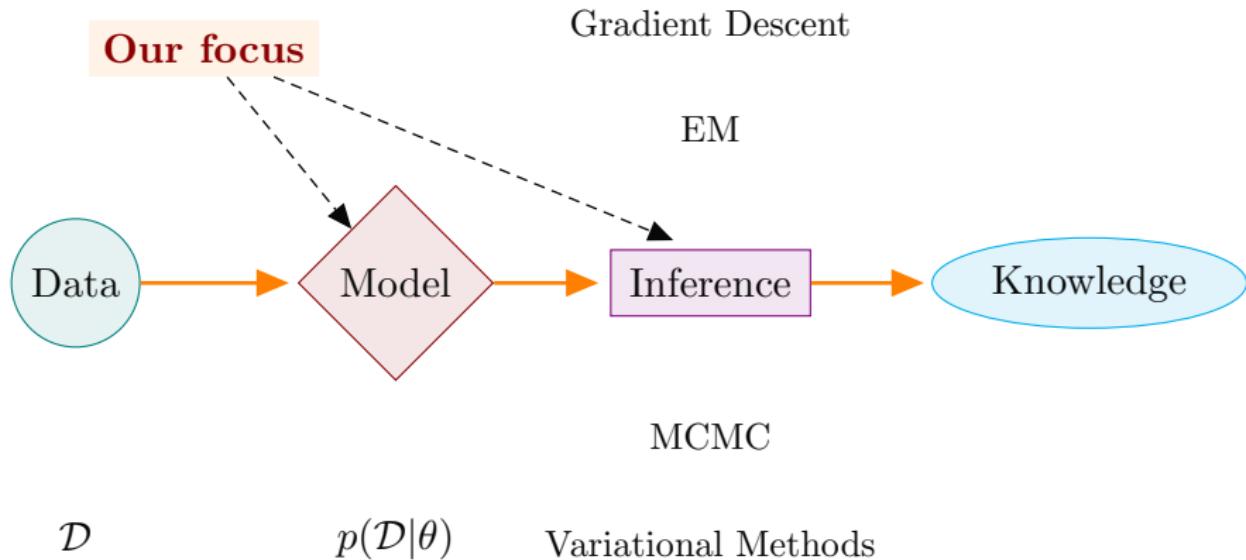


\mathcal{D}

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







“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}

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

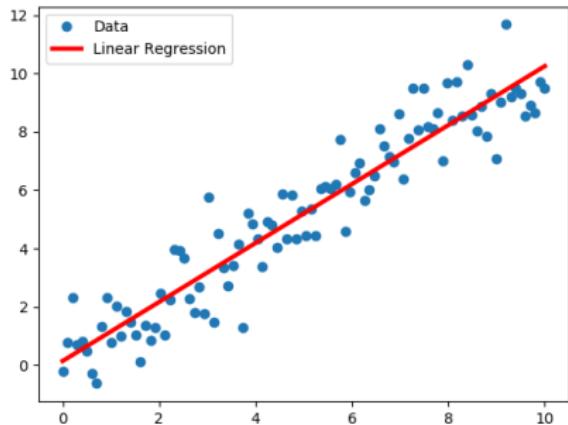
also known as the **likelihood**.

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

Model:

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

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



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

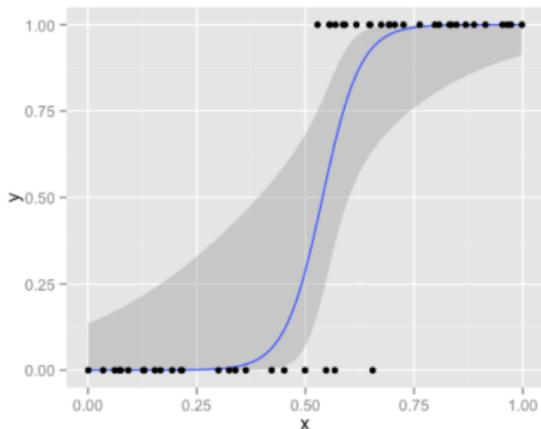
Data:

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

Model:

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

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



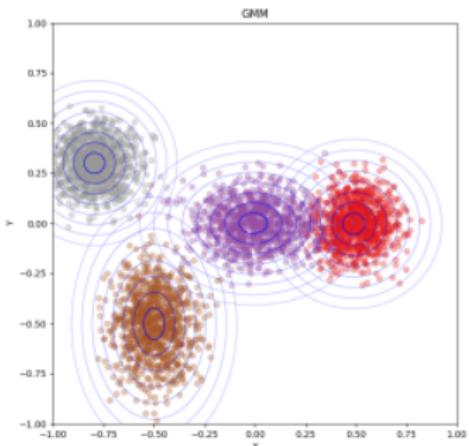
$$p(Y|X, \theta) = \prod_{i=1}^n p_i^{y_i} (1 - p_i)^{1-y_i}$$

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

Model:

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

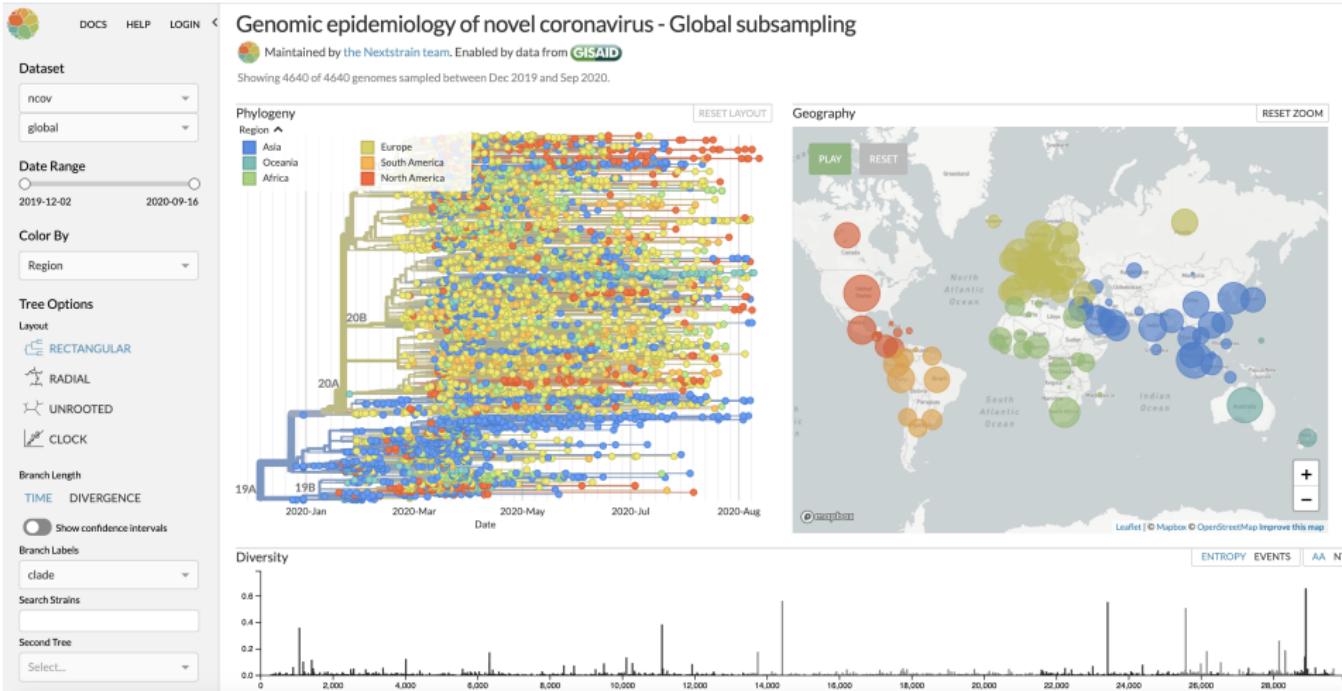
$$Z \sim \text{Categorical}(\alpha)$$



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

Examples: Phylogenetic Model

16/35



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

```
CTTTCAAGG AGTATTCCT ATGAACGAGT TAGACGGCAT
CATTGCAAAG GGAATAATCT ATGAACGCAA TAATTATTGA
CATTTCAGG ATAACTTCT ATGAAAGTAA ACTTAATACT
GAAAAGAAAT CGAGGCCAAA ATGAGCAAAG TCAGACTCGC
TGCAAAAAAA GGAAGACCAT ATGCTTGACG CTCAAACCAT
TTTTGTGGA GAAGACGCGT GTGATTGTTA AACGACCCGT
GTTATTAAAGG ATATGTTCAT ATGTTTTCA AAAAGAACCT
TACCCACCGG ATTTTACCC ATGCTCACCG TTAAGCAGAT
AATCAAAATG GAATAAAATC ATGCTACCAT CTATTCAAT
ATCACAGGGG AAGGTGAGAT ATGCACTCTC AAATCTGGGT
ACATCCAGTG AGAGAGACCG ATGCATCCGA TGCTGAACAT
```

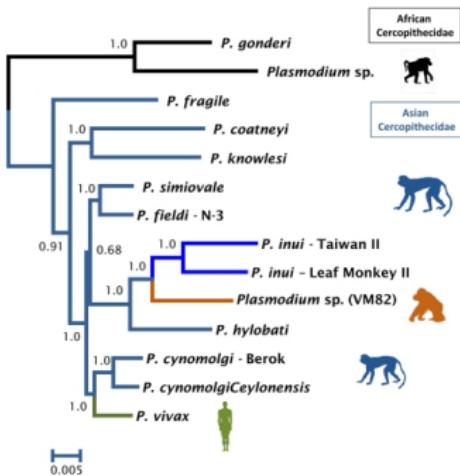


Examples: Phylogenetic Model

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

```
CTTTTCAGG AGTATTCCT ATGAACGAGT TAGACGGCAT
CATTGCAAAG GGAATAATCT ATGAACGCAA TAATTATTGA
CATTTCAGG ATAACTTCT ATGAAAGTAA ACTTAATACT
GAAAAGAAAT CGAGGCCAAA ATGAGCAAAG TCAGACTCGC
TGCAAAAAAA GGAAGACCAT ATGCTTGACG CTCAAACCAT
TTTTGTGGA GAAGACGCGT GTGATTGTTA AACGACCCGT
GTTATTAAAGG ATATGTTCAT ATGTTTTCA AAAAGAACCT
TACCCACCGG ATTTCACCC ATGCTCACCG TTAAGCAGAT
AATCAAATG GAATAAAATC ATGCTACCAT CTATTCAAT
ATCACAGGG AAGGTGAGAT ATGCACTCTC AAATCTGGGT
ACATCCAGTG AGAGAGACCG ATGCATCCGA TGCTGAACAT
```



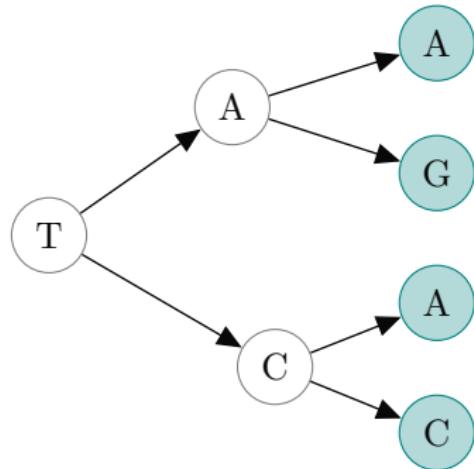
Data: DNA sequences $\mathcal{D} = \{y_i\}_{i=1}^n$

Model: Phylogenetic tree: (τ, q) .

Substitution model:

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

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



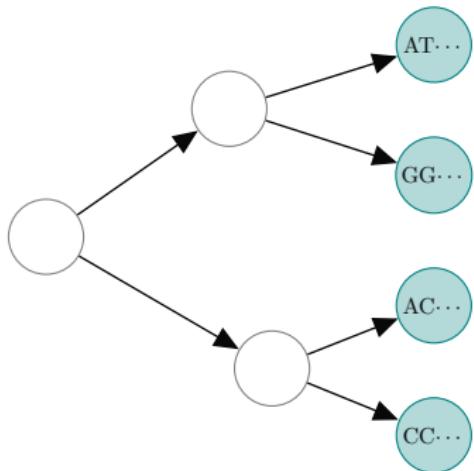
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$$p(Y|\tau, q) = \prod_{i=1}^n \sum_{a^i} \eta(a_\rho^i) \prod_{(u,v) \in E(\tau)} P_{a_u^i a_v^i}(q_{uv})$$

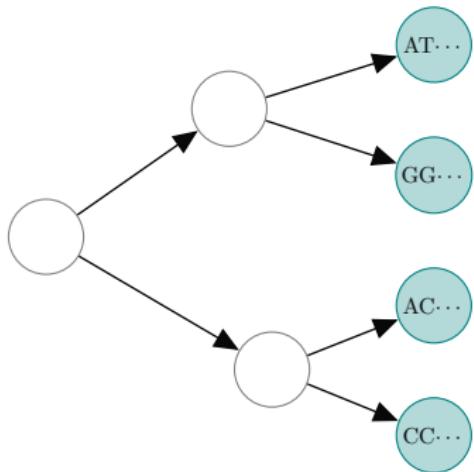
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where a^i agree with y_i at the tips

Topics

gene 0.04
dna 0.02
genetic 0.01
...

life 0.02
evolve 0.01
organism 0.01
...

brain 0.04
neuron 0.02
nerve 0.01
...

data 0.02
number 0.02
computer 0.01
...

Documents

Seeking Life's Bare (Genetic) Necessities

COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here,⁶ two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today's organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

Although the numbers don't match precisely, those predictions

"are not all that far apart," especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Umeå University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a numbers game. In particular, as more and more genomes are completely mapped and sequenced, "It may be a way of organizing any newly sequenced genome," explains

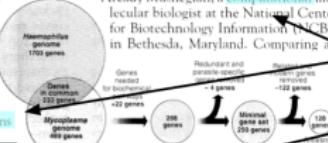
Aradush Mushegian, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing all

Topic proportions and assignments

*** Genome Mapping and Sequencing.** Cold Spring Harbor, New York, May 8 to 12.

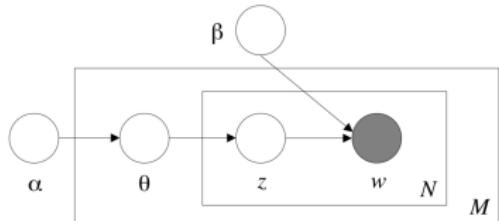
SCIENCE • VOL. 272 • 24 MAY 1996

Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.



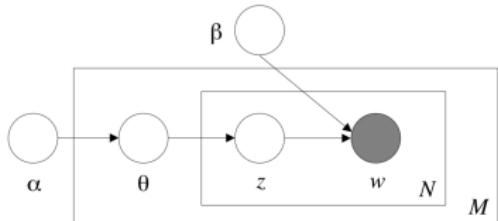
- ▶ Each topic is a distribution over words
- ▶ Documents exhibit multiple topics

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



Model: for each document \mathbf{w} in \mathcal{D} ,

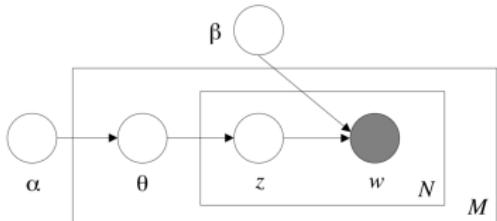
Data: a corpus $\mathcal{D} = \{\mathbf{w}_i\}_{i=1}^M$



Model: for each document \mathbf{w} in \mathcal{D} ,

- ▶ choose a mixture of topics $\theta \sim \text{Dir}(\alpha)$

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

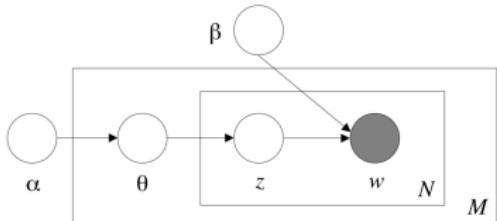


Model: for each document \mathbf{w} in \mathcal{D} ,

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

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

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



Model: for each document \mathbf{w} in \mathcal{D} ,

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

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

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

Many well-known distributions take the following form

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

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

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

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

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

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

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

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

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

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

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

The gradient of L with respect to θ 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 (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 θ' at $\theta' = \theta$

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

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

- ▶ **Consistency.** Under weak regularity condition, $\hat{\theta}_{MLE}$ is consistent: $\hat{\theta}_{MLE} \rightarrow \theta_0$ in probability as $n \rightarrow \infty$, where θ_0 is the “true” parameter
- ▶ **Asymptotical Normality.**

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

See Rao 1973 for more details.

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

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

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

By the **Law of large numbers**

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

By **central limit theorem**

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

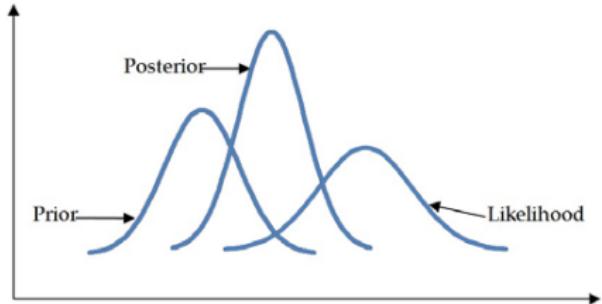
- ▶ Can we find an unbiased estimator with smaller variance than $\mathcal{I}^{-1}(\theta_0)$?
- ▶ **Cramér-Rao Lower Bound:** For any unbiased estimator $\hat{\theta}$ of θ_0 based on independent observations following the true distribution, the variance of the estimator is bounded by the reciprocal of the Fisher information

$$\text{Var}(\hat{\theta}) \geq \frac{1}{\mathcal{I}(\theta_0)}$$

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

$$\text{Cov}(T, s) = \mathbb{E}(Ts) = \psi'(\theta_0) \Rightarrow \text{Var}(T) \geq \frac{[\psi'(\theta_0)]^2}{\text{Var}(s)} = \frac{[\psi'(\theta_0)]^2}{\mathcal{I}(\theta_0)}$$

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 \iff 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

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

- ▶ Posterior

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

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 $\text{Dir}(\alpha)$ 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 $\{X_t\}, t = 0, 1, \dots$ with state space \mathcal{S}

Markov Property

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

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 π , then

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

and for any function h

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

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

- ▶ 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.

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