Bayesian methods

Machine Learning in High Energy Physics
Summer School 2019

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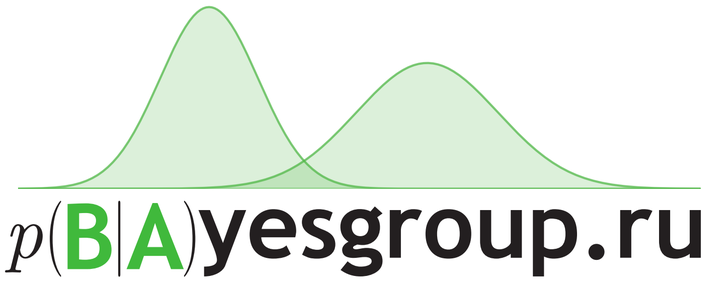

Slides are partially based on lectures of Dmitry Vetrov and Dmitry Kropotov, deepbayes.ru/2018

Outline: Intro to Bayesian methods

- Bayesian framework
- Bayesian ML models and full Bayesian inference
- Conjugate distributions
- Practice

Second part: Variational Inference

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How to work with distributions?

$$\text{Conditional} = \frac{\text{Joint}}{\text{Marginal}}, \quad p(x|y) = \frac{p(x,y)}{p(y)}$$

Product rule

any joint distribution can be expressed as a product of one-dimensional conditional distributions

$$p(x,y,z) = p(x|y,z)p(y|z)p(z)$$

Sum rule

any marginal distribution can be obtained from the joint distribution by integrating out

$$p(y) = \int p(x,y)dx$$

Example

- We have a joint distribution over three groups of variables $p(x, y, z)$
- We observe x and are interested in predicting y
- Values of z are unknown and irrelevant to us
- How to estimate $p(y|x)$ from $p(x, y, z)$?

Example

- We have a joint distribution over three groups of variables $p(x, y, z)$
- We observe x and are interested in predicting y
- Values of z are unknown and irrelevant to us
- How to estimate $p(y|x)$ from $p(x, y, z)$?

$$p(y|x) = \frac{p(x, y)}{p(x)} = \frac{\int p(x, y, z)dz}{\int p(x, y, z)dzdy}$$

Sum rule and product rule allow to obtain arbitrary conditional distributions from the joint one

Bayes theorem

Bayes theorem (follows from product and sum rules):

$$p(y|x) = \frac{p(x,y)}{p(x)} = \frac{p(x|y)p(y)}{p(x)} = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$$

Bayes theorem defines the rule for uncertainty conversion when new information arrives:

$$\text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

Statistical inference

Problem: given i.i.d. data $X = (x_1, ..., x_n)$ from distribution $p(x|\theta)$ one needs to estimate θ

Frequentist framework: use maximum likelihood estimation (MLE)

$$\theta_{ML} = \arg\max p(X|\theta) = \arg\max \prod_{i=1}^{n} p\left(x_i|\theta\right) = \arg\max \sum_{i=1}^{n} \log p\left(x_i|\theta\right)$$

Bayesian framework: encode uncertainty about θ in a prior $p(\theta)$ and apply Bayesian inference

$$p(\theta|X) = \frac{\prod_{i=1}^{n} p\left(x_i|\theta\right) p(\theta)}{\int \prod_{i=1}^{n} p\left(x_i|\theta\right) p(\theta) d\theta}$$

Example: coin tossing

- We have a coin which may be fair or not
- The task is to estimate a probability θ of landing heads up
- Data: 2 tries with a result (H,H)

Head (H) Tail (T)

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Head (H) Tail (T)

Frequentist framework:

In all experiments the coin landed heads up

$$\theta_{ML} = 1$$

→

The coin is not fair and always lands heads up

Example: coin tossing

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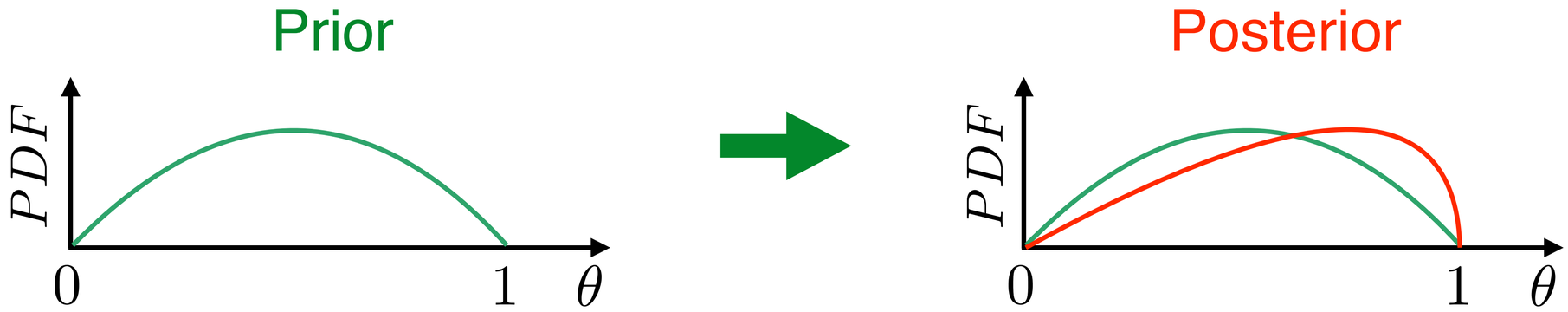
Bayesian framework:



Example: coin tossing

- We have a coin which may be fair or not
- The task is to estimate a probability θ of landing heads up
- Data: 1000 tries with a result (H,H,T,…) — 489 tails and 511 heads

Head (H) Tail (T)

Example: coin tossing

- We have a coin which may be fair or not
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Head (H) Tail (T)

Both frameworks:

Sufficient amount of data matches our expectations → The coin is fair

Frequentist vs. Bayesian frameworks

	Frequentist	Bayesian
Variables	random and deterministic	everything is random
Applicability	$n >> d$	$\forall n$

- The number of tunable parameters in modern ML models is comparable with the sizes of training data
- Frequentist framework is a limit case of Bayesian one:

$$\lim_{n/d \to \infty} p\left(\theta | x_1, \ldots, x_n\right) = \delta\left(\theta - \theta_{ML}\right)$$

Advantages of Bayesian framework

- We can encode our prior knowledge or desired properties of the final solution into a prior distribution
- Prior is a form of regularization
- Additionally to the point estimate of θ posterior contains information about the uncertainty of the estimate

Bayesian framework just provides an alternative point of view, it DOES NOT contradict or deny frequentist framework

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Probabilistic ML model

For each object in the data:

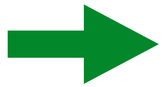
- x — set of observed variables (features)
- y — set of hidden / latent variables (class label / hidden representation, etc.)

Model:

- θ — model parameters (e.g. weights of the linear model)

Discriminative probabilistic ML model

Models $p(y, \theta \mid x)$



Cannot generate new objects — needs x as an input

Usually assumes that prior over θ does not depend on x:

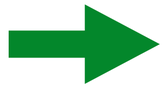
$$p(y, \theta \mid x) = p(y \mid x, \theta)p(\theta)$$

Examples:

- Classification or regression task (hidden space is much easier than the observed one)
- Machine translation (hidden and observed spaces have the same complexity)

Generative probabilistic ML model

Models joint distribution
$p(x, y, \theta) = p(x, y \mid \theta)p(\theta)$



Can generate new objects,
i.e. pairs (x, y)

May be quite difficult to train since the observed space is usually much more complicated than the hidden one

Examples:

- Generation of text, speech, images, etc.

Training Bayesian ML models

We are given training data (X_{tr}, Y_{tr}) and a discriminative model $p(y, \theta \mid x)$

Training stage — Bayesian inference over θ:

$$p\left(\theta \mid X_{tr}, Y_{tr}\right) = \frac{p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)}{\int p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta) d\theta}$$

Result: ensemble of algorithms rather than a single one θ_{ML}

- Ensemble usually outperforms single best model
- Posterior capture all dependencies from the training data that the model could extract and may be used as a new prior later

Predictions of Bayesian ML models

Testing stage:

- From training we have a posterior distribution $p\left(\theta \mid X_{tr}, Y_{tr}\right)$
- New data point x arrives
- We need to compute the predictive distribution on its hidden value y

Ensembling w.r.t. posterior over the parameters θ:

$$p\left(y \mid x, X_{tr}, Y_{tr}\right) = \int p(y \mid x, \theta) p\left(\theta \mid X_{tr}, Y_{tr}\right) d\theta$$

Full Bayesian inference

Training stage:

$$p\left(\theta \mid X_{tr}, Y_{tr}\right) = \frac{p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)}{\int p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta) d\theta}$$

Testing stage:

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May be intractable

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Conjugate distributions

Distribution $p(y)$ and $p(x \mid y)$ are conjugate iff $p(y \mid x)$ belongs to the same parametric family as $p(y)$:

$$p(y) \in \mathcal{A}(\alpha), \quad p(x \mid y) \in \mathcal{B}(y) \qquad \longrightarrow \qquad p(y \mid x) \in \mathcal{A}\left(\alpha'\right)$$

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Intuition:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{\int p(x \mid y)p(y)dy}$$

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Intuition:

$$p(y \mid x) = \frac{\boxed{p(x \mid y)p(y)}}{\int p(x \mid y)p(y)dy} \longleftarrow \text{conjugate}$$

- Denominator is tractable since any distribution in $\mathcal{A}$ is normalized

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Intuition:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{\int p(x \mid y)p(y)dy} \propto p(x \mid y)p(y)$$

- Denominator is tractable since any distribution in $\mathcal{A}$ is normalized
- All we need is to compute α'

Conjugate distributions

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In this case Bayesian inference can be done in closed form

Example: coin tossing

- We have a coin which may be fair or not
- The task is to estimate a probability θ of landing heads up
- Data: $X = (x_1, \ldots, x_n)\,, \quad x \in \{0, 1\}$

Head (H)

Tail (T)

Probabilistic model:

$$p(x, \theta) = p(x \mid \theta) p(\theta)$$

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$$p(x, \theta) = p(x \mid \theta) p(\theta)$$

Likelihood: $Bern(x \mid \theta) = \theta^x (1 - \theta)^{1-x}$

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Prior: ???

Example: coin tossing

How to choose a prior?

- Correct domain: $\theta \in [0, 1]$
- Include prior knowledge: a coin is most likely fair
- Inference complexity: use conjugate prior

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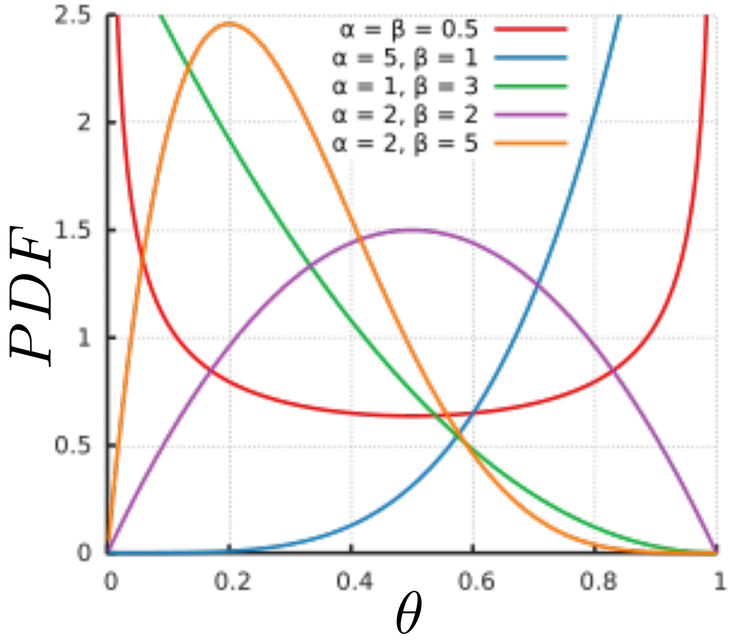
Beta distribution matches all requirements:

$$Beta(\theta \mid a, b) = \frac{1}{\mathrm{B}(a, b)} \theta^{a-1} (1-\theta)^{b-1}$$

Beta distribution



Example: coin tossing

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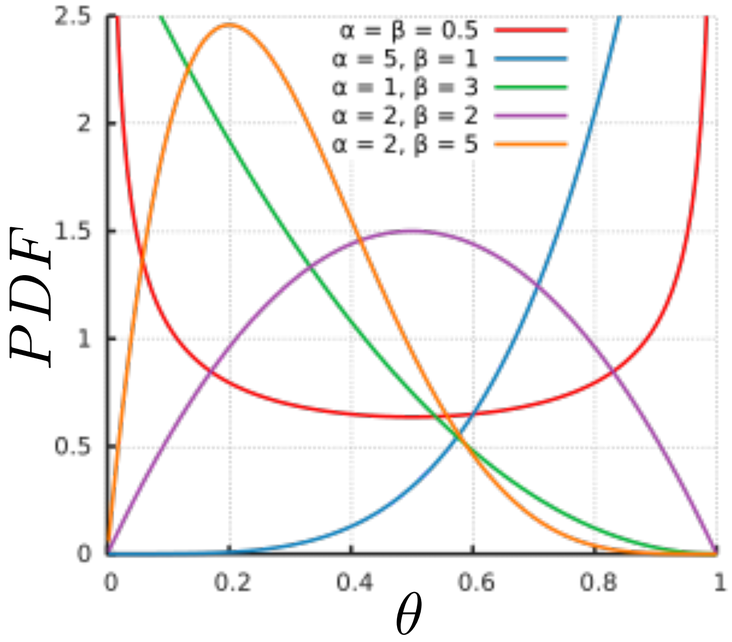

Beta distribution matches all requirements:

$$Beta(\theta \mid a, b) = \frac{1}{\mathrm{B}(a, b)} \theta^{a-1} (1-\theta)^{b-1}$$

* May be also used for the case of most likely unfair coin

Example: coin tossing

Let's check that our likelihood and prior are conjugate:

$$p(x \mid \theta) = \theta^x (1-\theta)^{1-x} \qquad p(\theta) = \frac{1}{\mathrm{B}(a,b)} \theta^{a-1} (1-\theta)^{b-1}$$

Idea — check that prior and posterior lay in the same parametric family:

Example: coin tossing

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Idea — check that prior and posterior lay in the same parametric family:

$$p(\theta) = C\theta^C (1-\theta)^C$$

Example: coin tossing

Let's check that our likelihood and prior are conjugate:

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Idea — check that prior and posterior lay in the same parametric family:

$$p(\theta) = C\theta^C (1-\theta)^C$$

$$p(\theta \mid x) = \frac{1}{C} p(x \mid \theta) p(\theta) = \frac{1}{C} \theta^x (1-\theta)^{1-x} \frac{1}{\mathrm{B}(a,b)} \theta^{a-1}(1-\theta)^{b-1} =$$

$$= C\theta^C (1-\theta)^C$$

Example: coin tossing

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Idea — check that prior and posterior lay in the same parametric family:

$$p(\theta) = \boxed{C\theta^C(1-\theta)^C}$$ conjugacy

$$p(\theta \mid x) = \frac{1}{C} p(x \mid \theta) p(\theta) = \frac{1}{C} \theta^x (1-\theta)^{1-x} \frac{1}{\mathrm{B}(a,b)} \theta^{a-1}(1-\theta)^{b-1} =$$

$$= \boxed{C\theta^C(1-\theta)^C}$$ conjugacy

Example: coin tossing

Bayesian inference after receiving data $X = (x_1, \ldots, x_n)$:

$$p(\theta \mid X) = \frac{1}{Z} p(X \mid \theta) p(\theta) = \frac{1}{Z} \prod_{i=1}^{n} p\left(x_i \mid \theta\right) p(\theta) =$$

Example: coin tossing

Bayesian inference after receiving data $X = (x_1, \ldots, x_n)$:

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$$= \frac{1}{Z} \prod_{i=1}^{n} \theta^{x_i} (1-\theta)^{1-x_i} \frac{1}{\mathrm{B}(a,b)} \theta^{a-1} (1-\theta)^{b-1} =$$

Example: coin tossing

Bayesian inference after receiving data $X = (x_1, \ldots, x_n)$:

$$
\begin{aligned}
p(\theta \mid X) &= \frac{1}{Z} p(X \mid \theta) p(\theta) = \frac{1}{Z} \prod_{i=1}^{n} p\left(x_i \mid \theta\right) p(\theta) = \\
&= \frac{1}{Z} \prod_{i=1}^{n} \theta^{x_i} (1-\theta)^{1-x_i} \frac{1}{\mathrm{B}(a,b)} \theta^{a-1} (1-\theta)^{b-1} = \\
&= \frac{1}{Z'} \theta^{a+\sum_{i=1}^{n} x_i - 1} (1-\theta)^{b+n-\sum_{i=1}^{n} x_i - 1}
\end{aligned}
$$

Example: coin tossing

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$$= \frac{1}{Z} \prod_{i=1}^{n} \theta^{x_i} (1-\theta)^{1-x_i} \frac{1}{\mathrm{B}(a,b)} \theta^{a-1} (1-\theta)^{b-1} =$$

$$= \frac{1}{Z'} \theta^{a+\sum_{i=1}^{n} x_i - 1} (1-\theta)^{b+n-\sum_{i=1}^{n} x_i - 1} = Beta\left(\theta \mid a', b'\right)$$

New parameters: $a' = a + \sum_{i=1}^{n} x_i \qquad b' = b + n - \sum_{i=1}^{n} x_i$

What to do if there is no conjugacy?

Simplest way — approximate posterior with delta function in θ_{MP}:

$$\theta_{MP} = \arg\max p\left(\theta \mid X_{tr}, Y_{tr}\right) = \arg\max p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)$$

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On the testing stage:

$$p\left(y \mid x, X_{tr}, Y_{tr}\right) = \int p(y \mid x, \theta) p\left(\theta \mid X_{tr}, Y_{tr}\right) d\theta \approx p\left(y | x, \theta_{MP}\right)$$

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We do not need to calculate normalisation constant

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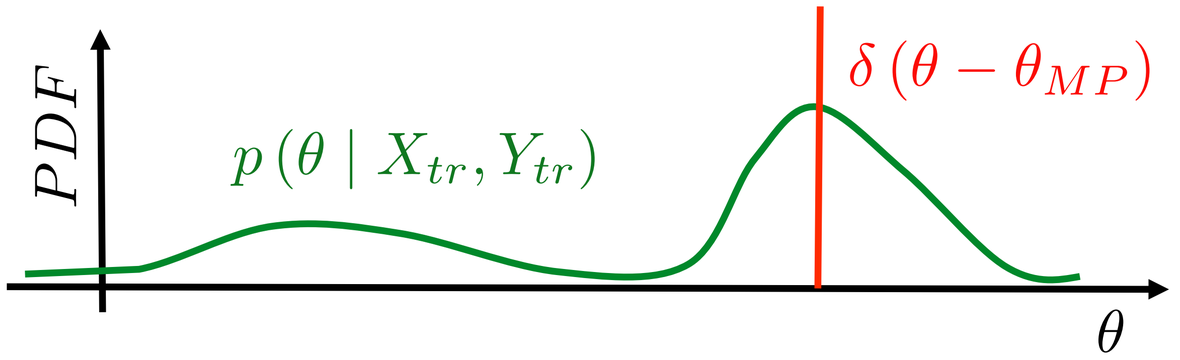

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More advanced techniques are needed
— next lecture.

Key takeaways

- Basic probabilistic rules: product rule, sum rule, Bayes theorem
- Bayesian framework as an alternative approach to building probabilistic models
- Bayesian ML models: training and predictions
- Full Bayesian inference and conjugate distributions

Now let’s practice =)

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The problem set is available here:

http://tiny.cc/c1t78y

Problem 1: basic Bayesian reasoning

Setting

During medical checkup, one of the tests indicates a serious disease. The test has high accuracy 99% (probability of true positive is 99%, probability of true negative is 99%). However, the disease is quite rare, and only one person in 10000 is affected.

Question

Calculate the probability that the examined person has the disease.

Problem 1: basic Bayesian reasoning

- $d \in \{0, 1\}$ — disease (1 means that the person has a disease)
- $t \in \{0, 1\}$ — test (1 means that test says that the person has a disease)

Setting: $p(t = 1 \mid d = 1) = p(t = 0 \mid d = 0) = 0.99, \quad p(d = 1) = 10^{-4}$

Question: $p(d = 1 \mid t = 1) = ?$

Problem 1: basic Bayesian reasoning

- $d \in \{0, 1\}$ — disease (1 means that the person has a disease)
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Setting: $p(t = 1 \mid d = 1) = p(t = 0 \mid d = 0) = 0.99, \quad p(d = 1) = 10^{-4}$

Question: $p(d = 1 \mid t = 1) = ?$

$$p(d = 1 \mid t = 1) = \frac{p(t = 1 \mid d = 1)p(d = 1)}{p(t = 1 \mid d = 1)p(d = 1) + p(t = 1 \mid d = 0)p(d = 0)} =$$

$$= \frac{0.99 \cdot 10^{-4}}{0.99 \cdot 10^{-4} + 0.01 \cdot (1 - 10^{-4})} \approx 1\%$$

Problem 2: frequentist framework

Setting

- $X = \{x_1, \ldots, x_N\}$ — independent dice rolls
- $N_k = \sum_{n=1}^{N} \mathbb{I}(x_n = k)$ — counts
- $p(X \mid \theta) = \prod_{k=1}^{K} \theta_k^{N_k}$ — multinomial likelihood, $\theta \in S_K$

Question

Maximum likelihood estimate for $\theta_{ML} = \arg\max_{\theta \in S_K} \log p(X \mid \theta)$

Problem 2: frequentist framework

θ is restricted to simplex. To omit the inequality restrictions change parameterization to $\mu_k = \log \theta_k, \quad \mu_k \in \mathbb{R}$

The Lagrangian has the form:

$$\mathcal{L}(\mu, \lambda) = \log p(X \mid \exp \mu) + \lambda(\sum_{k=1}^{K} \exp \mu_k - 1) =$$
$$= \sum_{k=1}^{K} (N_k \mu_k - \lambda \exp \mu_k) - \lambda$$

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The Lagrangian has the form:

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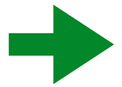
$$= \textstyle\sum_{k=1}^{K} (N_k \mu_k - \lambda \exp \mu_k) - \lambda$$

Differentiation:

$$0 = \frac{\partial \mathcal{L}(\boldsymbol{\mu}, \lambda)}{\partial \mu_k} = N_k - \lambda \exp \mu_k \Rightarrow \theta_k = \exp \mu_k = \frac{N_k}{\lambda}$$
$$0 = \frac{\partial \mathcal{L}(\boldsymbol{\mu}, \lambda)}{\partial \lambda} = \textstyle\sum_{k=1}^{K} \exp \mu_k - 1 \Rightarrow \lambda = \textstyle\sum_{k=1}^{K} N_k$$



$$\theta_k = \frac{N_k}{\sum_{l=1}^{K} N_l}$$

Problem 3: Bayesian framework

Setting

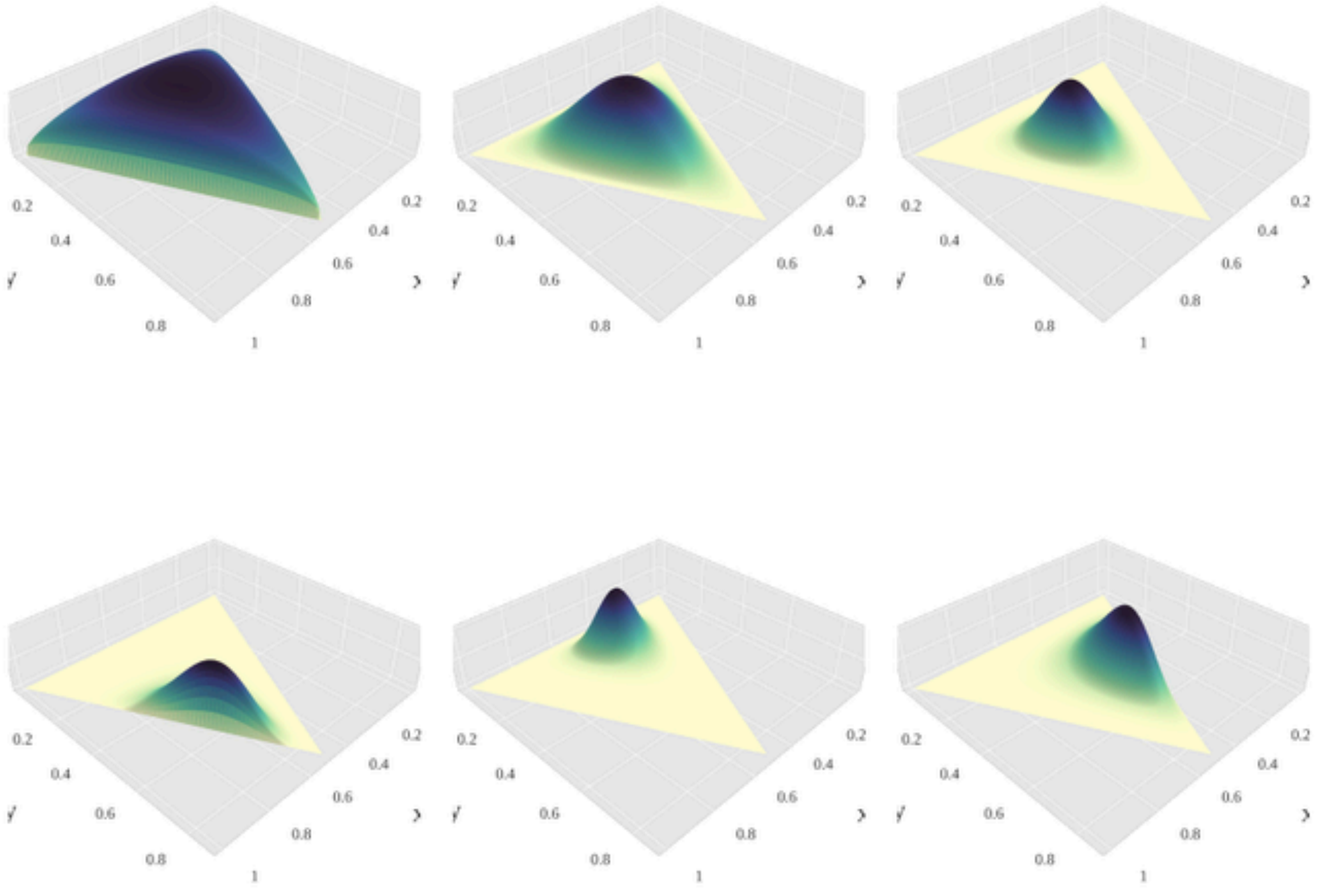
- $p(X \mid \theta) = \prod_{k=1}^{K} \theta_k^{N_k}$ — multinomial likelihood, $\theta \in S_K$
- Dirichlet prior:

$$\mathrm{Dir}(\theta \mid \alpha) = \frac{1}{B(\alpha_1, \ldots, \alpha_K)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}$$

Questions

- Check that likelihood and prior are conjugate
- Compute the posterior $p(\theta|X, \alpha)$
- Compute the predictive posterior $p(x_{N+1} = k|X, \alpha)$

Dirichlet distribution



Beta distribution is a special case of Dirichlet distribution:

$$\mathrm{Dir}(\theta \mid \alpha) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}$$

$$Beta(\theta \mid a, b) \propto \theta^{a-1}(1-\theta)^{b-1}$$

https://en.wikipedia.org/wiki/Dirichlet distribution

Problem 3: Bayesian framework

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Problem 3: Bayesian framework

Probabilistic model: $p(X, \theta) = p(X \mid \theta)p(\theta) = Dir(\theta \mid \alpha) \prod_{k=1}^{K} p\left(x_k \mid \theta\right)$

Problem 3: Bayesian framework

Probabilistic model: $p(X, \theta) = p(X \mid \theta)p(\theta) = Dir(\theta \mid \alpha) \prod_{k=1}^{K} p\left(x_k \mid \theta\right)$

Prior: $p(\theta) = \frac{1}{B(\alpha_1, \ldots, \alpha_K)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} = C \prod_{k=1}^{K} \theta_k^{C}$

Problem 3: Bayesian framework

Probabilistic model: $p(X, \theta) = p(X \mid \theta)p(\theta) = Dir(\theta \mid \alpha) \prod_{k=1}^{K} p\left(x_k \mid \theta\right)$

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Posterior: $p(\theta \mid X) \propto p(X \mid \theta)p(\theta) = \prod_{k=1}^{K} \theta_k^{N_k} \cdot \frac{1}{B(\alpha_1, \ldots, \alpha_K)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} =$

$$= C \prod_{k=1}^{K} \theta_k^{C}$$

Problem 3: Bayesian framework

Probabilistic model: $p(X, \theta) = p(X \mid \theta)p(\theta) = Dir(\theta \mid \alpha) \prod_{k=1}^{K} p\left(x_k \mid \theta\right)$

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$= C \prod_{k=1}^{K} \theta_k^{C}$

conjugate

Problem 3: Bayesian framework

Setting

- $p(X \mid \theta) = \prod_{k=1}^{K} \theta_k^{N_k}$ — multinomial likelihood, $\theta \in S_K$
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Questions

- Check that likelihood and prior are conjugate
- Compute the posterior $p(\theta|X, \alpha)$
- Compute the predictive posterior $p(x_{N+1} = k|X, \alpha)$

Problem 3: Bayesian framework

Likelihood and prior are conjugate → posterior is Dirichlet

$$p(\theta \mid X) \propto p(X \mid \theta)p(\theta) = \prod_{k=1}^{K} \theta_k^{N_k} \cdot \frac{1}{B(\alpha_1, \ldots, \alpha_K)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \propto$$

$$\propto \prod_{k=1}^{K} \theta_k^{N_k + \alpha_k - 1}$$

$$p(\theta \mid X) = Dir(\theta \mid \alpha'), \quad \alpha' = (\alpha_1 + N_1, \ldots, \alpha_K + N_K)$$

Problem 3: Bayesian framework

Setting

- $p(X \mid \theta) = \prod_{k=1}^{K} \theta_k^{N_k}$ — multinomial likelihood, $\theta \in S_K$
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Questions

- Check that likelihood and prior are conjugate
- Compute the posterior $p(\theta|X, \alpha)$
- Compute the predictive posterior $p(x_{N+1} = k|X, \alpha)$

Problem 3: Bayesian framework

$$p(x_{N+1} = k \mid X, \alpha) = \int_{S_K} p(x_{N+1} = k \mid \theta) p(\theta \mid X, \alpha) \mathrm{d}\theta =$$

$$= \frac{\int_{S_K} \theta_k \prod_{k=1}^{K} \theta_k^{N_k + \alpha_k - 1} \mathrm{d}\theta}{B(\alpha_1 + N_1, \ldots, \alpha_K + N_K)} = \frac{B(\alpha_1 + N_1, \ldots, \alpha_k + N_k + 1, \ldots, \alpha_K + N_K)}{B(\alpha_1 + N_1, \ldots, \alpha_k + N_k, \ldots, \alpha_K + N_K)} =$$

$$= \frac{\Gamma(\alpha_1 + N_1) \ldots \Gamma(\alpha_k + N_k + 1) \ldots \Gamma(\alpha_K + N_K)}{\Gamma(\alpha_1 + N_1) \ldots \Gamma(\alpha_k + N_k) \ldots \Gamma(\alpha_K + N_K)} \cdot \frac{\Gamma(\sum_l (\alpha_l + N_l))}{\Gamma(\sum_l (\alpha_l + N_l) + 1)} =$$

$$= \frac{\alpha_k + N_k}{\sum_k \alpha_k + N}$$

Second part: Variational Inference

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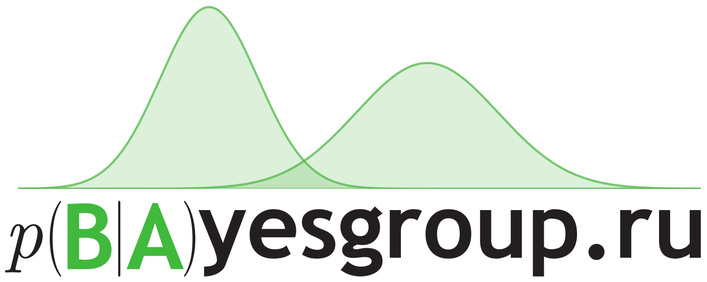
Higher School of Economics, Moscow, Russia



Slides are partially based on lectures of Dmitry Vetrov and Dmitry Kropotov, deepbayes.ru/2018

Outline: Variational Inference

- Variational inference
- Variational mean field approximation
- Variational parametric approximation
- Practice: Gaussian mixture model

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Full Bayesian inference

Training stage:

$$p\left(\theta \mid X_{tr}, Y_{tr}\right) = \frac{p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)}{\int p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta) d\theta}$$

Testing stage:

$$p\left(y \mid x, X_{tr}, Y_{tr}\right) = \int p(y \mid x, \theta) p\left(\theta \mid X_{tr}, Y_{tr}\right) d\theta$$

Full Bayesian inference

Training stage:

$$p\left(\theta \mid X_{tr}, Y_{tr}\right) = \frac{p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)}{\int p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta) d\theta}$$

May be intractable

Testing stage:

$$p\left(y \mid x, X_{tr}, Y_{tr}\right) = \int p(y \mid x, \theta) p\left(\theta \mid X_{tr}, Y_{tr}\right) d\theta$$

Posterior distributions can be calculated analytically only for simple conjugate models!

Approximate inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta)$

Variational Inference

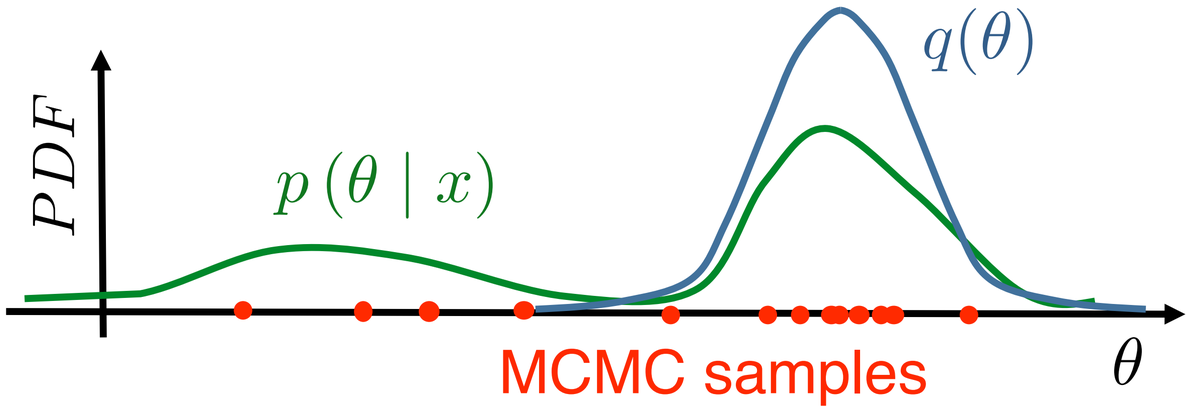
Approximate $p(\theta \mid x) \approx q(\theta) \in \mathcal{Q}$

- Biased
- Faster and more scalable

MCMC

Samples from unnormalized $p(\theta \mid x)$

- Unbiased
- Need a lot of samples



Variational inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta)$

Main idea: find posterior approximation $p(\theta \mid x) \approx q(\theta) \in \mathcal{Q}$, using the following criterion function:

$$F(q) := KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}}$$

Kullback-Leibler divergence
a good mismatch measure between
two distributions over the **same domain**

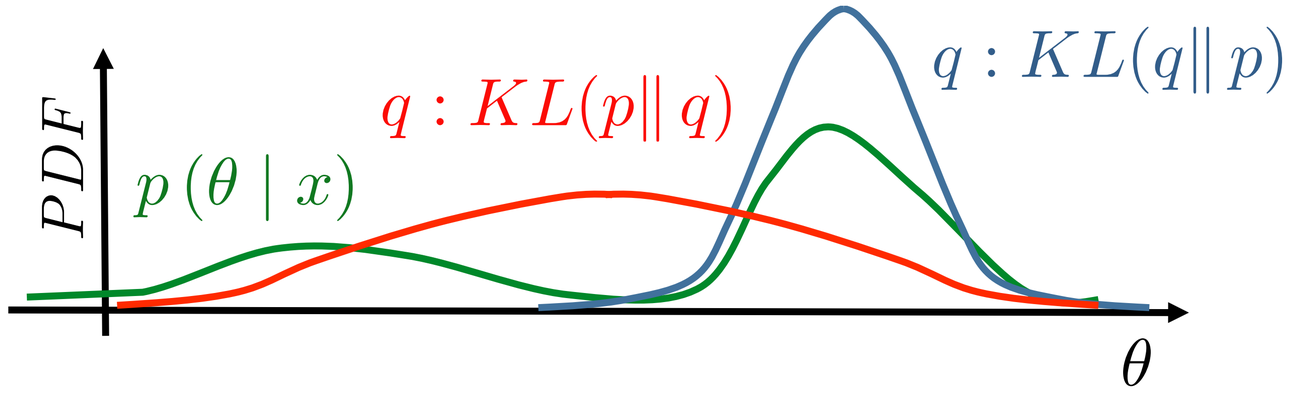
Kullback-Leibler divergence

A good mismatch measure between two distributions over the **same domain**

$$KL(q(\theta) \| \, p(\theta \mid x)) = \int q(\theta) \log \frac{q(\theta)}{p(\theta \mid x)} d\theta$$

Properties:

- $KL(q \| \, p) \geq 0$
- $KL(q \| \, p) = 0 \;\Leftrightarrow\; q = p$
- $KL(q \| \, p) \neq KL(p \| \, q)$



Variational inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta)$

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We could not compute the posterior in the first place

How to perform an optimization w.r.t. a distribution?

Mathematical magic

$$\log p(x)$$

Mathematical magic

$$\log p(x) = \int q(\theta) \log p(x) d\theta$$

Mathematical magic

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Mathematical magic

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$$= \mathcal{L}(q(\theta)) + KL(q(\theta) \| p(\theta \mid x))$$

Mathematical magic

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$$= \boxed{\mathcal{L}(q(\theta))} + \boxed{KL(q(\theta) \| p(\theta \mid x))}$$

Evidence lower bound (ELBO)

KL-divergence we need for VI

ELBO = Evidence Lower Bound

$$\log p(x) = \mathcal{L}(q(\theta)) + KL(q(\theta) \| p(\theta \mid x))$$

Evidence:

$$p(\theta \mid x) = \frac{p(x \mid \theta)p(\theta)}{p(x)} = \frac{p(x \mid \theta)p(\theta)}{\int p(x \mid \theta)p(\theta)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

Evidence of the probabilistic model shows the total probability of observing the data.

Lower Bound: KL is non-negative $\rightarrow$ $\log p(x) \geq \mathcal{L}(q(\theta))$

Variational inference

Optimization problem with intractable posterior distribution:

$$F(q) := KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}}$$

Variational inference

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Let's use our magic:

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does not depend on q

depend on q

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does not depend on q

depend on q

$$KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}} \quad \Leftrightarrow \quad \mathcal{L}(q(\theta)) \to \max_{q(\theta) \in \mathcal{Q}}$$

Variational inference

Final optimisation problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x, \theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

Variational inference: ELBO interpretation

Final optimisation problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x, \theta)}{q(\theta)} d\theta = \int q(\theta) \log \frac{p(x \mid \theta) p(\theta)}{q(\theta)} d\theta =$$

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$$= \mathbb{E}_{q(\theta)} \log p(x \mid \theta) - KL(q(\theta) \| \, p(\theta))$$

Variational inference: ELBO interpretation

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data term

regularizer

Variational inference: ELBO interpretation

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data term

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this is not the same KL-divergence!

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$$= \mathbb{E}_{q(\theta)} \log p(x \mid \theta) - KL(q(\theta) \| p(\theta))$$

data term

regularizer

this is not the same KL-divergence!

$$\log p(x) = \mathbb{E}_{q(\theta)} \log p(x \mid \theta) - KL(q(\theta) \| p(\theta)) + KL(q(\theta) \| p(\theta \mid x))$$

Variational inference

Final optimisation problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x, \theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

How to perform an optimization w.r.t. a distribution?

Variational inference

Final optimisation problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x, \theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

How to perform an optimization w.r.t. a distribution?

Mean field approximation

Factorized family

$$q(\theta) = \prod_{j=1}^{m} q_j\left(\theta_j\right), \quad \theta = [\theta_1, \ldots, \theta_m]$$

Parametric approximation

Parametric family

$$q(\theta) = q(\theta \mid \lambda)$$

Outline: Variational Inference

- Variational inference
- Variational mean field approximation
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Mean Field Approximation

Factorized family of variational distributions:

$$q(\theta) = \prod_{j=1}^{m} q_j\left(\theta_j\right), \quad \theta = [\theta_1, \ldots, \theta_m]$$

Why is it a restriction?

Mean Field Approximation

Factorized family of variational distributions:

$$q(\theta) = \prod_{j=1}^{m} q_j\left(\theta_j\right), \quad \theta = [\theta_1, \ldots, \theta_m]$$

Why is it a restriction? From product rule:

$$q(\theta) = \prod_{j=1}^{m} q_j\left(\theta_j \mid \theta_{<j}\right)$$

We assume that $\theta_1, \ldots, \theta_m$ are independent $\longrightarrow$ simpler approximation

Mean Field Approximation

Optimization problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x,\theta)}{q(\theta)} d\theta \rightarrow \max_{q(\theta)=q_1(\theta_1)\cdot\ldots\cdot q_m(\theta_m)}$$

Block coordinate assent:

At each step fix all factors $\{q_i(\theta_i)\}_{i\neq j}$ except one and optimise w.r.t. to it:

$$\mathcal{L}(q(\theta)) \rightarrow \max_{q_j(\theta_j)}$$

Mean Field Approximation

$$\mathcal{L}(q(\theta)) = \mathbb{E}_{q(\theta)} \log p(x, \theta) - \mathbb{E}_{q(\theta)} \log q(\theta) =$$

Mean Field Approximation

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Mean Field Approximation

$$\mathcal{L}(q(\theta)) = \mathbb{E}_{q(\theta)} \log p(x,\theta) - \mathbb{E}_{q(\theta)} \log q(\theta) =$$

$$= \mathbb{E}_{q(\theta)} \log p(x,\theta) - \sum_{k=1}^{m} \mathbb{E}_{q_k(\theta_k)} \log q_k(\theta_k) =$$

$$= \mathbb{E}_{q_j(\theta_j)} \left[\mathbb{E}_{q_{i \neq j}} \log p(x,\theta) \right] - \mathbb{E}_{q_j(\theta_j)} \log q_j(\theta_j) + Const =$$

Mean Field Approximation

$$\mathcal{L}(q(\theta)) = \mathbb{E}_{q(\theta)} \log p(x,\theta) - \mathbb{E}_{q(\theta)} \log q(\theta) =$$

$$= \mathbb{E}_{q(\theta)} \log p(x,\theta) - \sum_{k=1}^{m} \mathbb{E}_{q_k(\theta_k)} \log q_k(\theta_k) =$$

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$$= \left\{ r_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i \neq j}} \log p(x,\theta) \right) \right\} =$$

Mean Field Approximation

$$\mathcal{L}(q(\theta)) = \mathbb{E}_{q(\theta)} \log p(x,\theta) - \mathbb{E}_{q(\theta)} \log q(\theta) =$$

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$$= \mathbb{E}_{q_j(\theta_j)} \left[\mathbb{E}_{q_{i \neq j}} \log p(x,\theta) \right] - \mathbb{E}_{q_j(\theta_j)} \log q_j(\theta_j) + Const =$$

$$= \left\{ r_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i \neq j}} \log p(x,\theta) \right) \right\} =$$

$$= \mathbb{E}_{q_j(\theta_j)} \log \frac{r_j(\theta_j)}{q_j(\theta_j)} + Const = -KL\left(q_j(\theta_j) \| \, r_j(\theta_j) \right) + Const$$

Mean Field Approximation

Optimization problem at each step of the block coordinate assent:

$$\mathcal{L}(q(\theta)) = -KL\left(q_j(\theta_j) \| \, r_j(\theta_j)\right) + Const \rightarrow \max_{q_j(\theta_j)}$$

Mean Field Approximation

Optimization problem at each step of the block coordinate assent:

$$\mathcal{L}(q(\theta)) = -KL\left(q_j(\theta_j) \| \, r_j(\theta_j)\right) + Const \rightarrow \max_{q_j(\theta_j)}$$

Solution:

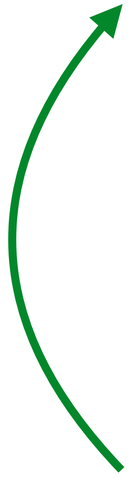
$$q_j\left(\theta_j\right) = r_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i \neq j}} \log p(x, \theta)\right)$$

Mean Field Variational Inference

Algorithm:

Initialize $q(\theta) = \prod_{j=1}^{m} q_j(\theta_j)$

Iterations:



- Update each factor $q_1, \ldots, q_m$:

$$q_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i \neq j}} \log p(x, \theta)\right)$$

- Compute ELBO $\mathcal{L}(q(\theta))$

Repeat until convergence of ELBO

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Assumption:
we can compute the update analytically

Mean Field Variational Inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta), \quad \theta = [\theta_1, \ldots, \theta_m]$

When applicable?

Conditional conjugacy of likelihood and prior on each θ_j conditional on all other $\{\theta_i\}_{i \neq j}$:

$$p(\theta_j \mid \theta_{i \neq j}) \in \mathcal{A}(\alpha), \quad p(x \mid \theta) \in \mathcal{B}(y) \quad \longrightarrow \quad p(\theta_j \mid x, \theta_{i \neq j}) \in \mathcal{A}(\alpha')$$

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How to check in practice?

For each θ_j :

- Fix all other $\{\theta_i\}_{i \neq j}$ (look at them as some constants)
- Check whether $p(x \mid \theta)$ and $p(\theta)$ are conjugate w.r.t. θ_j

Mean Field Variational Inference

In practice:

$$q_j(\theta_j) = \frac{1}{Z_j} \exp\left(\mathbb{E}_{q_{i\neq j}} \log p(x, \theta)\right)$$

$$\log q_j(\theta_j) = \mathbb{E}_{q_{i\neq j}} \log p(x, \theta) + Const$$

Conditional conjugacy → $q_j(\theta_j)$ from the same family as prior on θ_j → Normalization constant is tractable

Outline: Variational Inference

- Variational inference
- Variational mean field approximation
- Variational parametric approximation
- Practice: Gaussian mixture model

Parametric approximation

Parametric family of variational distributions:

$$q(\theta) = q(\theta \mid \lambda), \qquad \lambda \text{ — some parameters}$$

Why is it a restriction? We choose a family of some fixed form:

- It may be too simple and insufficient to model the data
- If it is complex enough then there is no guaranty we can train it well to fit the data

Parametric approximation

Parametric family of variational distributions:

$$q(\theta) = q(\theta \mid \lambda), \qquad \lambda \text{ — some parameters}$$

Variational inference transforms to parametric optimization problem:

$$\mathcal{L}(q(\theta \mid \lambda)) = \int q(\theta \mid \lambda) \log \frac{p(x, \theta)}{q(\theta \mid \lambda)} d\theta \to \max_{\lambda}$$

If we're able to calculate derivatives of ELBO w.r.t. then we can solve this problem using some numerical optimization solver.

Inference methods: summary

Full Bayesian inference: $p(\theta \mid x)$

MP inference: $p(\theta \mid x) \approx \delta(\theta - \theta_{MP})$

Mean field variational inference: $p(\theta \mid x) \approx q(\theta) = \prod_{j=1}^{m} q_j(\theta_j)$

Parametric variational inference: $p(\theta \mid x) \approx q(\theta) = q(\theta \mid \lambda)$

Inference methods: summary

Inference	Full $q(\theta)$	Factorized $q(\theta)$
Bayesian	Full Bayesian inference	Mean field VI
Parametric approx.	Parametric VI	Parametric mean field VI
Delta function approx.	MP inference	
No prior	MLE	

In factorised case different factors could be approximated in different ways

Inference methods: summary

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Common example: Expectation-Maximization (EM) algorithm

two factors: Bayesian + No prior

Outline: Variational Inference

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The problem set is available here:

http://tiny.cc/c1t78y

Problem 4: Clustering

Clustering problem:

- Dataset $X = \{x_i\}_{i=1}^{n}$
- We want to group these objects into K clusters

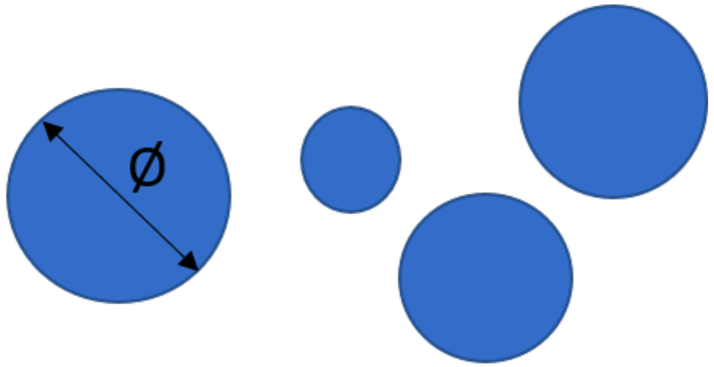
Gaussian mixture model:

- K Gaussian components with probabilities $\pi = (\pi_1, \ldots, \pi_K)$
- Each Gaussian has parameters μ_k, Σ_k
- Each object has latent variable which shows affiliation to a cluster:

$$z_i \in \{0, 1\}^K, \quad \sum_{k=1}^{K} z_{ik} = 1$$

Problem 4: Clustering

K-means



- Hard clustering
- Diagonal covariance matrices

GMM

- Soft clustering
- Trainable covariance matrices
- We may use priors for μ, Σ, π

Problem 4: Gaussian mixture model

Probabilistic model: $p(X, Z, \pi|\mu, \Sigma) = p(\pi) \prod_{i=1}^{n} p(z_i|\pi) p(x_i|z_i, \mu, \Sigma)$

$$= \mathrm{Dir}(\pi|\alpha) \prod_{i=1}^{n} \prod_{k=1}^{K} [\pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)]^{z_{ik}}$$

Approximation: $p(Z, \pi|X, \mu, \Sigma) \approx q(Z, \pi) = q(Z)q(\pi)$

Questions

- Check that likelihood and prior are not conjugate
- Check that there is a conditional conjugacy
- Write down update rules for $q(Z)$ and $q(\pi)$ for Variational Inference

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no conjugacy

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$= C \prod_{i=k}^{K} \pi_k^C$

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conjugacy

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Fix π

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Conditional conjugacy

↓

$q(Z, \pi) = q(Z)q(\pi)$

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Update rule for Variational inference:

$$\log q_j(\theta_j) = \mathbb{E}_{q_{i \neq j}} \log p(X, \theta) + Const, \quad \theta = (Z, \pi)$$

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$$\log q(Z) = \mathbb{E}_{q(\pi)} \log p(X, Z, \pi) + Const =$$

$$= \mathbb{E}_{q(\pi)} \left[\sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} (\log \pi_k + \log \mathcal{N}(x_i|\mu_k, \Sigma_k)) \right] + Const =$$

$$= \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} (\mathbb{E}_{q(\pi)} \log \pi_k + \log \mathcal{N}(x_i|\mu_k, \Sigma_k)) + Const =$$

$$= \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} \log \rho_{ik} + Const$$

$$q(Z) = \prod_{i=1}^{n} q(z_i), \quad q(z_i) = \frac{\prod_{k=1}^{K} \rho_{ik}{}^{z_{ik}}}{\sum_{k=1}^{K} \rho_{ik}}$$

Problem 4: Gaussian mixture model

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$$\log q(\pi) = \mathbb{E}_{q(Z)} \log p(X, Z, \pi) + Const =$$

$$= \mathbb{E}_{q(Z)} \left[\sum_{k=1}^{K} (\alpha_k - 1) \log \pi_k + \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} \log \pi_k \right] + Const =$$

$$= \sum_{k=1}^{K} (\alpha_k - 1) \log \pi_k + \sum_{i=1}^{n} \sum_{k=1}^{K} [\mathbb{E}_{q(Z)} z_{ik}] \log \pi_k + Const =$$

$$= \sum_{k=1}^{K} \log \pi_k \left(\alpha_k - 1 + \sum_{i=1}^{n} \mathbb{E}_{q(Z)} z_{ik} \right) + Const$$

$$q(\pi) = Dir(\pi|\alpha')$$

$$\alpha_k{}' = \alpha_k + \sum_{n=1}^{n} \mathbb{E}_{q(Z)} z_{ik}$$