10-701: Introduction to Machine Learning Lecture 6 – MLE & MAP

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Front Matter

• Announcements:

- HW1 released 9/6, due 9/20 (Wednesday) at 11:59 PM
- HW2 released 9/20 (Wednesday), due 10/4 at 11:59 PM
- Recommended Readings:
 - Mitchell, Estimating Probabilities
 - Murphy, <u>Sections 15.1 & 15.2</u>

Probabilistic Learning

- Previously:
 - (Unknown) Target function, $c^*: \mathcal{X} \to \mathcal{Y}$
 - Classifier, $h: \mathcal{X} \to \mathcal{Y}$
 - Goal: find a classifier, h, that best approximates c^*
- Now:
 - (Unknown) Target *distribution*, $y \sim p^*(Y|\mathbf{x})$
 - Distribution, $p(Y|\mathbf{x})$
 - Goal: find a distribution, p, that best approximates p^*

Likelihood

• Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, ..., x^{(N)}\}$ of a random variable X • If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *likelihood* of \mathcal{D} is $\int_{L(\theta)}^{N} \int_{u=1}^{N} p(x^{(n)}|\theta)$

• If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *likelihood* of \mathcal{D} is

$$L(\theta) = \prod_{n=1}^{N} f(x^{(n)}|\theta)$$

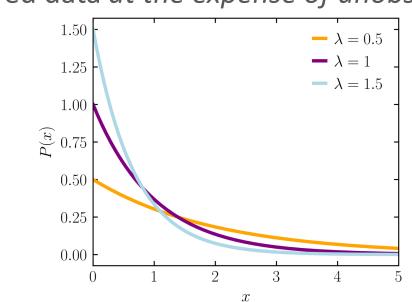
Log-Likelihood

• Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ of a random variable X • If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *log-likelihood* of \mathcal{D} is $\ell(\theta) = \log \prod^{n} p(x^{(n)}|\theta) = \sum^{n} \log p(x^{(n)}|\theta)$ • If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *log-likelihood* of \mathcal{D} is

$$\ell(\theta) = \log \prod_{n=1}^{N} f(x^{(n)}|\theta) = \sum_{n=1}^{N} \log f(x^{(n)}|\theta)$$

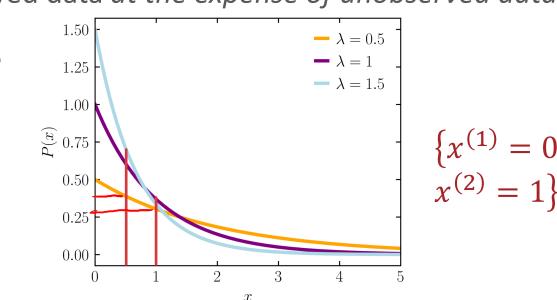
Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



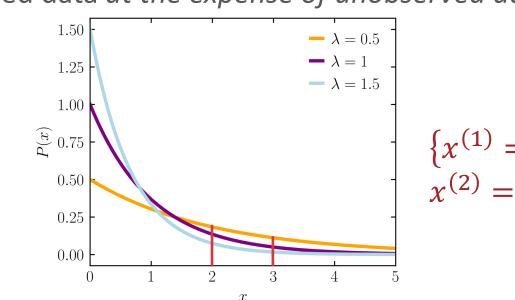
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Exponential Distribution MLE • The pdf of the exponential distribution is $f(x|\lambda) = \lambda e^{-\lambda x}$

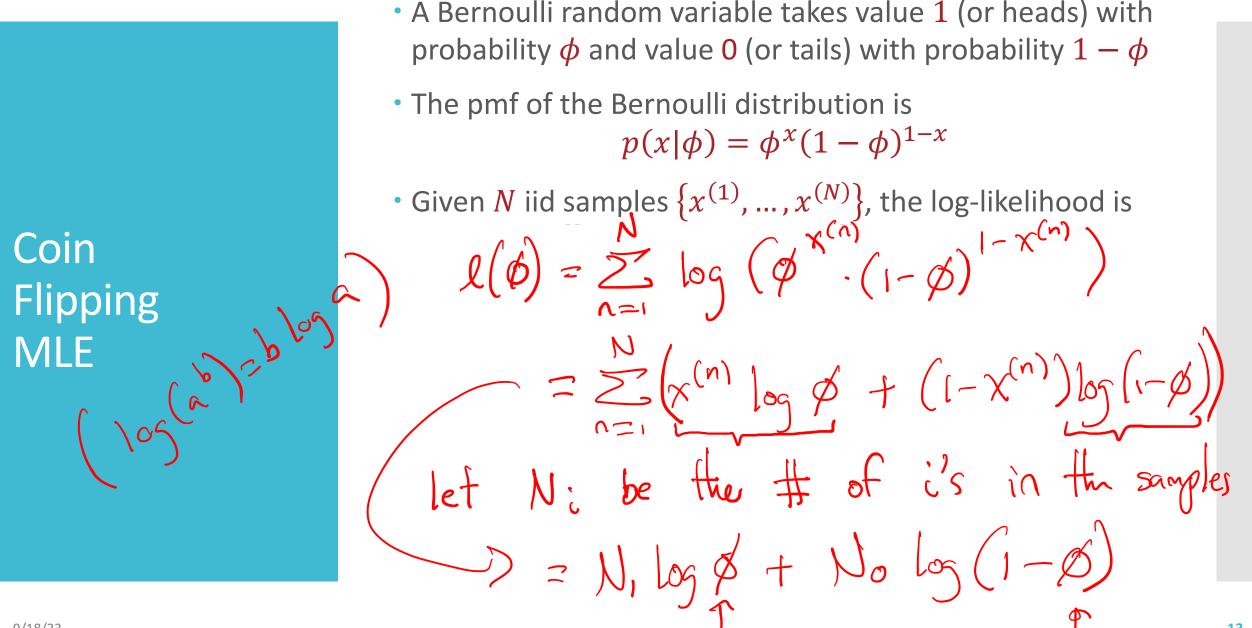
• Given Niid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the likelihood is $L(\lambda) = \prod_{n=1}^{N} \lambda e^{-\lambda x^{(n)}}$ Exponential Distribution MLE

- The pdf of the exponential distribution is $f(x|\lambda) = \lambda e^{-\lambda x}$
- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is $\mathcal{L}(\lambda) = \log \prod_{n=1}^{N} \lambda e^{-\lambda x^{(n)}} = \sum_{n=1}^{N} \log(\lambda e^{-\lambda x^{(n)}})$ $= \sum_{n=1}^{N} (\log \lambda + \log e^{-\lambda \chi(n)})$ $= \sum_{q=1}^{N} (\log \lambda - \lambda x^{(n)})$ (n) × $- \sum' \lambda$ $\frac{N}{3} - \sum_{n=1}^{N} \chi(n) - .$ $-\sum_{n}^{N} \chi^{(n)}$

Bernoulli Distribution MLE

- A Bernoulli random variable takes value 1 with probability ϕ and value 0 with probability 1ϕ
- The pmf of the Bernoulli distribution is

 $p(x|\phi) = \phi^x (1-\phi)^{1-x}$



Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability 1ϕ
- The pmf of the Bernoulli distribution is $p(x|\phi) = \phi^x (1-\phi)^{1-x}$
- The partial derivative of the log-likelihood is 6

Maximum a Posteriori (MAP) Estimation

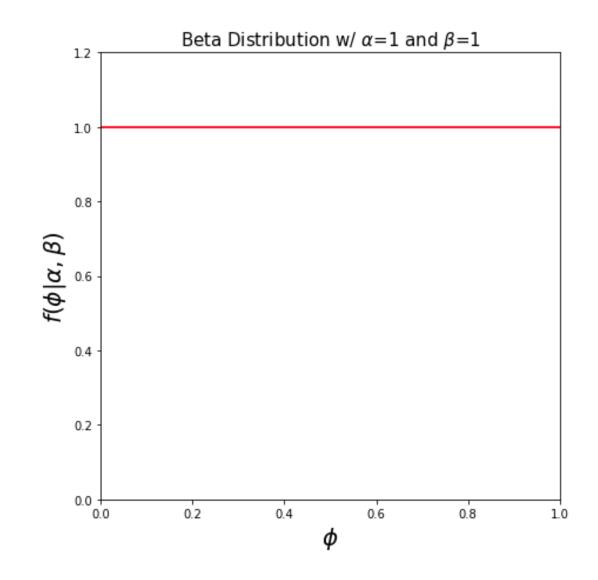
- Insight: sometimes we have *prior* information we want to incorporate into parameter estimation
- Idea: use Bayes rule to reason about the *posterior* distribution over the parameters

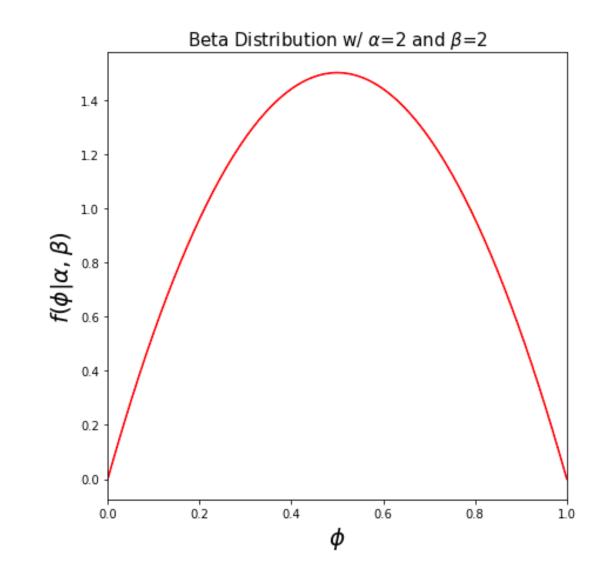
MLE: ÔMIF. = MAP: ÔMAP = argmax 17 Coin Flipping MAP

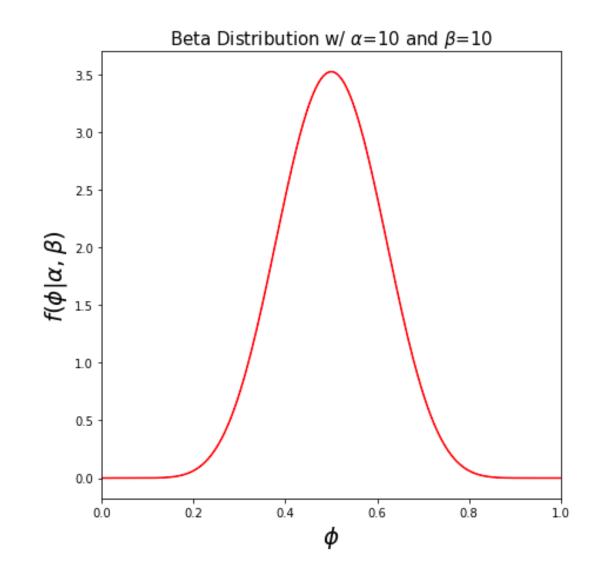
- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1-\phi$
- The pmf of the Bernoulli distribution is $p(x|\phi) = \phi^x (1-\phi)^{1-x}$
- Assume a Beta prior over the parameter ϕ , which has pdf $f(\phi|\alpha,\beta) = \frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{B(\alpha,\beta)}$

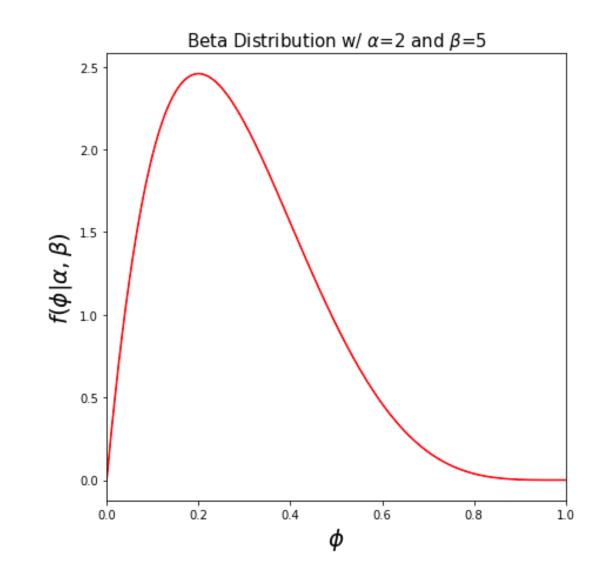
where $B(\alpha,\beta) = \int_0^1 \phi^{\alpha-1}(1-\phi)^{\beta-1}d\phi$ is a normalizing

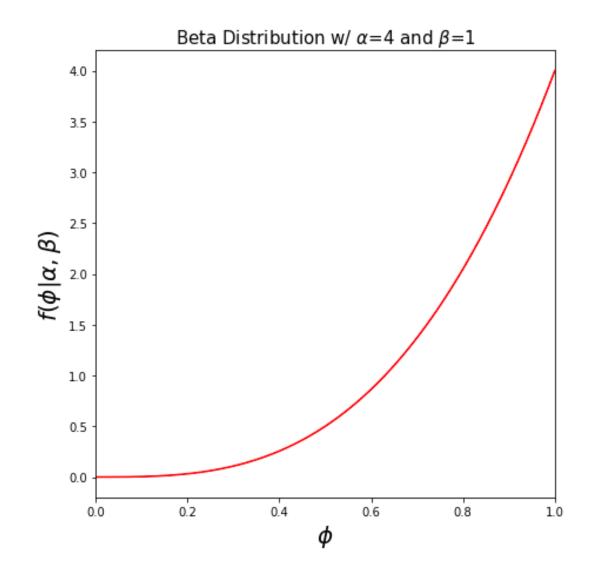
constant to ensure the distribution integrates to 1



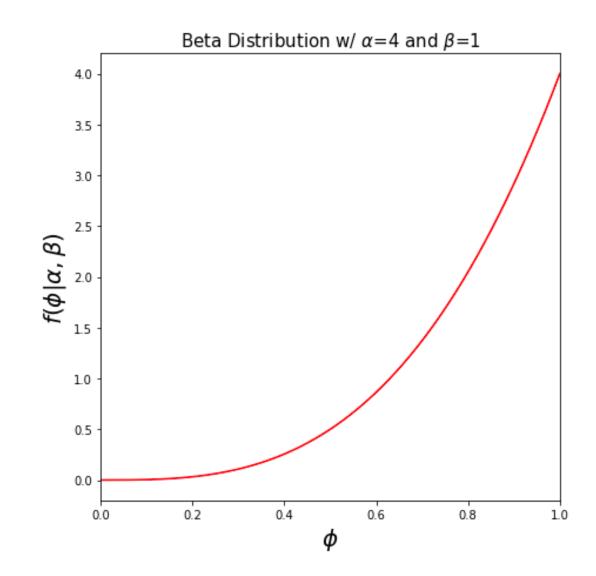








Okay, but why should we use this strange distribution as a prior?



Conjugate Priors

For a given likelihood function p(D|θ), a prior p(θ) is called a *conjugate prior* if the resulting posterior distribution p(θ|D) is in the same family as p(θ) i.e., p(θ|D) and p(θ) are the same type of random variable just with different parameters

- We like conjugate priors because they are mathematically convenient
- However, we do not have to use a conjugate prior if it doesn't align with our actual prior belief.

Example: Beta-Binomial Conjugacy

(pt-1/1-

 $f(\phi|x,\alpha,\beta) = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{p(x|\alpha,\beta)}$ $P(x | \alpha, \beta) = \int p(x | \beta) f(\beta) \alpha, \beta)$ Ø^{a-1} D €⁶, ⁶, ²¢ $\frac{1}{B(\alpha,\beta)} \int_{0}^{1} \varphi^{(\alpha+\chi-1)} \\ B(\alpha+\chi, B+(1-\chi))$ $\left(1-\phi\right)^{\beta-\chi}$ ² B(a, B). $p(x | \alpha, \beta) =$

B(d,B)=,

Example: Beta-Binomial Conjugacy

 $f(\phi|x,\alpha,\beta) = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{p(x|\alpha,\beta)} = \frac{p(x|\phi)f(\phi|\alpha,\beta)}{\int p(x|\phi)f(\phi|\alpha,\beta)d\phi}$ $\beta^{x}(1-\beta)^{x} \frac{\beta^{\alpha-1}}{R}$ $f(\emptyset|x,a,\beta) =$ BCaje $B(\alpha + x, \beta + (1 - x))$ $= \phi^{\alpha+\kappa-1} \left(\left(-\phi \right)^{\beta+\left(1-\kappa \right)} \right)$ B(d+X, B+(1-X))A Beta distribution w/ parameters d+X ~ B+(I-X)

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Beta-Binomial MAP

• Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-posterior is $\mathcal{L}(\phi) = \log\left(f(\phi \mid \chi^{(i)}, \dots, \chi^{(N)}, d, \beta)\right)$ $=\log\left(f(\phi \mid \alpha + \sum_{n=1}^{N} x^{(n)}, \beta + \sum_{n=1}^{N} (i - x^{(n)})\right)$ = log (Prost (Ø l a + N, B+ No)) $= \log \left(\frac{\varphi^{\alpha+N_1-1}(1-\varphi)^{\beta+N_2-1}}{B(\alpha+N_1,\beta+N_2)} \right)$ $= (\alpha + N_1 - 1) \log (\beta + (\beta + N_0 - 1) \log (r - \alpha)) \\ - \log (\beta (\alpha + N_1, \beta + N_0))$ 28

Beta-Binomial MAP

• Given N iid samples
$$\{x^{(1)}, \dots, x^{(N)}\}$$
, the partial derivative of the log-posterior is

$$\frac{\partial l}{\partial \varphi} = \frac{(\alpha + N_1 - 1)}{(\alpha + N_1 - 1)} \frac{(\beta + N_0 - 1)}{(1 - \beta)}$$

$$\frac{\partial l}{\partial \varphi} = \frac{\alpha + N_1 - 1}{(\alpha + N_1 - 1) + (\beta + N_0 - 1)}$$

Coin Flipping MAP: Example • Suppose \mathcal{D} consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$): $\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$ • Using a Beta prior with $\alpha = 2$ and $\beta = 5$, then

$$P_{MAP} = \frac{10 + 2 - 1}{11 + 16} = \frac{11}{17} < \frac{10}{12}$$

Coin Flipping MAP: Example • Suppose \mathcal{D} consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$): $\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$

• Using a Beta prior with $\alpha = 101$ and $\beta = 101$, then

.

Coin Flipping MAP: Example • Suppose \mathcal{D} consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$): $\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$

• Using a Beta prior with $\alpha = 1$ and $\beta = 1$, then

M(C)LE for Linear Regression • If we assume a linear model with additive Gaussian noise

$$y = \boldsymbol{\omega}^{T} \boldsymbol{x} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(0, \sigma^{2}) \rightarrow \boldsymbol{y} \sim N(\boldsymbol{\omega}^{T} \boldsymbol{x}, \sigma^{2}) \dots$$
then given $X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^{T}} \\ 1 & \boldsymbol{x}^{(2)^{T}} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^{T}} \end{bmatrix}$ and $\boldsymbol{y} = \begin{bmatrix} \boldsymbol{y}^{(1)} \\ \boldsymbol{y}^{(2)} \\ \vdots \\ \boldsymbol{y}^{(N)} \end{bmatrix}$, the MLE of $\boldsymbol{\omega}$ is
 $\hat{\boldsymbol{\omega}} = \underset{\boldsymbol{\omega}}{\operatorname{argmax}} \log P(\boldsymbol{y}|X, \boldsymbol{\omega})$
 \vdots

$$= (X^{T}X)^{-1}X^{T}\boldsymbol{y}$$

MAP for Linear Regression • If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2)$... and **independent, identical** Gaussian priors on the weights ... $\omega_d \sim N(0, s^2) \rightarrow \boldsymbol{\omega} \sim N(\mathbf{0}, s^2 I_{D+1})$

then, the MAP of $\boldsymbol{\omega}$ is the ridge regression solution!

 $\widehat{\boldsymbol{\omega}} = \underset{\boldsymbol{\omega}}{\operatorname{argmax}} \log P(\boldsymbol{\omega} | X, \boldsymbol{y})$

:]

 $= (X^T X + \lambda(s^2) I_{D+1})^{-1} X^T y$

• If we assume a linear model with additive Gaussian noise $y = \omega^T x + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\omega^T x, \sigma^2) \dots$ and a **general** (zero-mean) Gaussian prior on the weights \dots $\omega \sim N(0, \Sigma)$ then the distribution over y is $\gamma \equiv \chi \omega + \mathcal{E}$ $y \sim N(X0 + 0 = 0, X\Sigma X^T + \sigma^2 I)$

• If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \dots$ and a general (zero-mean) Gaussian prior on the weights ... $\boldsymbol{\omega} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$ then the *joint* distribution over y and ω is $\begin{bmatrix} \mathbf{y} \\ \boldsymbol{\omega} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} X \Sigma X^T + \sigma^2 I & ??? \\ (???) & \Sigma \end{bmatrix} \right)$ Cov(y, w) = Cov(Xw+G, w)= $\chi Cov(w,w) = \chi \Sigma$

• If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim N(0, \sigma^2) \rightarrow \boldsymbol{y} \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2)$... and a **general** (zero-mean) Gaussian prior on the weights ... $\boldsymbol{\omega} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$

then the *joint* distribution over \boldsymbol{y} and $\boldsymbol{\omega}$ is $\mathcal{N}\begin{bmatrix}\boldsymbol{y}\\\boldsymbol{\omega}\end{bmatrix} \sim N\left(\begin{bmatrix}\boldsymbol{0}\\\boldsymbol{0}\end{bmatrix}, \begin{bmatrix}\boldsymbol{X}\boldsymbol{\Sigma}\boldsymbol{X}^T + \sigma^2\boldsymbol{I} & \boldsymbol{\Sigma}\boldsymbol{X}^T\\\boldsymbol{X}\boldsymbol{\Sigma} & \boldsymbol{\Sigma}\end{bmatrix}\right)$

• If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim N(0, \sigma^2) \rightarrow \boldsymbol{y} \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \dots$ and a **general** (zero-mean) Gaussian prior on the weights \dots $\boldsymbol{\omega} \sim N(\mathbf{0}, \Sigma)$

then the *conditional* distribution of $\boldsymbol{\omega}$ given \boldsymbol{y} is

 $\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{POST}, \boldsymbol{\Sigma}_{POST})$ where $\boldsymbol{\mu}_{POST} = \boldsymbol{\Sigma} X^T (\boldsymbol{X} \boldsymbol{\Sigma} \boldsymbol{X}^T + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{y},$ $\boldsymbol{\Sigma}_{POST} = \boldsymbol{\Sigma} - \boldsymbol{\Sigma} X^T (\boldsymbol{X} \boldsymbol{\Sigma} \boldsymbol{X}^T + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{X} \boldsymbol{\Sigma}$

• If we assume a linear model with additive Gaussian noise $y = \omega^T x + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\omega^T x, \sigma^2)$... and a **general** (zero-mean) Gaussian prior on the weights ... $\omega \sim N(0, \Sigma)$

then the *conditional* distribution of $h(x') = {x'}^T \omega$ given y is

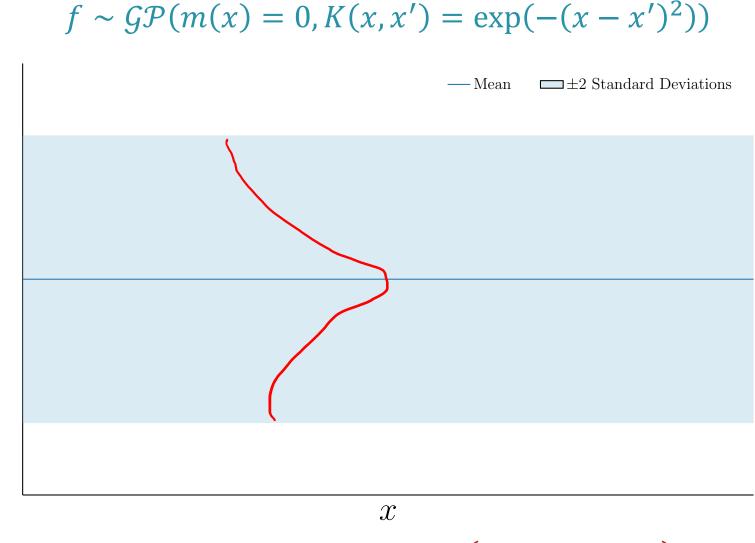
 $h(\mathbf{x}') \mid \mathbf{y} \sim N(\boldsymbol{\mu}_{PRED}, \boldsymbol{\Sigma}_{PRED})$ $\downarrow \qquad \text{where}$ $\boldsymbol{\mu}_{PRED} = \mathbf{x}'^{T} \boldsymbol{\Sigma} \boldsymbol{X}^{T} (\boldsymbol{X} \boldsymbol{\Sigma} \boldsymbol{X}^{T} + \sigma^{2} I)^{-1} \mathbf{y},$ $\boldsymbol{\Sigma}_{PRED} = \mathbf{x}'^{T} \boldsymbol{\Sigma} \mathbf{x}' - \mathbf{x}'^{T} \boldsymbol{\Sigma} \boldsymbol{X}^{T} (\boldsymbol{X} \boldsymbol{\Sigma} \boldsymbol{X}^{T} + \sigma^{2} I)^{-1} \boldsymbol{X} \boldsymbol{\Sigma} \mathbf{x}'$ Kernelized Bayesian Linear Regression

• If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2)$... and a general (zero-mean) Gaussian prior on the weights ... $\boldsymbol{\omega} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$ then the *conditional* distribution of $h(\mathbf{x}') = {\mathbf{x}'}^T \boldsymbol{\omega}$ given \mathbf{y} is $h(\mathbf{x}') \mid \mathbf{y} \sim N(\boldsymbol{\mu}_{PRED}, \boldsymbol{\Sigma}_{PRED})$ where $K(\boldsymbol{a}, \boldsymbol{b}) = \Phi(\boldsymbol{a})^T \Sigma \Phi(\boldsymbol{b})$ $\boldsymbol{\mu}_{PRED} = K(\boldsymbol{x}', \boldsymbol{X})(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 \boldsymbol{I})^{-1}\boldsymbol{y},$ $\Sigma_{PRFD} = K(\mathbf{x}', \mathbf{x}') - K(\mathbf{x}', X)(K(X, X) + \sigma^2 I)^{-1}K(X, \mathbf{x}')$ Kernelized Bayesian Linear Regression = Gaussian Process (GP)

 If we assume a linear model with additive Gaussian noise $y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon$ where $\epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \dots$ and a general (zero-mean) Gaussian prior on the weights ... $\boldsymbol{\omega} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$ then the *conditional* distribution of $h(\mathbf{x}') = {\mathbf{x}'}^T \boldsymbol{\omega}$ given \mathbf{y} is $h(\mathbf{x}') \mid \mathbf{y} \sim N(\boldsymbol{\mu}_{PRED}, \boldsymbol{\Sigma}_{PRED})$ where $K(\boldsymbol{a}, \boldsymbol{b}) = \Phi(\boldsymbol{a})^T \Sigma \Phi(\boldsymbol{b})$

> $\boldsymbol{\mu}_{PRED} = K(\boldsymbol{x}', \boldsymbol{X})(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 I)^{-1} \boldsymbol{y}_{\boldsymbol{i}}$ $\boldsymbol{\Sigma}_{PRED} = K(\boldsymbol{x}', \boldsymbol{x}') - K(\boldsymbol{x}', \boldsymbol{X})(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 I)^{-1} K(\boldsymbol{X}, \boldsymbol{x}')$

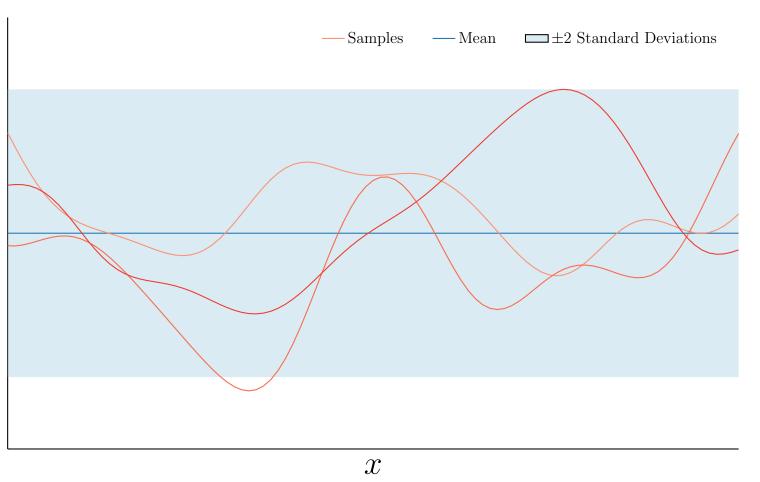
Gaussian Process (GP)



 $f \sim \mathcal{GP}(m, K) \rightarrow f(x) \sim \mathcal{N}(m(x), K(x, x))$

Gaussian Process (GP)

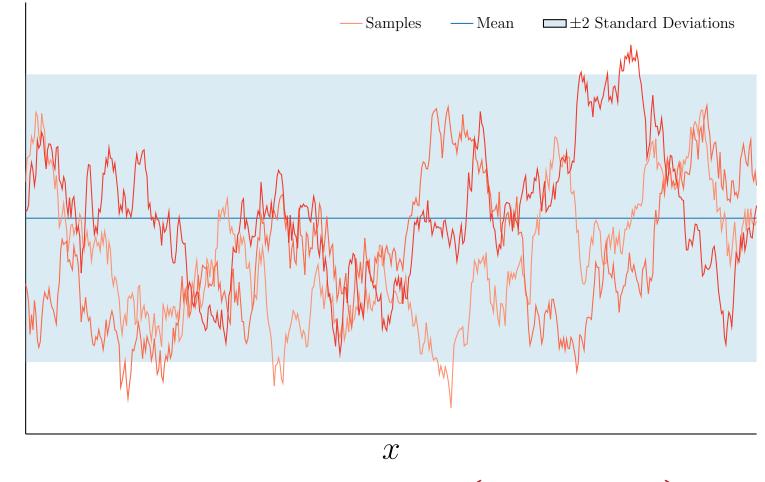
$$f \sim \mathcal{GP}(m(x) = 0, K(x, x') = \exp(-(x - x')^2))$$



 $f \sim \mathcal{GP}(m, K) \rightarrow f(x) \sim \mathcal{N}(m(x), K(x, x))$

Gaussian Process (GP)





 $f \sim \mathcal{GP}(m, K) \rightarrow f(x) \sim \mathcal{N}(m(x), K(x, x))$



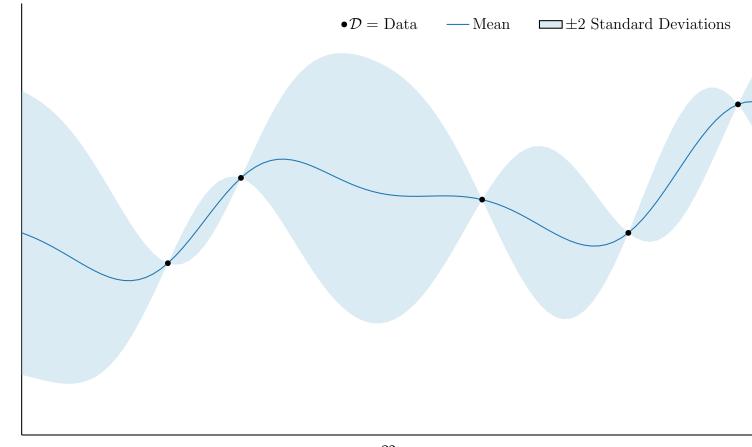


— Mean $\square \pm 2$ Standard Deviations



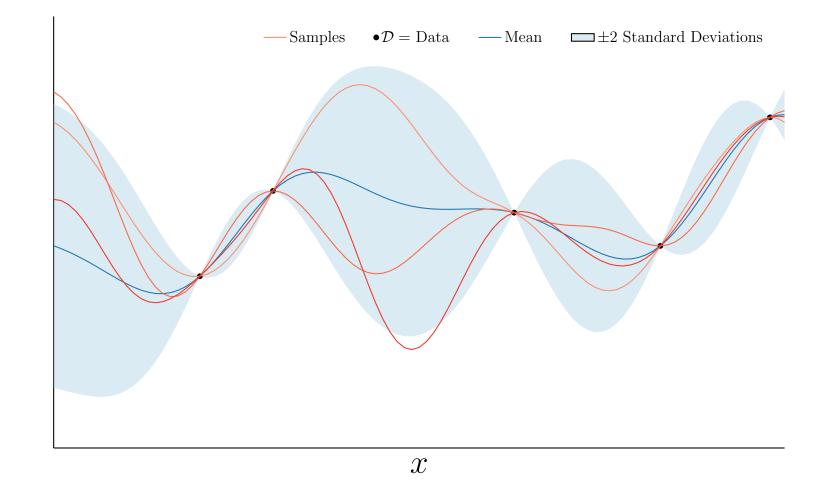
GP Posterior





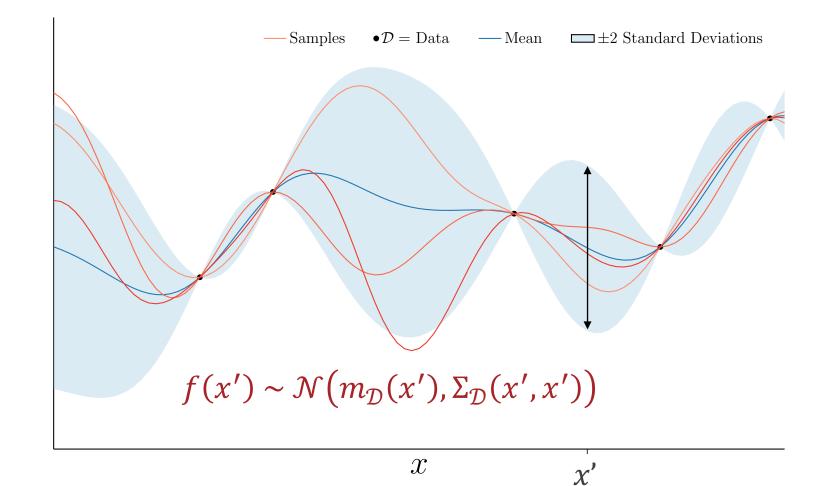
GP Posterior

$f \mid \mathcal{D} \sim \mathcal{GP}(m_{\mathcal{D}}, K_{\mathcal{D}})$



GP Posterior

$f \mid \mathcal{D} \sim \mathcal{GP}(m_{\mathcal{D}}, K_{\mathcal{D}})$



Key Takeaways

- Two ways of estimating the parameters of a probability distribution given samples of a random variable:
 - Maximum likelihood estimation maximize the (log-)likelihood of the observations
 - Maximum a posteriori estimation maximize the (log-)posterior of the parameters conditioned on the observations
 - Requires a prior distribution, drawn from background knowledge or domain expertise
- Linear/ridge regression can be interpreted as MLE/MAP estimators under certain likelihood/prior models
 - A Gaussian process is the kernelization of Bayesian
 - linear regression or MAP estimation for linear regression 49