Probabilistic Models for Regression

Piyush Rai

Probabilistic Machine Learning (CS772A)

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Background: Linear Regression

- Supervised Learning. Training data as N i.i.d. examples $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$, $\boldsymbol{x}_n \in \mathbb{R}^D$, $y_n \in \mathbb{R}$

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- Nice, convex objective with unique solution

Probabilistic Linear Regression

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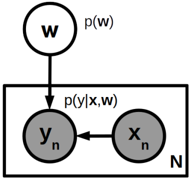

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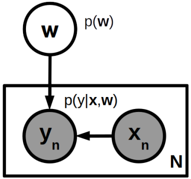

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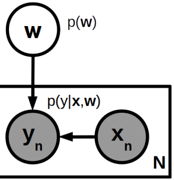

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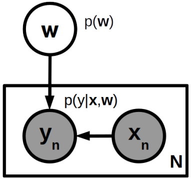

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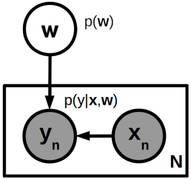

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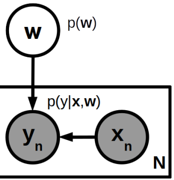

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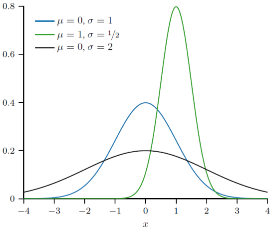
  - Note: In some supervised learning problems (especially classification), inputs are also modeled (more on this when we discuss "generative classification")
- Only $\boldsymbol{w}$ and y_n $(n = 1, \ldots, N)$ are the random variables in this model (not $\boldsymbol{x}_n$'s, which are fixed)

Background: Univariate Gaussian Distribution

- Distribution over real-valued scalar r.v. x
- Defined by a scalar **mean** μ and a scalar **variance** $\sigma^2 > 0$
- Mean: $\mathbb{E}[x] = \mu$, Variance: $\text{var}[x] = \sigma^2$
- Precision (inverse variance) $\beta = 1/\sigma^2$
- Distribution defined as

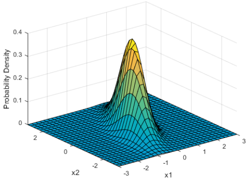
$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}(x-\mu)^2}$$



Background: Multivariate Gaussian Distribution

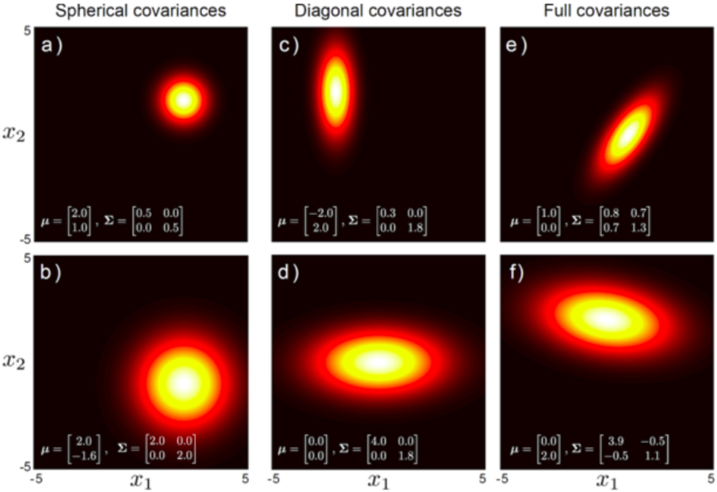
- Distribution over a multivariate r.v. vector $\mathbf{x} \in \mathbb{R}^D$ of real numbers
- Defined by a **mean vector** $\boldsymbol{\mu} \in \mathbb{R}^D$ and a $D \times D$ **cov. matrix** $\boldsymbol{\Sigma}$ (its inverse is precision matrix)

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$



- The covariance matrix $\boldsymbol{\Sigma}$ must be symmetric and positive definite
  - All eigenvalues are positive
  - $\boldsymbol{z}^\top \boldsymbol{\Sigma} \boldsymbol{z} > 0$ for any real vector $\boldsymbol{z}$
- Inverse of the covariance matrix is known as the **precision matrix** $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$ (also positive definite)

The covariance matrix can be spherical, diagonal, or full



Picture courtesy: Computer vision: models, learning and inference (Simon Price)

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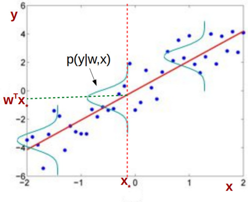

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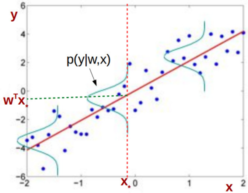

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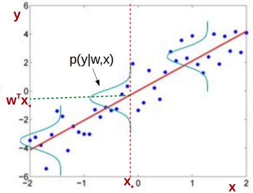

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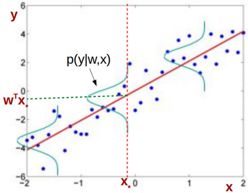

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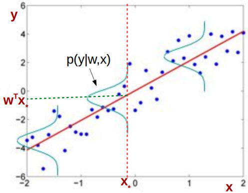

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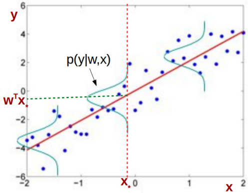

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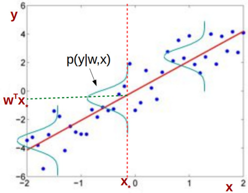

- $p(y_n|\boldsymbol{x}_n, \boldsymbol{w})$ is our likelihood model - Gaussian distribution in this case
- Note: We are only modeling the outputs y; the inputs $\boldsymbol{x}$ are not being modeled (fixed)
- Denoting $\mathbf{X} = [\boldsymbol{x}_1 \dots \boldsymbol{x}_N]^\top$ $(N \times D)$, $\boldsymbol{y} = [y_1 \dots y_N]^\top$ $(N \times 1)$, the overall likelihood for i.i.d. data

$$p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \prod_{n=1}^{N} \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2} \propto e^{-\frac{\beta}{2}\sum_{n=1}^{N}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2} \propto e^{-\frac{\beta}{2}(\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{w})}$$

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$$P(\boldsymbol{w}|\lambda) = \mathcal{N}(\boldsymbol{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}_D)$$

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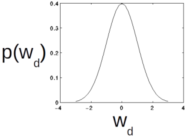

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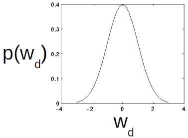

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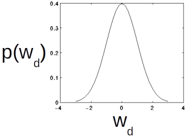

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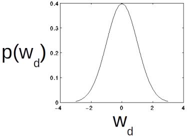

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  - We'll see that the Gaussian prior exactly corresponds to having an ℓ_2 (squared Euclidean norm) regularizer on $\boldsymbol{w}$, of the form $\boldsymbol{w}^\top \boldsymbol{w} = \sum_{d=1}^{D} w_d^2$

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$$NLL(\boldsymbol{w}) = -\log p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}) = -\log \prod_{n=1}^{N} \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2}$$

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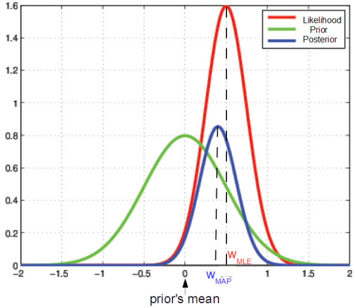
- $\boldsymbol{w}_{MAP}$ is a compromise between prior's mean (zero in this case) and $\boldsymbol{w}_{MLE}$



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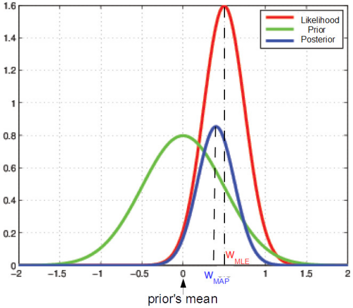

- Doing MAP shrinks the estimate of $\boldsymbol{w}$ towards the prior's mean
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MLE vs MAP for Probabilistic Linear Regression

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  - Basically, the conjugacy helps here (Gaussian prior is conjugate to Gaussian likelihood)
- The posterior over the weight vector $\boldsymbol{w}$ (with β and λ known)

$$p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) = \frac{p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta)p(\boldsymbol{w}|\lambda)}{p(\boldsymbol{y}|\mathbf{X}, \beta, \lambda)}$$

- Computing $P(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda)$ (like Bernoulli-Beta case, doing it only upto proportionality constant)

$$P(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) \propto P(\boldsymbol{w}|\lambda)P(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta)$$

- After some algebra, this gets simplified into the following (proof on the next two slides)

$$\begin{aligned}
P(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) &= \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad \text{(The posterior must be Gaussian due to conjugacy)} \\
\text{where} \quad \boldsymbol{\Sigma} &= (\beta \sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^\top + \lambda \mathbf{I}_D)^{-1} = (\beta \mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \\
\boldsymbol{\mu} &= \boldsymbol{\Sigma}(\beta \sum_{n=1}^{N} y_n \boldsymbol{x}_n) = \boldsymbol{\Sigma}(\beta \mathbf{X}^\top \boldsymbol{y}) = (\mathbf{X}^\top \mathbf{X} + \frac{\lambda}{\beta} \mathbf{I}_D)^{-1} \mathbf{X}^\top \boldsymbol{y}
\end{aligned}$$

The "Completing The Square" Trick for Gaussian Posterior

- Plugging in the respective distributions for $p(\boldsymbol{w}|\lambda)$ and $p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta)$, we will get

$$p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) \propto p(\boldsymbol{w}|\lambda)p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta) \quad = \quad \mathcal{N}(\boldsymbol{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}_D)\mathcal{N}(\boldsymbol{y}|\mathbf{X}\boldsymbol{w}, \beta^{-1}\mathbf{I}_N)$$

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$$\begin{aligned} p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) \propto p(\boldsymbol{w}|\lambda)p(\boldsymbol{y}|\mathbf{X}, \boldsymbol{w}, \beta) &= \mathcal{N}(\boldsymbol{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}_D)\mathcal{N}(\boldsymbol{y}|\mathbf{X}\boldsymbol{w}, \beta^{-1}\mathbf{I}_N) \\ &\propto \exp\left(-\frac{\lambda}{2}\boldsymbol{w}^\top\boldsymbol{w}\right)\exp\left(-\frac{\beta}{2}(\boldsymbol{y}-\mathbf{X}\boldsymbol{w})^\top(\boldsymbol{y}-\mathbf{X}\boldsymbol{w})\right) \end{aligned}$$

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&= \exp\left[-\frac{\lambda}{2}\boldsymbol{w}^\top\boldsymbol{w} - \frac{\beta}{2}(\boldsymbol{y}^\top\boldsymbol{y} + \boldsymbol{w}^\top\mathbf{X}^\top\mathbf{X}\boldsymbol{w} - 2\boldsymbol{w}^\top\mathbf{X}^\top\boldsymbol{y})\right]
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\end{aligned}$$

- We will now try to bring the exponent into a quadratic form to see if it corresponds to some Gaussian. So basically, we will use the "complete the square" trick

The “Completing The Square” Trick for Gaussian Posterior

- So we had.. $p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) \propto \exp\left[-\frac{1}{2}\left(\boldsymbol{w}^\top(\lambda \mathbf{I}_D + \beta \mathbf{X}^\top \mathbf{X})\boldsymbol{w} - 2\beta \boldsymbol{w}^\top \mathbf{X}^\top \boldsymbol{y}\right)\right]$

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- Let's see if we can bring the above posterior into the form of the following Gaussian

$$\mathcal{N}(\boldsymbol{w}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto \exp\left[-\frac{1}{2}(\boldsymbol{w} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{w} - \boldsymbol{\mu})\right] = \exp\left[-\frac{1}{2}(\boldsymbol{w}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{w} - 2\boldsymbol{w}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} + \boldsymbol{\mu}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu})\right]$$

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- Note: The above expression for the posterior can also be directly obtained using properties of Gaussian distributions (we will see those in the coming lectures)

Information within the Posterior

- As we saw, the posterior over the weight vector $\boldsymbol{w}$

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- Setting λ to 0 makes μ equivalent to the MLE solution
- However, MLE and MAP are only point estimates whereas we now have the full posterior over $\boldsymbol{w}$
- Therefore, the solution given by the full posterior in a way subsumes MAP/MLE solutions

Posterior Predictive Distribution

- Now we want to use the posterior over $\boldsymbol{w}$ to make predictions (response y_* for a new input $\boldsymbol{x}_*$)

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- Both terms on RHS are Gaussians: $p(y_*|\boldsymbol{x}_*, \boldsymbol{w}, , \beta) = \mathcal{N}(y_*|\boldsymbol{w}^\top \boldsymbol{x}_*, \beta^{-1})$ and $p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, \beta, \lambda) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

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$$\boxed{p(y_*|\boldsymbol{x}_*, \mathbf{X}, \boldsymbol{y}, , \beta, \lambda) = \mathcal{N}(\boldsymbol{\mu}^\top \boldsymbol{x}_*, \beta^{-1} + \boldsymbol{x}_*^\top \boldsymbol{\Sigma} \boldsymbol{x}_*)}$$

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Posterior Predictive Distribution

- Now we want to use the posterior over $\boldsymbol{w}$ to make predictions (response y_* for a new input $\boldsymbol{x}_*$)
- The posterior predictive distribution in this case will be

$$p(y_*|\boldsymbol{x}_*, \mathbf{X}, \boldsymbol{y}, , \beta, \lambda) = \int p(y_*|\boldsymbol{x}_*, \boldsymbol{w}, , \beta) p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y}, , \beta, \lambda) d\boldsymbol{w}$$

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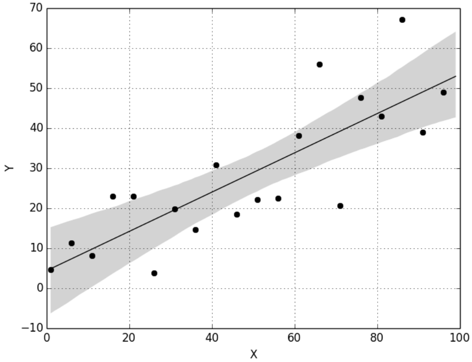
- Important: Unlike MLE/MAP, the variance of y_* also depends on the input $\boldsymbol{x}_*$ (this, as we will see later, will be very useful in sequential decision-making problems such as active learning)

Posterior Predictive Distribution: An Illustration

Black dots are training examples



Regions with more training examples have smaller predictive variance

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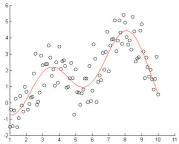
Probabilistic (Nonlinear) Regression



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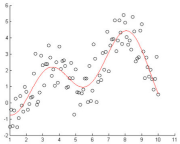

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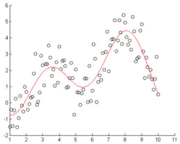

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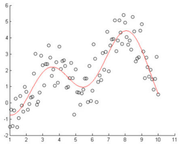

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