# Learning via Probabilistic Modeling, Probabilistic Linear Regression

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Machine Learning (CS771A)

Aug 12, 2016

# Some Announcements

- Homework 1 out tomorrow. Will be due in two weeks.
  - Will cover topics from up to the previous lecture
- Project discussion next week.
- Class TA's finalized. Will soon announce their/mine office hours
- Watch out the class webpage regularly for readings/reference materials
- Please participate on Piazza actively. Share and learn from each other.

# Recap

# Learning as Optimization

- Supervised learning problem with training data $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^{N}$
- Goal: Find $f : \boldsymbol{x} \to y$ that fits the training data well and is also "simple"
- The function $f$ is learned by solving the following optimization problem

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- This is called **Regularized** Empirical Risk Minimization
- Regularization hyperparameter $\lambda$ controls the amount of regularization

# $\ell_2$ Regularized Linear Regression: Ridge Regression

- Linear regression model $f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}$
- Loss function: squared loss, regularizer: $\ell_2$ norm of $\boldsymbol{w}$
- The resulting Ridge Regression problem is solved as

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2 + \lambda ||\boldsymbol{w}||^2$$

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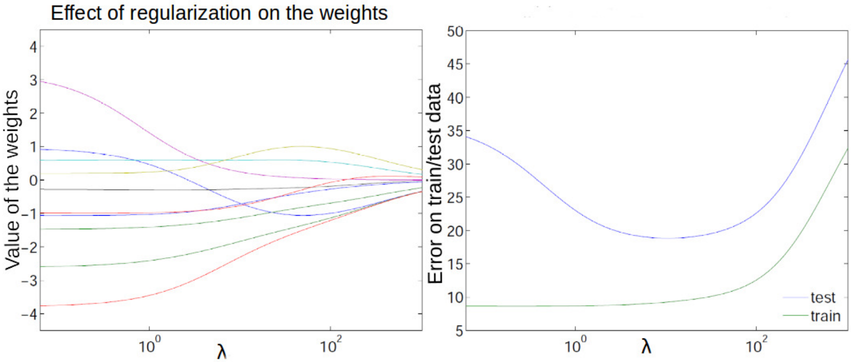
- Can also used iterative methods (e.g., gradient-descent) to optimize the objective function and solve for $\boldsymbol{w}$ (for better efficiency)

# Ridge Regression: Effect of Regularization

- Consider ridge regression on some data with 10 features (thus the weight vector $\boldsymbol{w}$ has 10 components)



# Learning via Probabilistic Modeling

# Probabilistic Modeling of Data

- Assume the data $\boldsymbol{y} = \{y_1, y_2, \ldots, y_N\}$ as generated from a probability model

$$y_n \sim p(y|\theta) \qquad \forall n$$

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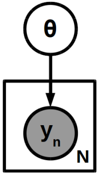


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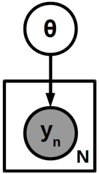


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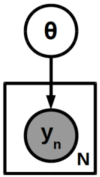


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- Almost any learning problem can be formulated like this

# Parameter Estimation in Probabilistic Models

- Since data is i.i.d., the probability of observing data $\boldsymbol{y} = \{y_1, y_2, \ldots, y_N\}$

$$p(\boldsymbol{y}|\theta) = p(y_1, y_2, \ldots, y_N|\theta) = \prod_{n=1}^{N} p(y_n|\theta)$$

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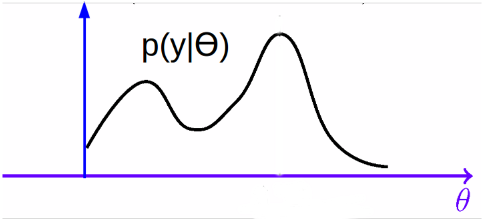

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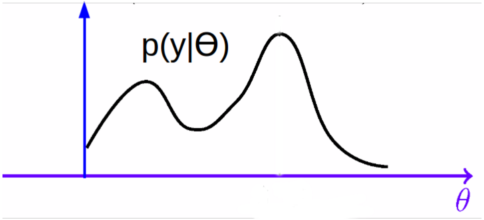


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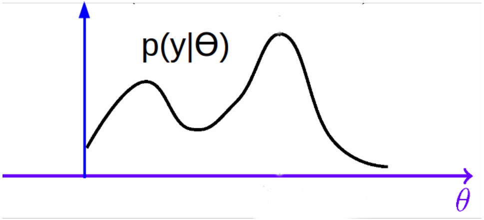


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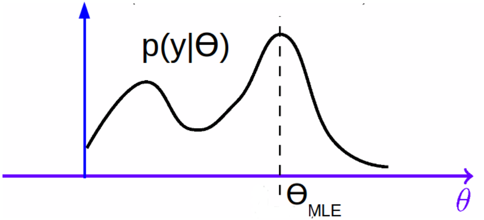


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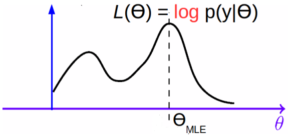


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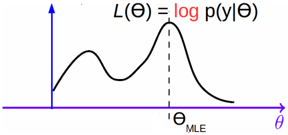


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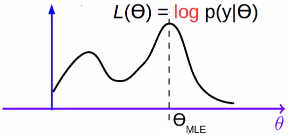


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- Now this becomes an optimization problem w.r.t. $\theta$

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- Maximum Likelihood parameter estimation

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- Something is still missing (we will look at that shortly)

# MLE: An Example

- Consider a sequence of $N$ coin toss outcomes (observations)
- Each observation $y_n$ is a binary random variable. Head = 1, Tail = 0
- Since each $y_n$ is binary, let's use a **Bernoulli distribution** to model it

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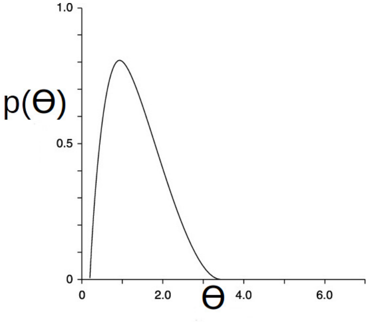
- What can go wrong with this approach (or MLE in general)?
  - We haven't "regularized" $\theta$. Can do badly (i.e., overfit) if there are outliers or if we don't have enough data to learn $\theta$ reliably.

# Prior Distributions

- In probabilistic models, we can specify a prior distribution $p(\theta)$ on parameters



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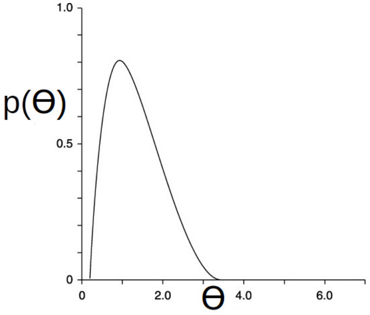


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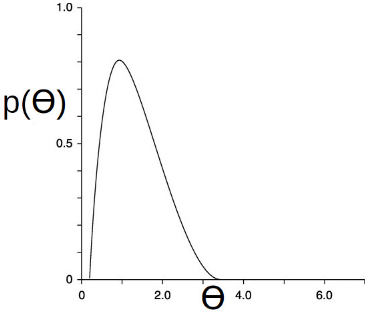


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  - The prior helps us specify that some values of $\theta$ are more likely than others

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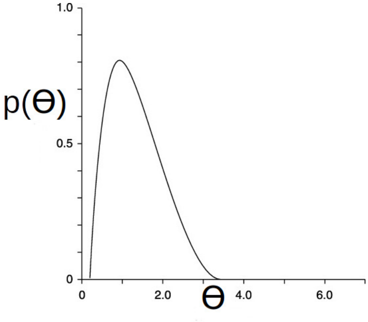


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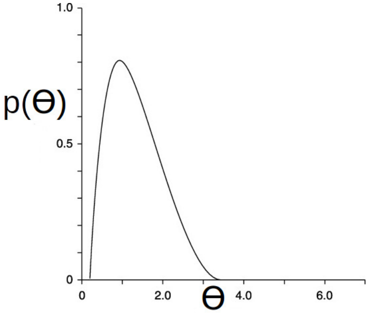


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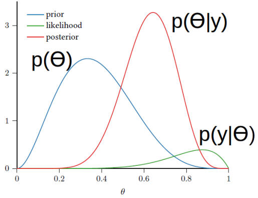
  - The prior also works as a regularizer for $\theta$ (we will see this soon)
- Note: A uniform prior distribution is the same as using no prior!

# Using a Prior in Parameter Estimation

- We can **combine** the prior $p(\theta)$ with the likelihood $p(\boldsymbol{y}|\theta)$ using Bayes rule and define the posterior distribution over the parameters $\theta$

$$p(\theta|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\theta)p(\theta)}{p(\boldsymbol{y})}$$



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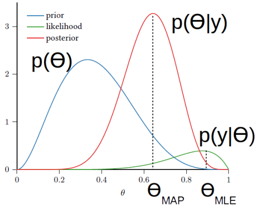


- Now, instead of doing MLE which maximizes the likelihood, we can find the $\theta$ that maximizes the posterior probability $p(\theta|\boldsymbol{y})$

$$\hat{\theta}_{MAP} = \arg\max_{\theta} p(\theta|\boldsymbol{y})$$

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- When $p(\theta)$ is a uniform prior, MAP reduces to MLE

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- Let's again consider the coin-toss problem (estimating the bias of the coin)
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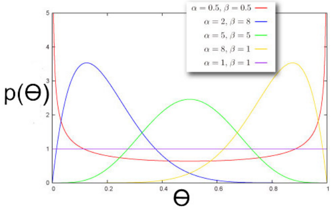

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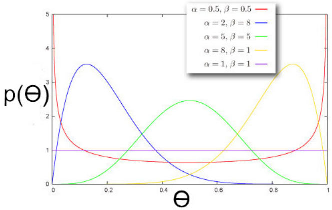


- For Beta, using $\alpha = \beta = 1$ corresponds to using a uniform prior distribution

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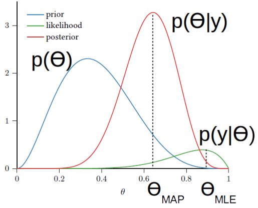
- **Note:** Hyperparameters of a prior distribution usually have intuitive meaning. E.g., in the coin-toss example, $\alpha - 1$, $\beta - 1$ are like "pseudo-observations" - expected numbers of heads and tails, respectively, before tossing the coin

# Inferring the full Posterior (aka Bayesian Inference)

- MLE/MAP only give us a point estimate of $\theta$. Doesn't capture the uncertainty in $\theta$



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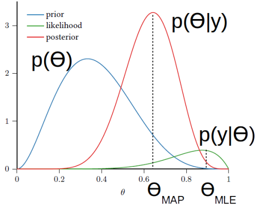


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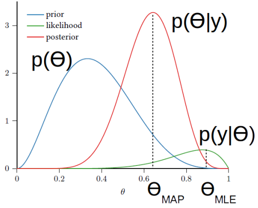


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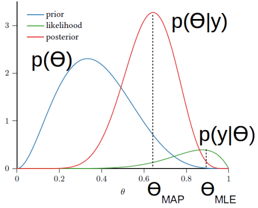


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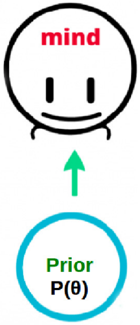
- A very nice aspect is that Bayesian inference is naturally "online" (the posterior can be treated as a prior for next batch of data and updated recursively as we see more and more data)

# Bayesian Inference

- Bayesian inference fits naturally into an "online" learning setting



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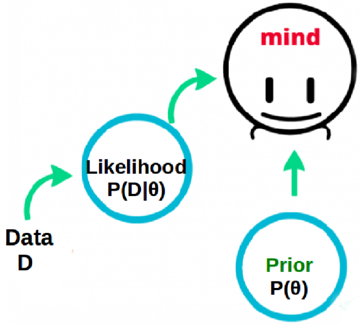

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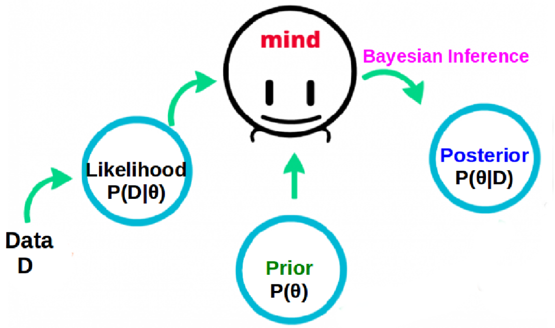

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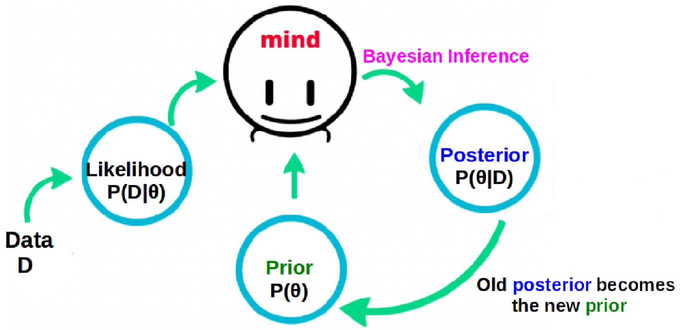

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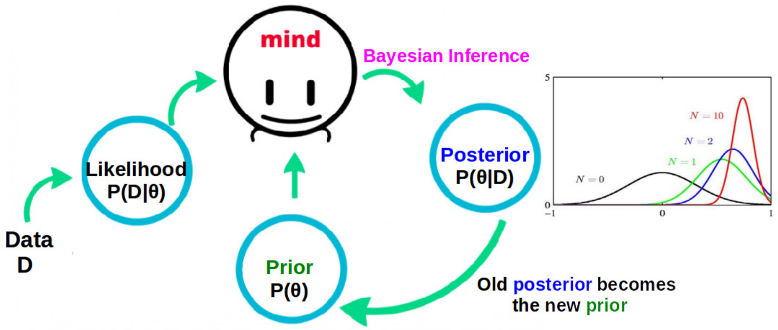

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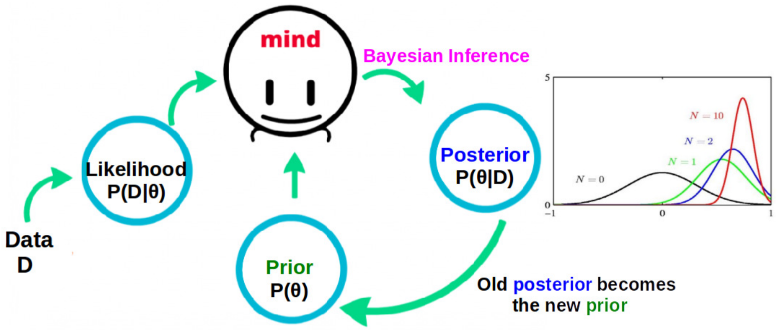


- Our belief about $\theta$ keeps getting updated as we see more and more data

# Bayesian Inference: An Example

- Let's again consider the coin-toss example
- With Bernoulli likelihood and Beta prior (a conjugate pair), the posterior is also Beta

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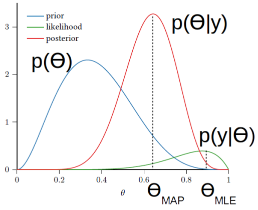
- Exercise: Can verify the above by simply plugging in the expressions of likelihood and prior into the Bayes rule and identifying the form of resulting posterior (note: this may not always be easy)



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- Note that the fully Bayesian approach to prediction averages over all possible values of $\theta$, weighted by their respective posterior probabilities (easy in this example, but a hard problem in general)

# Probabilistic Linear Regression

# Linear Regression: A Probabilistic View

- Given: $N$ training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, features: $\boldsymbol{x}_n \in \mathbb{R}^D$, response $y_n \in \mathbb{R}$
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- Thus each $y_n$ can be thought of as drawn from a Gaussian, as follows

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$$\boxed{y_n = \boldsymbol{w}^\top \boldsymbol{x}_n + \epsilon_n}$$

- Gaussian noise: $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$, $\sigma^2$: variance of Gaussian noise
- Thus each $y_n$ can be thought of as drawn from a Gaussian, as follows

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- Goal: Learn weight vector $\boldsymbol{w}$ (note: $\sigma^2$ assumed known but can be learned)

# Linear Regression: A Probabilistic View

- Given: $N$ training examples $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, features: $\boldsymbol{x}_n \in \mathbb{R}^D$, response $y_n \in \mathbb{R}$
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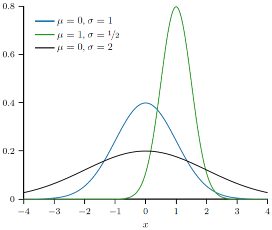
- Let's look at both MLE and MAP estimation for this probabilistic model

# Gaussian Distribution: Brief Review

# Univariate Gaussian Distribution

- Distribution over real-valued scalar r.v. $x$
- Defined by a scalar **mean** $\mu$ and a scalar **variance** $\sigma^2$
- Distribution defined as

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

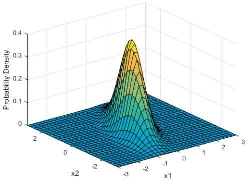



- Mean: $\mathbb{E}[x] = \mu$
- Variance: $\text{var}[x] = \sigma^2$

# 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 $D \times D$ **covariance matrix** $\boldsymbol{\Sigma}$

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




- 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 $\boldsymbol{z}$

# MLE for Probabilistic Linear Regression

- Assuming Gaussian distributed responses $y_n$, we have

$$p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2}{2\sigma^2}\right\}$$

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- Thus the likelihood (assuming i.i.d. responses) or *probability* of data:

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- Note that **negative** log likelihood (NLL) is similar to squared loss function
- MLE will give the same solution as in the (unregularized) least squares

# MAP Estimation for Probabilistic Linear Regression

- We want to regularize our model, so we will use a prior distribution on the weight vector $\boldsymbol{w}$. We will use a **multivariate Gaussian prior** with zero mean

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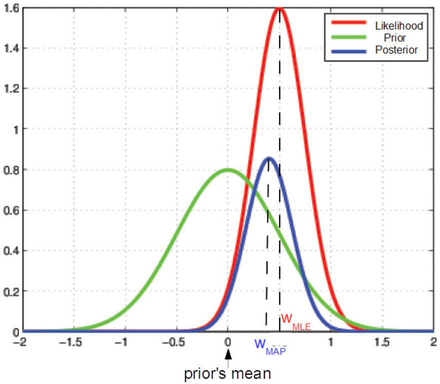
- Assuming $\lambda = \frac{\sigma^2}{\rho^2}$ (regularization hyperparam), it's equivalent to regularized (i.e., ridge) regression

# MLE vs MAP Estimation: An Illustration

$\boldsymbol{w}_{MAP}$ is a compromise between prior's mean and $\boldsymbol{w}_{MLE}$




In this case, doing MAP shrinks the estimate of $\boldsymbol{w}$ towards the prior's mean

# MLE vs MAP for Linear Regression: Summary

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  - Note: Full Bayesian inference can be performed as well (not a focus of this course though)

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- MLE/MAP estimation is also related to the optimization view of ML

# Next Class:
# Probabilistic Models for Classification
# (Logistic Regression)