Machine Learning

Lecture 6: Linear Regression

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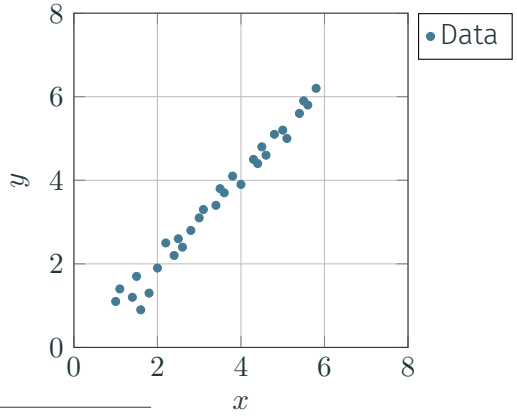
Outline

Regression problem

Given a dataset $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$ of observations, predict y_{new} for a x_{new}?

Given features $\boldsymbol{x}_i \in \mathbb{R}^D$ and labels $y_i \in \mathbb{R}$, find a mapping f such that $y_i \approx f(\boldsymbol{x}_i)$



On the figure $x_i \in \mathbb{R}$ is one dimensional.

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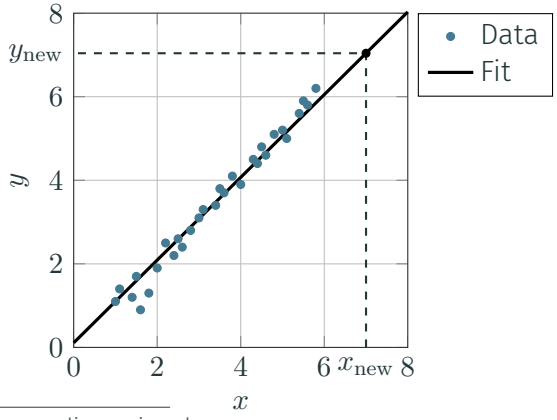

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Linear model

Target y is generated by a deterministic function f of $\boldsymbol{x}$ plus Gaussian noise

$$y_i = f(\boldsymbol{x}_i) + \epsilon_i, \qquad \epsilon_i \sim \mathcal{N}(0, \beta^{-1})$$

We choose $f(\boldsymbol{x})$ to be a linear function

$$\begin{aligned} f_{\boldsymbol{w}}(\boldsymbol{x}_i) &= w_0 + w_1 x_{i1} + w_2 x_{i2} + ... + w_D x_{iD} \\ &= w_0 + \boldsymbol{w}^T \boldsymbol{x}_i \end{aligned}$$

Here w_0 is called the bias or offset term.

Absorbing the bias term

The linear function is given by

$$\begin{aligned} f_{\boldsymbol{w}}(\boldsymbol{x}) &= w_0 + w_1 x_1 + w_2 x_2 + ... + w_D x_D \\ &= w_0 + \boldsymbol{w}^T \boldsymbol{x} \end{aligned}$$

For simplicity, we can "absorb" it by prepending a 1 to the feature vector $\boldsymbol{x}$ and respectively adding w_0 to the weight vector $\boldsymbol{w}$:

$$\tilde{\boldsymbol{x}} = (1, x_1, ..., x_D)^T \qquad \tilde{\boldsymbol{w}} = (w_0, w_1, ..., w_D)^T$$

The function $f_{\boldsymbol{w}}$ can compactly be written as $f_{\boldsymbol{w}}(\boldsymbol{x}) = \tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}}$.

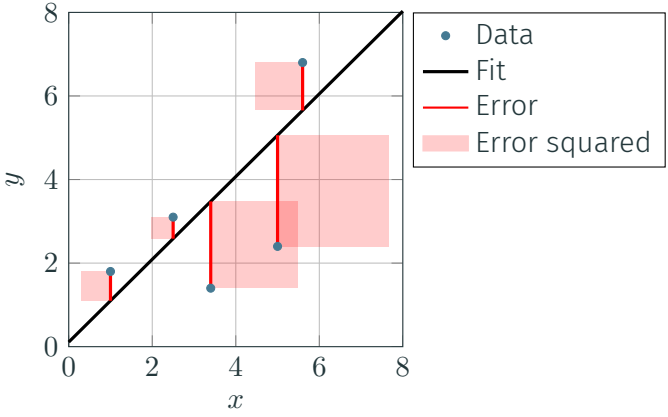
To unclutter the notation, we will assume the bias term is always absorbed and write $\boldsymbol{w}$ and $\boldsymbol{x}$ instead of $\tilde{\boldsymbol{w}}$ and $\tilde{\boldsymbol{x}}$.

Now, how do we choose the "best" $\boldsymbol{w}$ that fits our data?

The least squares loss

Standard choice to measure the error between our model (parametrized by $\boldsymbol{w}$) and the observed data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$ is the **least squares** loss.

$$\begin{aligned}\mathcal{L}_{\text{LS}}(\boldsymbol{w}) &= \frac{1}{2}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2 \\ &= \frac{1}{2}\sum_{i=1}^{N}(f_{\boldsymbol{w}}(\boldsymbol{x}_i) - y_i)^2 \\ &= \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_i - y_i)^2\end{aligned}$$



The factor $\frac{1}{2}$ is for later convenience.

Minimizing the loss

Find the optimal weight vector $\boldsymbol{w}^\star$ that minimizes the loss

$$\begin{aligned}\boldsymbol{w}^* &= \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) \\ &= \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{x}_i^T \boldsymbol{w} - y_i)^2\end{aligned}$$

By stacking the observations $\boldsymbol{x}_i$ as rows of a matrix $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)^T \in \mathbb{R}^{N \times D}$ and the targets y_i into a vector $\boldsymbol{y} = (y_1, \ldots, y_N) \in \mathbb{R}^N$.

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \frac{1}{2} (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

We omit the LS subscript in $\mathcal{L}_{\mathrm{LS}}(\boldsymbol{w})$ when it is clear from the context.

Optimal solution

To find the minimum of the loss $\mathcal{L}(\boldsymbol{w})$, compute the gradient $\nabla_{\boldsymbol{w}}\mathcal{L}(\boldsymbol{w})$:

$$\begin{aligned}\nabla_{\boldsymbol{w}}\mathcal{L}(\boldsymbol{w}) &= \nabla_{\boldsymbol{w}}\frac{1}{2}(\boldsymbol{X}\boldsymbol{w}-\boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{w}-\boldsymbol{y}) \\ &= \nabla_{\boldsymbol{w}}\frac{1}{2}\left(\boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}-2\boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{y}+\boldsymbol{y}^T\boldsymbol{y}\right) \\ &= \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}-\boldsymbol{X}^T\boldsymbol{y}\end{aligned}$$

See Equations (69), (81) from The Matrix Cookbook for details.

Optimal solution

Now set the gradient to zero and solve for $\boldsymbol{w}$ to obtain the minimizer[1]

$$\begin{aligned} \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^T\boldsymbol{y} &\stackrel{!}{=} 0 \\ \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} &= \boldsymbol{X}^T\boldsymbol{y} \end{aligned}$$

This leads to the so-called normal equation of the least squares problem

$$\boldsymbol{w}^* = \underbrace{(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T}_{=\boldsymbol{X}^\dagger}\boldsymbol{y} \tag{1}$$

$\boldsymbol{X}^\dagger$ is called the **Moore-Penrose pseudo-inverse** of $\boldsymbol{X}$ because for an invertible square matrix, $\boldsymbol{X}^\dagger = \boldsymbol{X}^{-1}$.

[1] Because the Hessian $\nabla_{\boldsymbol{w}}\nabla_{\boldsymbol{w}}E(\boldsymbol{w}) = \boldsymbol{X}^T\boldsymbol{X}$ is positive (semi)definite.

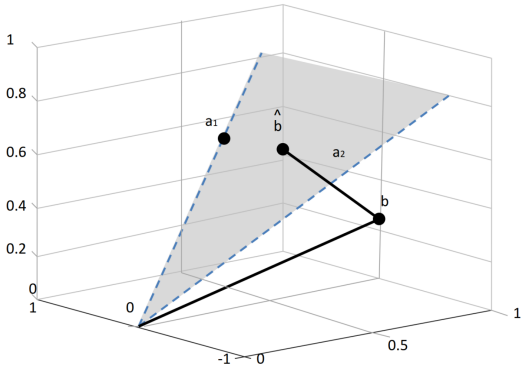
Geometric interpretation

Assume more observations than unknowns ($N > D$) – an overdetermined system.

Example $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ for $\boldsymbol{A} \in \mathbb{R}^{3\times 2}$.
3 equations and 2 unknowns.

The columns of $\boldsymbol{A}$, $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, define a 2D linear subspace embedded in $\mathbb{R}^3$.

$\hat{\boldsymbol{b}}$ is the orthogonal projection of the target $\boldsymbol{b}$ onto the linear subspace.



In the special case that $\boldsymbol{X} = \boldsymbol{x}$ is a column vector, the orthogonal projection of y onto the line x becomes $\boldsymbol{x}\frac{\boldsymbol{x}^T\boldsymbol{y}}{\boldsymbol{x}^T\boldsymbol{x}}$.

Algorithmic issues

The closed from ordinary least squares (OLS) solution is $\boldsymbol{w}^* = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$.

Possible numerical issues if $\boldsymbol{X}^T\boldsymbol{X}$ is ill-conditioned or singular leading.

Alternatives:

- Compute the pseudo-inverse using the SVD (default in sklearn)
- If $\boldsymbol{X}$ is tall and skinny ($N \gg D$) we can use QR decomposition[2]
- Iterative solvers such as conjugate gradient methods and GMRES[3]

[2] Here $\boldsymbol{w}^* = \boldsymbol{R}^{-1}\boldsymbol{Q}^T\boldsymbol{y}$, where $\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R}$ and $\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{I}$ and $\boldsymbol{R}$ is upper triangular.

[3] Suitable when $\boldsymbol{X}$ is sparse or structured since they only need the ability to perform matrix-vector multiplications.

Outline

Simple linear regression

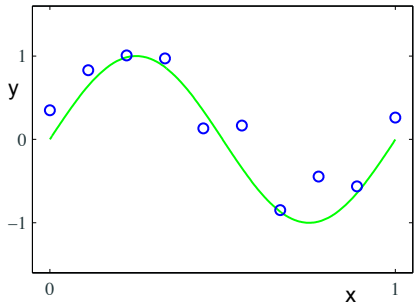
Non-linear relationships

Probabilistic Interpretation

Nonlinear dependency in data

What if the dependency between y and $\boldsymbol{x}$ is not linear?

Example data generating process: $y_i = \sin(2\pi x_i) + \epsilon_i, \qquad \epsilon_i \sim \mathcal{N}(0, \beta^{-1})$



For this example assume that the data dimensionality is $D = 1$.

Polynomials

Solution: Polynomials are universal function approximators.

So for a 1-dimensional x we can define f as

$$f_{\boldsymbol{w}}(x) = w_0 + \sum_{j=1}^{M} w_j x^j$$

or more generally for any basis function $\phi_j(x)$

$$= w_0 + \sum_{j=1}^{M} w_j \phi_j(x)$$

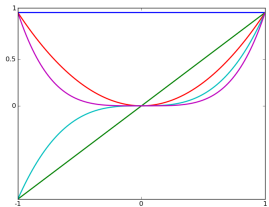
Absoribing the bias term by defining $\phi_0 = 1$

$$f_{\boldsymbol{w}}(x) = \boldsymbol{w}^T \boldsymbol{\phi}(x) = \boldsymbol{w}^T \left[\phi_0(x), \phi_1(x), \ldots, \phi_M(x)\right]$$

The function f is still linear in $\boldsymbol{w}$ despite being potentially non-linear in x!

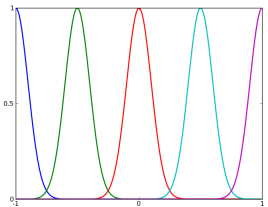
Typical basis functions

Polynomials



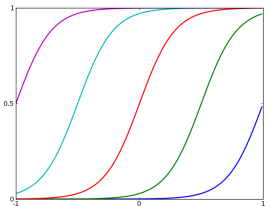
$$\phi_j(x) = x^j$$

Gaussian



$$\phi_j(x) = \exp^{\frac{-(x-\mu_j)^2}{2s^2}}$$

Logistic Sigmoid



$$\phi_j(x) = \sigma(\frac{x-\mu_j}{s}),$$

where $\sigma(a) = \frac{1}{1+\exp^{-a}}$ is the sigmoid, and μ_j and s are hyperparameters.

Linear basis function model

For D-dimensional data $\boldsymbol{x}$, $\phi_j : \mathbb{R}^D \to \mathbb{R}$ and we have

$$f_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + \sum_{j=1}^{M} w_j \phi_j(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})$$

Using the same least squares error function as before

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{2} \sum^{N} \left(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i \right)^2 = \frac{1}{2} (\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y})^T (\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y})$$

$$\text{with } \boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\boldsymbol{x}_1) & \phi_1(\boldsymbol{x}_1) & \dots & \phi_M(\boldsymbol{x}_1) \\ \phi_0(\boldsymbol{x}_2) & \phi_1(\boldsymbol{x}_2) & & \vdots \\ \vdots & \vdots & \ddots & \\ \phi_0(\boldsymbol{x}_N) & \phi_1(\boldsymbol{x}_N) & \dots & \phi_M(\boldsymbol{x}_N) \end{pmatrix} \in \mathbb{R}^{N \times (M+1)}$$

$\boldsymbol{\Phi}$ is called the **design matrix** of $\boldsymbol{\phi}$.

Optimal solution

Recall least squares loss for the original feature matrix $\boldsymbol{X}$

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{2}(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

and compare it to the expression we found with the design matrix $\boldsymbol{\Phi} \in \mathbb{R}^{N\times(M+1)}$

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{2}(\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y})^T(\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}).$$

The optimal weights $\boldsymbol{w}^*$ can be obtained in the same way

$$\boldsymbol{w}^* = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\boldsymbol{y} = \boldsymbol{\Phi}^\dagger\boldsymbol{y} \tag{2}$$

Compare this to Equation 1: $\boldsymbol{w}^* = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^\dagger\boldsymbol{y}$

Only thing we've done is transformed our original features $\boldsymbol{X}$ into new features $\boldsymbol{\Phi}$.

Choosing the degree of the polynomial

How do we choose the degree of the polynomial M?

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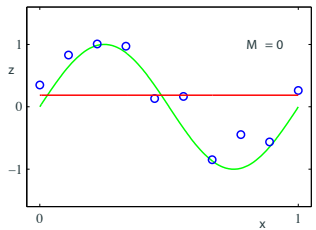

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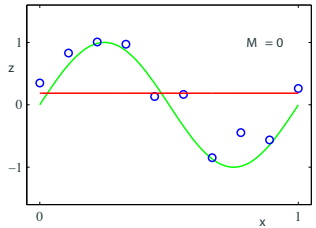

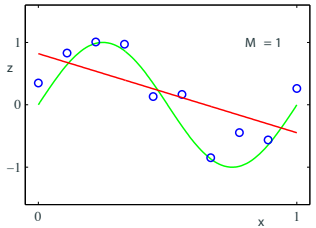

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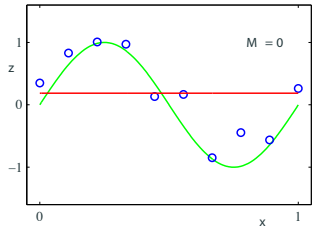

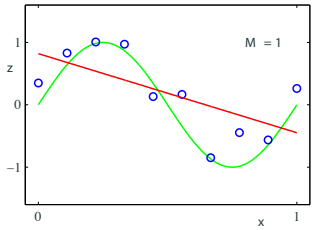

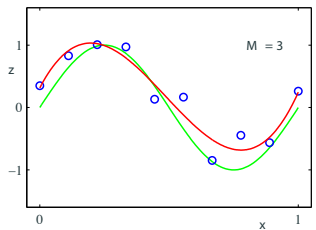

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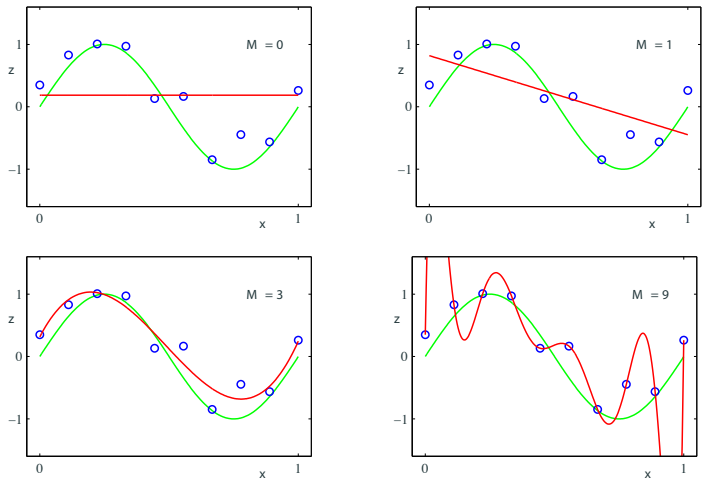
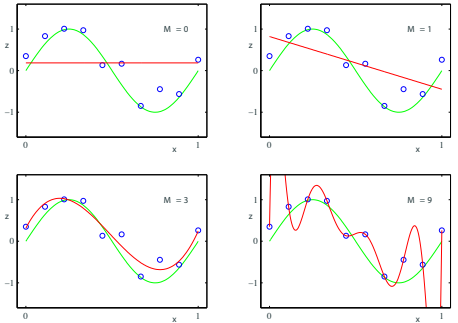
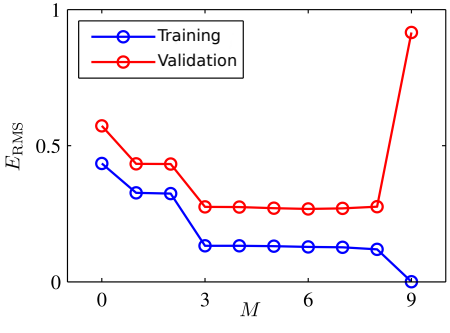


Choosing the degree of the polynomial

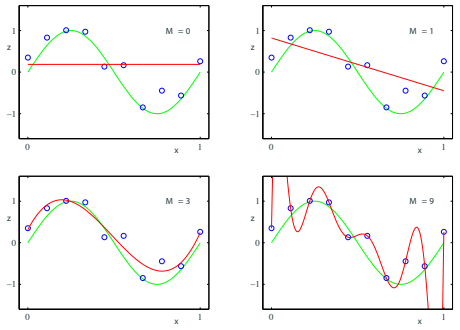
One valid solution is to choose M using the train-validation split.





Manifestation of overfitting

Observation: overfitting occurs when the coefficients $\boldsymbol{w}$ become large.



	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

What if we penalize large weights?

Controlling overfitting with regularization

Least squares loss with **L2 regularization**, also called **ridge regression**

$$\mathcal{L}_{\text{ridge}}(\boldsymbol{w}) = \frac{1}{2}\sum^{N}\left[\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_i) - y_i\right]^2 + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2 \tag{3}$$

where $\|\boldsymbol{w}\|_2^2 \equiv \boldsymbol{w}^T\boldsymbol{w} = w_0^2 + w_1^2 + w_2^2 + \cdots + w_M^2$ is the squared L2 norm of $\boldsymbol{w}$ and λ is the regularization strength.

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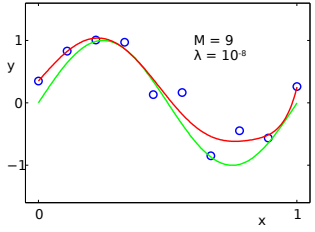
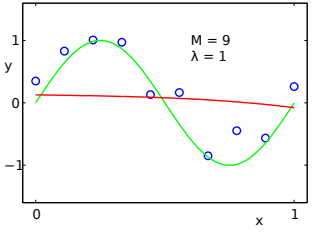
Larger regularization strength λ leads to smaller weights $\boldsymbol{w}$.





Bias-variance trade-off

Increasing the degree of the polynomial M

Increasing the regularization strength λ

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Increasing the regularization strength λ

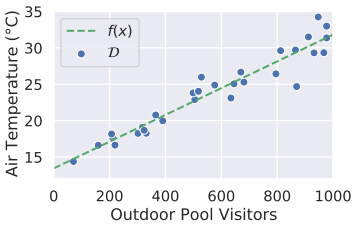
- increases bias
- decreases variance

Intepretation and correlation vs. causation

The weight w_d can be interpreted as the strength of the (linear) relationship between feature x_d and y.

Least squares fit $f(x) = 0.018x + 13.43$.

A weight of 0.018 shows a strong correlation (considering the different scales).



Correlation $\not\Rightarrow$ causation: Increasing pool visitors doesn't increase temperature.

If you normalize the data to handle the different scales of $\boldsymbol{x}$ and $\boldsymbol{y}$ (as we often do in practice) we find a weight of about 1.

Outline

Simple linear regression

Non-linear relationships

Probabilistic Interpretation

Maximum likelihood

Assuming Gaussian likelihood (with a fixed precision β) for a single sample

$$p(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta) = \mathcal{N}(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta^{-1})$$

and assuming that the samples are drawn independently, the likelihood of the entire dataset $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N = \{\boldsymbol{X}, \boldsymbol{y}\}$ is

$$p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) = \prod_{i=1}^{N} p(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta)$$

We use the same approach as previously – maximize the likelihood w.r.t. $\boldsymbol{w}$ and β

$$\boldsymbol{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}} = \arg\max_{\boldsymbol{w}, \beta} p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$$

Maximum likelihood

Like in the coin flip example, we can make a few simplifications

$$\begin{aligned}\boldsymbol{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}} &= \arg\max_{\boldsymbol{w},\beta} p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \\ &= \arg\max_{\boldsymbol{w},\beta} \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \\ &= \arg\min_{\boldsymbol{w},\beta} -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)\end{aligned}$$

We need to minimize the negative log-likelihood which is our loss

$$\mathcal{L}_{\mathrm{NLL}}(\boldsymbol{w}, \beta) = -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$$

Simplifing the loss

$$
\begin{aligned}
\mathcal{L}_{\text{NLL}}(\boldsymbol{w}, \beta) &= -\ln \left[\prod_{i=1}^{N} \mathcal{N}(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta^{-1}) \right] \\
&= -\ln \left[\prod_{i=1}^{N} \sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{2} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 \right) \right] \\
&= -\sum_{i=1}^{N} \ln \left[\sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{2} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 \right) \right] \\
&= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi
\end{aligned}
$$

Minimizing the negative log-likelihood w.r.t. $\boldsymbol{w}$

$$
\begin{aligned}
\boldsymbol{w}_{\mathrm{ML}} &= \arg\min_{\boldsymbol{w}} \mathcal{L}_{\mathrm{NLL}}(\boldsymbol{w}, \beta) \\
&= \arg\min_{\boldsymbol{w}} \left[\frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 \underbrace{- \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi}_{=\text{const}} \right] \\
&= \arg\min_{\boldsymbol{w}} \underbrace{\frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2}_{\text{least squares loss}} \\
&= \arg\min_{\boldsymbol{w}} \mathcal{L}_{\mathrm{LS}}(\boldsymbol{w})
\end{aligned}
$$

Maximizing the likelihood is equivalent to minimizing the least squares loss!

Thus, we have $\boldsymbol{w}^* = \boldsymbol{w}_{\mathrm{LS}} = \boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T \boldsymbol{y} = \boldsymbol{\Phi}^\dagger \boldsymbol{y}$

Minimizing the negative log-likelihood w.r.t. β

Plug in the estimate for $\boldsymbol{w}$ and minimize w.r.t. β

$$\begin{aligned}\beta_{\mathrm{ML}} &= \arg\min_{\beta} E_{\mathrm{ML}}(\boldsymbol{w}_{\mathrm{ML}}, \beta) \\ &= \arg\min_{\beta} \left[\frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}_{\mathrm{ML}}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi \right]\end{aligned}$$

Take derivative w.r.t. β and set it to zero

$$\frac{\partial}{\partial \beta} \mathcal{L}_{\mathrm{ML}}(\boldsymbol{w}_{\mathrm{ML}}, \beta) = \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}_{\mathrm{ML}}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2\beta} \stackrel{!}{=} 0$$

Solving for β

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{i=1}^{N} (\boldsymbol{w}_{\mathrm{ML}}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2$$

Posterior distribution

Since MLE can overfit with little data consider the posterior distribution instead.

$$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot) = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)}^{\text{likelihood}} \cdot \overbrace{p(\boldsymbol{w} \mid \cdot)}^{\text{prior}}}{\underbrace{p(\boldsymbol{y} \mid \boldsymbol{X}, \beta, \cdot)}_{\text{normalizing constant}}} \propto p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)$$

The precision $\beta = 1/\sigma^2$ is treated as a known parameter to simplify the calculations.

Posterior distribution

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$$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot) = \frac{\overbrace{p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)}^{\text{likelihood}} \cdot \overbrace{p(\boldsymbol{w} \mid \cdot)}^{\text{prior}}}{\underbrace{p(\boldsymbol{y} \mid \boldsymbol{X}, \beta, \cdot)}_{\text{normalizing constant}}} \propto p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)$$

Connection to the coin flip example

	train data	likelihood	prior	posterior
coin:	$\mathcal{D} = \boldsymbol{x}$	$p(\mathcal{D} \mid \theta)$	$p(\theta \mid a, b)$	$p(\theta \mid \mathcal{D})$
regr.:	$\mathcal{D} = \{\boldsymbol{X}, \boldsymbol{y}\}$	$p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$	$p(\boldsymbol{w} \mid \cdot)$	$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot)$

The precision $\beta = 1/\sigma^2$ is treated as a known parameter to simplify the calculations.

Choosing the prior for $\boldsymbol{w}$

Isotropic multivariate normal distribution with zero mean as prior for $\boldsymbol{w}$

$$p(\boldsymbol{w} \mid \alpha) = \mathcal{N}(\boldsymbol{w} \mid \mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w}\right)$$

where α is the precision, and M is the dimension.

Motivation:

- Higher probability is assigned to small values of $\boldsymbol{w} \implies$ prevents overfitting (recall slide 20)
- Likelihood is also Gaussian - simplified calculations

Maximum a posteriori (MAP)

We are looking for $\boldsymbol{w}$ that corresponds to the mode of the posterior

$$\begin{aligned}\boldsymbol{w}_{\text{MAP}} &= \arg\max_{\boldsymbol{w}} \; p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \alpha, \beta) \\ &= \arg\max_{\boldsymbol{w}} \; \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) + \ln p(\boldsymbol{w} \mid \alpha) - \underbrace{\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \beta, \alpha)}_{=\text{const}} \\ &= \arg\min_{\boldsymbol{w}} - \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) - \ln p(\boldsymbol{w} \mid \alpha)\end{aligned}$$

Similar to ML, define the MAP loss function as the negative log-posterior

$$\begin{aligned}\mathcal{L}_{\text{MAP}}(\boldsymbol{w}) &= - \ln p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \alpha, \beta) \\ &= - \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) - \ln p(\boldsymbol{w} \mid \alpha) + \text{const}\end{aligned}$$

We ignore the constant terms in the loss function, as they are independent of $\boldsymbol{w}$.

Simplify the MAP loss function

$$
\begin{aligned}
\mathcal{L}_{\text{MAP}} &= -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) - \ln p(\boldsymbol{w} \mid \alpha) \\
&= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi - \frac{M}{2} \ln \left(\frac{\alpha}{2\pi} \right) + \frac{\alpha}{2} \boldsymbol{w}^T \boldsymbol{w} \\
&= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 + \frac{\alpha}{2} \|\boldsymbol{w}\|_2^2 + \text{ const} \\
&\propto \underbrace{\frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 + \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2}_{\text{ridge regression loss}} + \text{const} \qquad \text{where } \lambda = \frac{\alpha}{\beta} \\
&= E_{\text{ridge}}(\boldsymbol{w}) + \text{const}
\end{aligned}
$$

MAP estimation with Gaussian prior is equivalent to ridge regression!

Full Bayesian approach

Full posterior $p(\boldsymbol{w} \mid \mathcal{D}) \propto p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)\, p(\boldsymbol{w} \mid \alpha)$ instead of a point estimate $\boldsymbol{w}_{\text{MAP}}$. Since both likelihood and prior are Gaussian, the posterior is Gaussian as well![4]

$$p(\boldsymbol{w} \mid \mathcal{D}) = \mathcal{N}(\boldsymbol{w} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\boldsymbol{\mu} = \beta \boldsymbol{\Sigma} \boldsymbol{\Phi}^T \boldsymbol{y}$ and $\boldsymbol{\Sigma}^{-1} = \alpha \boldsymbol{I} + \beta \boldsymbol{\Phi}^T \boldsymbol{\Phi}$.

Observations

- The posterior is Gaussian, so its mode is the mean and $\boldsymbol{w}_{\text{MAP}} = \boldsymbol{\mu}$
- In the limit of an infinitely broad prior $\alpha \to 0$, $\boldsymbol{w}_{\text{MAP}} \to \boldsymbol{w}_{\text{ML}}$
- For $N = 0$, i.e. no data points, the posterior equals the prior
- Even though we assume an isotropic prior $p(\boldsymbol{w})$, the posterior covariance is in general not diagonal

[4] The Gaussian distribution is a *conjugate prior* to itself.

Predictions for new data: MLE and MAP

After observing data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$, we can compute the MLE/MAP.

Usually, what we are actually interested in is the prediction $\hat{y}_{\text{new}}$ for a new data point $\boldsymbol{x}_{\text{new}}$ - the model parameters $\boldsymbol{w}$ are just a means to achieve this.

Recall, that $y \sim \mathcal{N}(f_{\boldsymbol{w}}(\boldsymbol{x}), \beta^{-1})$

Plugging in the estimated parameters we get a predictive distribution that lets us make prediction $\hat{y}_{\text{new}}$ for new data $\boldsymbol{x}_{\text{new}}$.

Maximum likelihood given $\boldsymbol{w}_{\text{ML}}$ and β_{ML}:

$$p(\hat{y}_{\text{new}} \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{w}_{\text{ML}}, \beta_{\text{ML}}) = \mathcal{N}\left(\hat{y}_{\text{new}} \mid \boldsymbol{w}_{\text{ML}}^T \boldsymbol{\phi}(\boldsymbol{x}_{\text{new}}), \beta_{\text{ML}}^{-1}\right)$$

Maximum a posteriori given $\boldsymbol{w}_{\text{MAP}}$:

$$p(\hat{y}_{\text{new}} \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{w}_{\text{MAP}}, \beta) = \mathcal{N}\left(\hat{y}_{\text{new}} \mid \boldsymbol{w}_{\text{MAP}}^T \boldsymbol{\phi}(\boldsymbol{x}_{\text{new}}), \beta^{-1}\right)$$

For MAP we assume β to be known a priori to simplify the calculations.

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After observing data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$, we can compute the MLE/MAP.

Usually, what we are actually interested in is the prediction $\hat{y}_{\text{new}}$ for a new data point $\boldsymbol{x}_{\text{new}}$ - the model parameters $\boldsymbol{w}$ are just a means to achieve this.

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Maximum likelihood given $\boldsymbol{w}_{\text{ML}}$ and β_{ML}:

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Maximum a posteriori given $\boldsymbol{w}_{\text{MAP}}$:

$$p(\hat{y}_{\text{new}} \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{w}_{\text{MAP}}, \beta) = \mathcal{N}\left(\hat{y}_{\text{new}} \mid \boldsymbol{w}_{\text{MAP}}^T \boldsymbol{\phi}(\boldsymbol{x}_{\text{new}}), \beta^{-1}\right)$$

For MAP we assume β to be known a priori to simplify the calculations.

Posterior predictive distribution

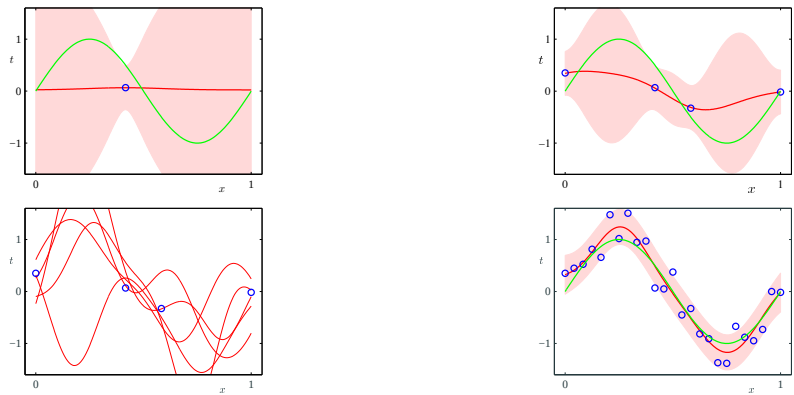
Alternatively, we can use the full posterior distribution $p(\boldsymbol{w} \mid \mathcal{D})$.

This allows us to compute the **posterior predictive** distribution

$$
\begin{aligned}
p(\hat{y}_{\text{new}} \mid \boldsymbol{x}_{\text{new}}, \mathcal{D}) &= \int p(\hat{y}_{\text{new}}, \boldsymbol{w} \mid \boldsymbol{x}_{\text{new}}, \mathcal{D}) \, \mathrm{d}\boldsymbol{w} \\
&= \int p(\hat{y}_{\text{new}} \mid \boldsymbol{x}_{\text{new}}, \boldsymbol{w}) \, p(\boldsymbol{w} \mid \mathcal{D}) \, \mathrm{d}\boldsymbol{w} \\
&= \mathcal{N}\left(\hat{y}_{\text{new}} \mid \boldsymbol{\mu}^T \phi(\boldsymbol{x}_{\text{new}}), \beta^{-1} + \phi(\boldsymbol{x}_{\text{new}})^T \boldsymbol{\Sigma} \phi(\boldsymbol{x}_{\text{new}})\right)
\end{aligned}
$$

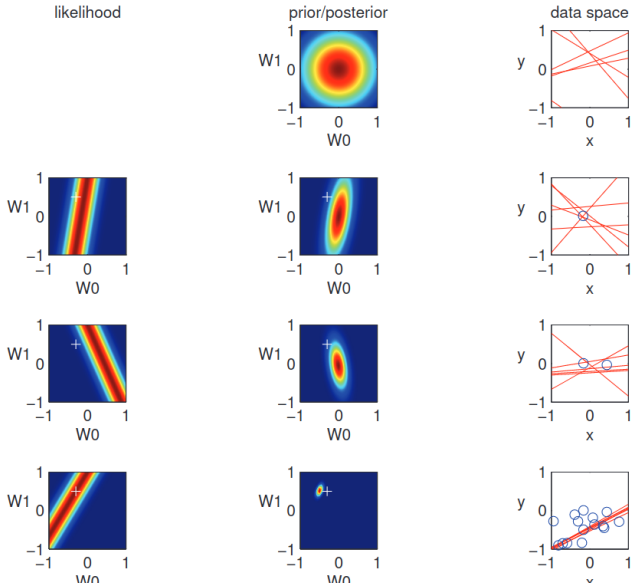
Advantage: We get a data-dependent uncertainty estimate – the variance of the Gaussian now also depends on the input $\boldsymbol{x}_{\text{new}}$.

Example of posterior predictive distribution



True function (green), observations (blue), mode (dark red), variance (light red).

Sequential Bayesian updating



Summary

Optimization-based approaches to regression have probabilistic interpretations:

- Least squares regression $\iff$ Maximum likelihood (Slide 27)
- Ridge regression $\iff$ Maximum a posteriori (Slide 32)

Even non-linear dependencies can be captured by a model linear w.r.t. weights $\boldsymbol{w}$ by applying a non-linear transformation to the input features (Slide 13).

Penalizing large weights helps to reduce overfitting (Slide 20).

Full Bayesian gives us data-dependent uncertainty estimates (Slide 35).

Reading material

Main reading

”Pattern Recognition and Machine Learning” by Bishop
[ch. 1.1, 3.1 – 3.6]

Extra reading

”Machine Learning: A Probabilistic Perspective” by Murphy
[ch. 7.2, 7.3, 7.5.1, 7.6.1, 7.6.2]

Slides are based on an older version by G. Jensen, C. Osendorfer, and S. Günnemann. Some figures are from Bishop’s “Pattern Recognition and Machine Learning”.