Lecture 3: Linear Models for Regression

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SoE, Westlake University

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This lecture:

- Normal Equation and Least Squares
- Probabilistic Interpretation of Linear Regression
- Maximum Likelihood Estimation (MLE)
- Over-fitting and Under-fitting
- Polynomial Regression, Ridge Regression, and Lasso

Next lecture:

- Generalization Gap and Model Selection
- Bias-Variance Decomposition

Reading materials

- Chapter 1, Stanford CS 229 Lecture Notes, `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Chapter 3.1 & 3.2, Bishop, Pattern Recognition and Machine Learning
- Read about over-fitting in the paper by Pedro Domingos (Sections 3 and 5 of “A few useful things to know about machine learning”)

Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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Gradient Descent for linear regression with MSE

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$ for $f_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w}$.

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We define the error vector $\mathbf{e}$:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{2}$$

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and then the gradient is given by $\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N} \mathbf{X}^\top \mathbf{e}$.

Stochastic Gradient Descent (SGD)

- **Sum Objectives:** In machine learning, most cost functions are formulated as a sum over the training examples, that is

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- **Theoretical Motivation:** In expectation over the random choice of n, we have

$$\mathbb{E}[\nabla\mathcal{L}_n(\mathbf{w})] = \nabla\mathcal{L}(\mathbf{w})$$

which is the true gradient direction.

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- Note that in the extreme case $B := [N]$, we obtain (batch) gradient descent, i.e. $\mathbf{g} = \nabla \mathcal{L}$.

An alternative view of SGD

Finite-sum empirical risk minimization problem:

$$f(\mathbf{x}^\star) = \min_{\mathbf{x}\in\mathbb{R}^d} \left\{ f(\mathbf{x}) := \frac{1}{N}\sum_{i=1}^{N} \left(f_i(\mathbf{x}) := \boxed{F(\mathbf{x}, \boldsymbol{\xi}_i)} \right) \right\}$$

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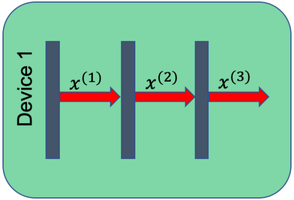

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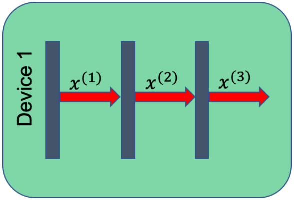

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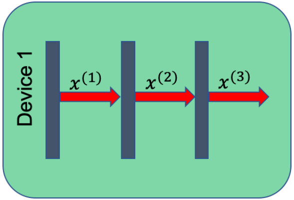

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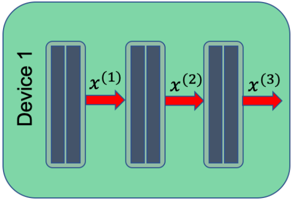
(Using *mini-batching*)



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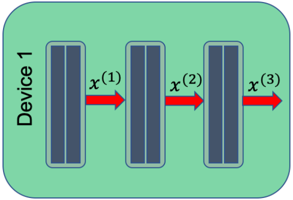

Alternative view: Stochastic reformulation of finite-sum problems (SGD with arbitrary sampling)

Random sampling vector $\mathbf{v} = (v_1, \ldots, v_N) \sim \mathcal{D}$ with $\mathbb{E}\left[v_i\right] = 1 \qquad$ for $i = 1, \ldots, N$.

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Sample $v_i^{(t)} \sim \mathcal{D}$

$$\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} - \eta \nabla f_{v_i^{(t)}}(\mathbf{x}^{(t)})$$

The distribution $\mathcal{D}$ encodes any form of mini-batching / non-uniform sampling.

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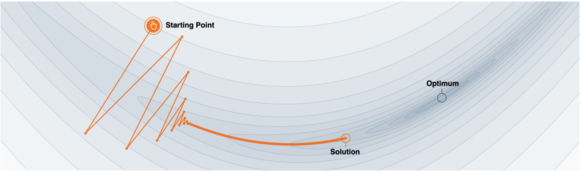
Motivation

Recall that *GD for Linear Regression with MSE loss* is an iterative optimization algorithm, computationally flexibility for handling large datasets.



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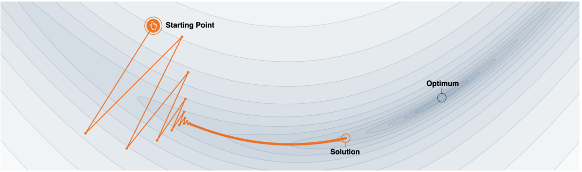
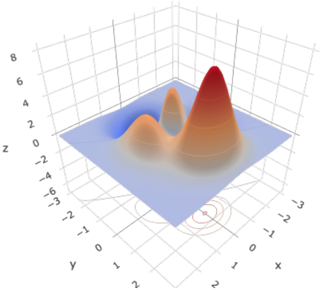
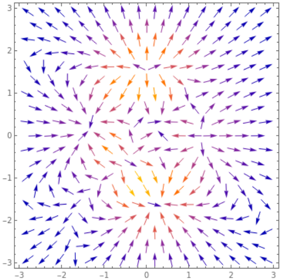


Can we compute the optimum of the cost function analytically?

- Linear regression using an MSE cost function is one such case.



Cost function $f(x, y)$.



Gradient of f plotted as a vector field.

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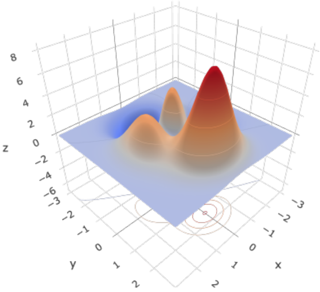

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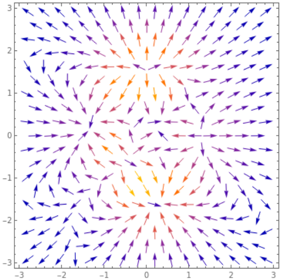

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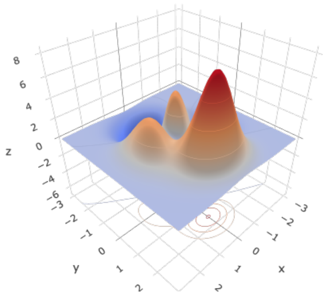

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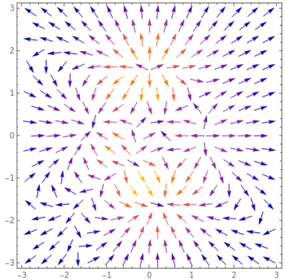

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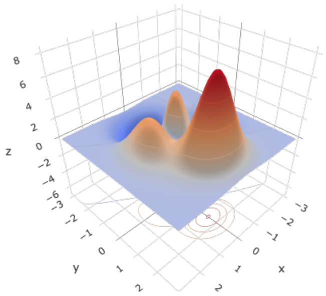

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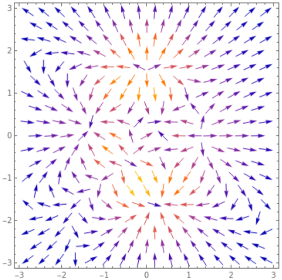

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$\Rightarrow$ Solving the normal equations is called the least squares.

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What is the meaning of finding the analytical solution?

Steps to form normal equations

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Definition 1 (Convexity)

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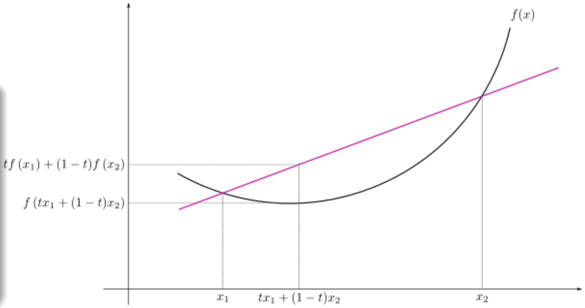

Steps to form normal equations

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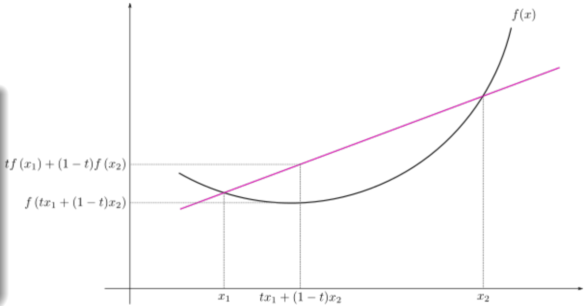

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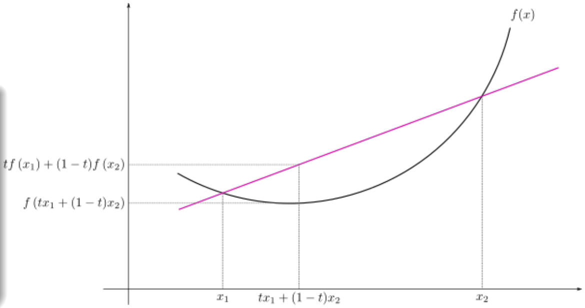

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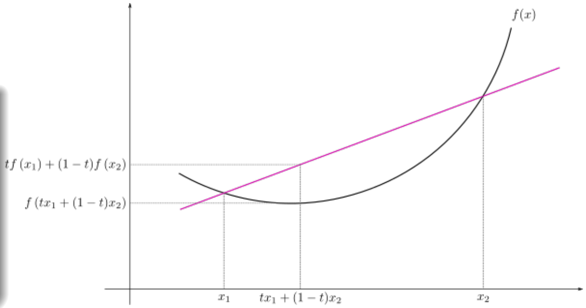

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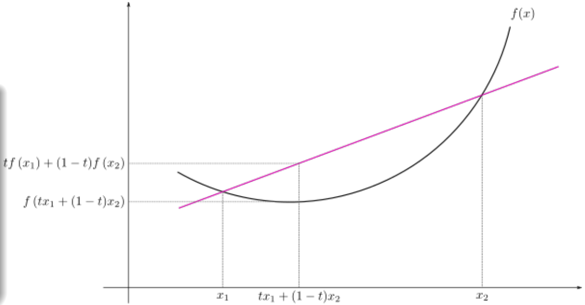

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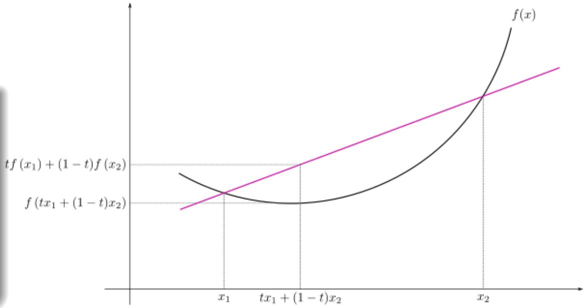

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$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \quad (7)$$

where $\mathbf{w}^\star$ corresponds to the parameter at the optimum point.

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Given the property of convexity $\nabla\mathcal{L}(\mathbf{w}^\star) = \mathbf{0}$, we can get the normal equations for linear regression:

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}\,, \tag{11}$$

where the error $\mathbf{e} := \mathbf{y} - \mathbf{X}\mathbf{w}$ is orthogonal to all columns of $\mathbf{X}$.

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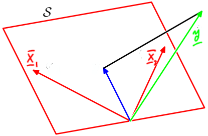

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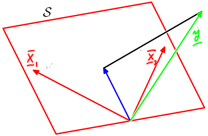

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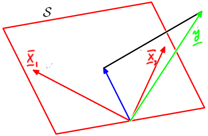

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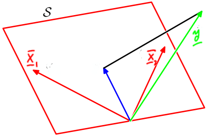

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- $\mathbf{u}^\star$ should be equal to *the projection of* $\mathbf{y}$ *onto* $span(\mathbf{X})$.

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We need to solve the linear system of the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, where

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We need to solve the linear system of the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, where

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Remark 3

The Gram matrix $\mathbf{X}^\top\mathbf{X} \in \mathbb{R}^{D\times D}$ is invertible if and only if $\mathbf{X}$ has full column rank, or in other words $rank(\mathbf{X}) = D$.

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Can we solve least squares if $\mathbf{X}$ is rank deficient?
Yes, using a linear system solver, e.g., $\mathrm{np.linalg.solve}(\mathbf{X}, \mathbf{y})$.

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Two random variables X and Y are called *independent* when $p(x, y) = p(x)p(y)$.

A probabilistic model for linear regression

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The probabilistic view point: maximize this likelihood over the choice of model $\mathbf{w}$.

Maximum-likelihood estimator (MLE)

Instead of maximizing the likelihood, we can maximize the logarithm of the likelihood:

$$\mathcal{L}_{\mathsf{LL}}(\mathbf{w}) := \log p(\mathbf{y} \,|\, \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst}. \qquad \text{(log-likelihood (LL))}$$

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Maximizing the LL is equivalent to minimizing the MSE:

$$\arg\min_{\mathbf{w}}\ \mathcal{L}_{\text{MSE}}(\mathbf{w}) = \arg\max_{\mathbf{w}}\ \mathcal{L}_{\text{LL}}(\mathbf{w}). \tag{21}$$

Properties of MLE

MLE is a *sample* approximation to the *expected log-likelihood*:

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where $\mathbf{F}(\mathbf{w}) = -\mathbb{E}_{p(\mathbf{y})}\left[\frac{\partial^2 \mathcal{L}}{\partial \mathbf{w} \partial \mathbf{w}^\top}\right]$ is the Fisher information.

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4. MLE is efficient, i.e. it achieves the Cramer-Rao lower bound.

Another example

What if we replace the Gaussian distribution with a Laplace distribution?

$$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b}\left|y_n - \mathbf{x}_n^\top \mathbf{w}\right|} \tag{26}$$

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We can recover the MAE cost function!

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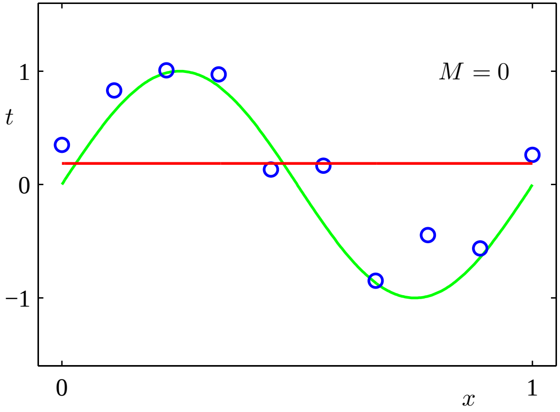

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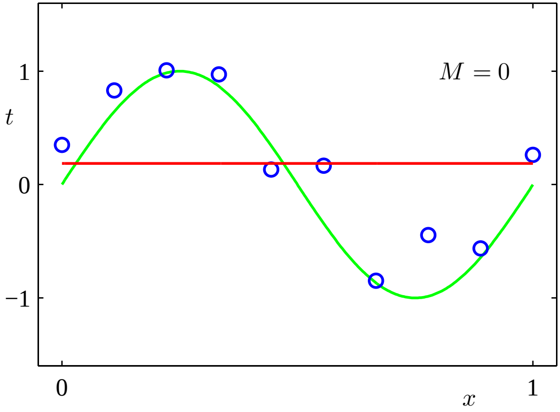

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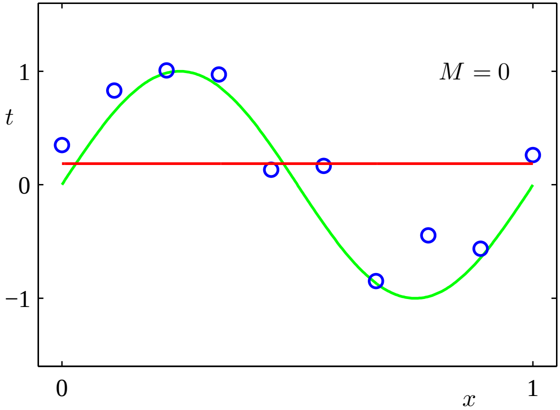

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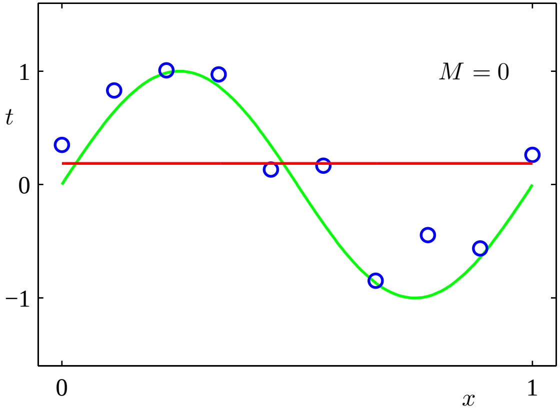

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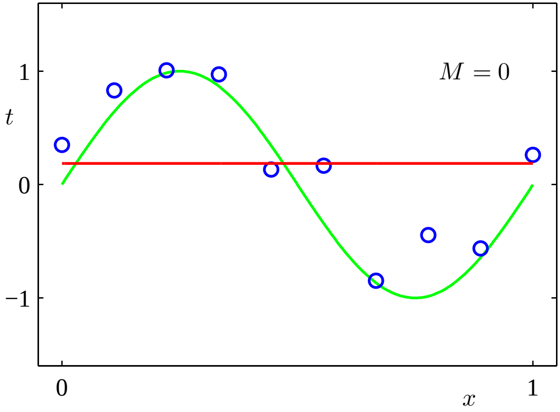

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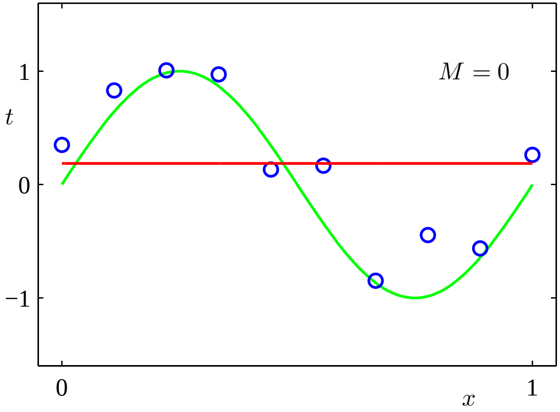

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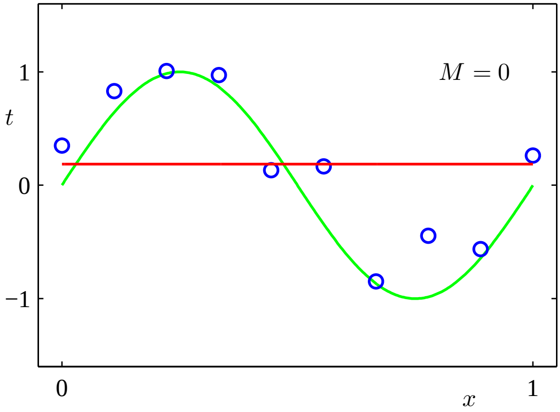

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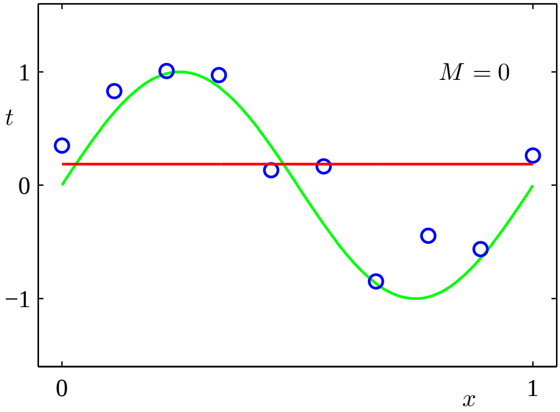

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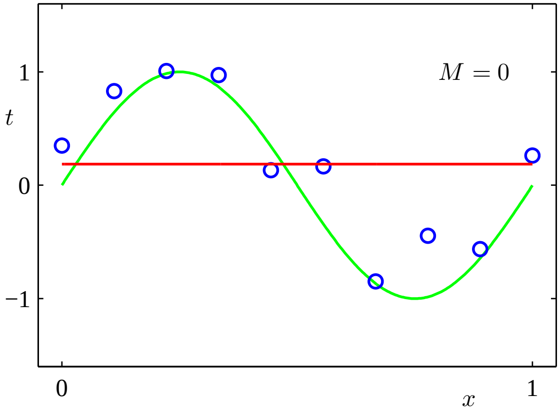

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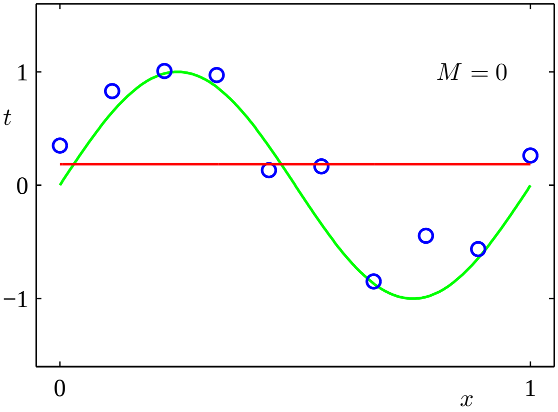

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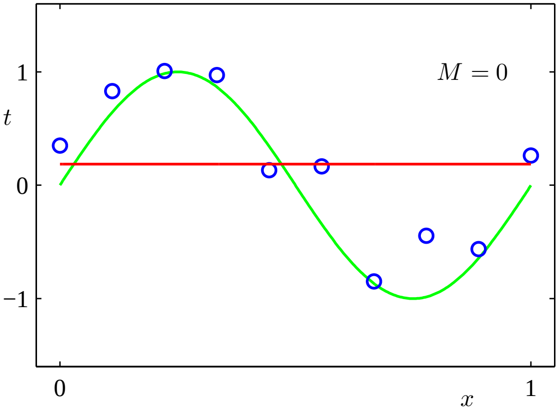

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- The y_n are shown as blue circles.
- Our model family consists of only linear functions of the scalar input x:

$$\mathcal{F} = \{f_w(x) = xw\} \,. \tag{28}$$

Linear Model might under-fit!

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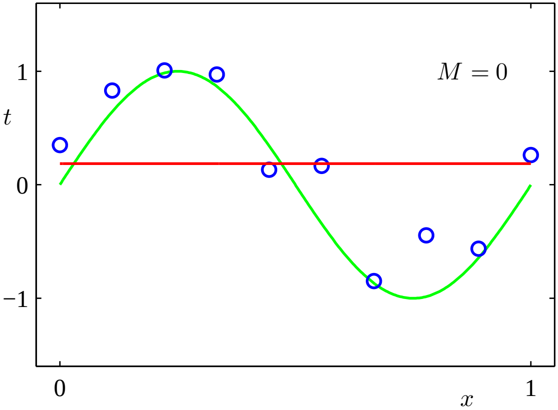

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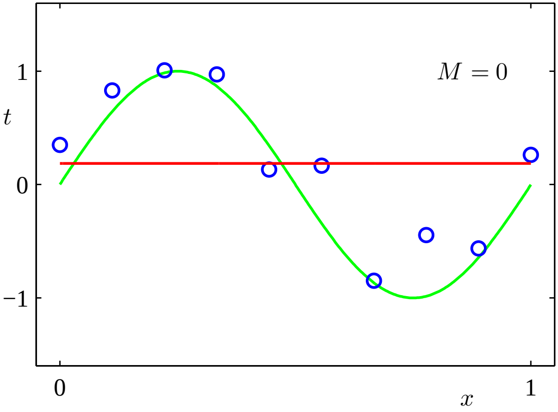

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Is it all good?

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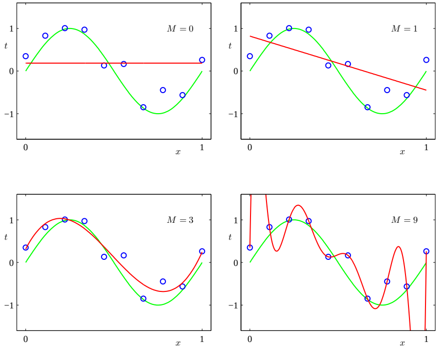

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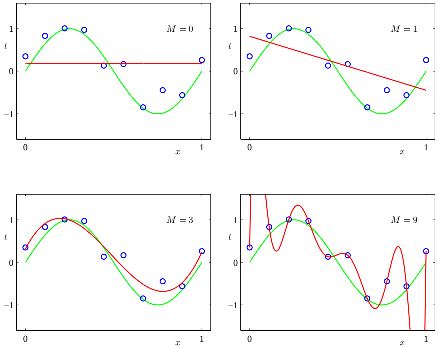

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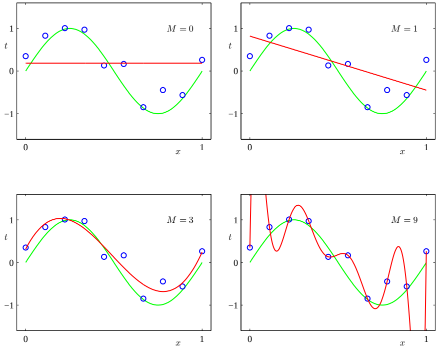

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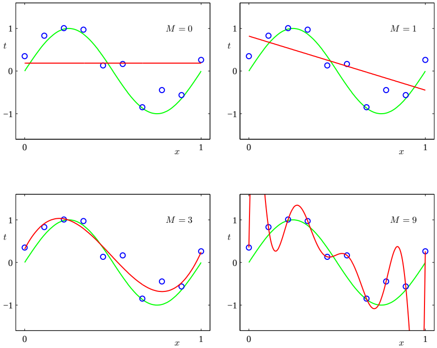

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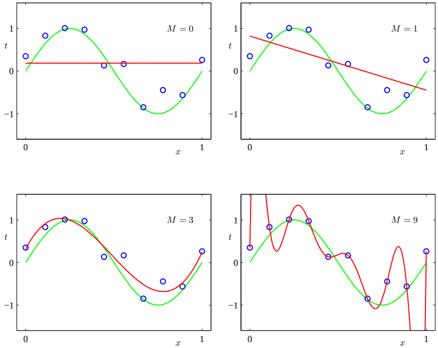

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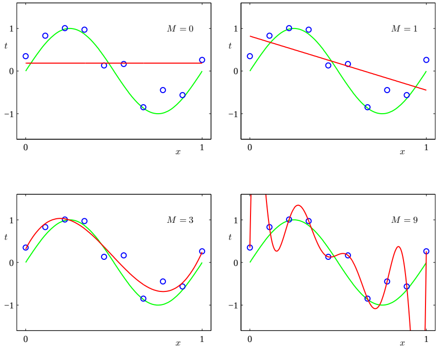

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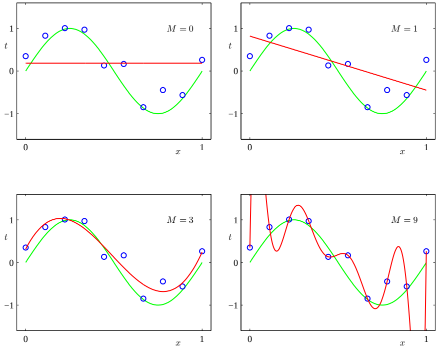

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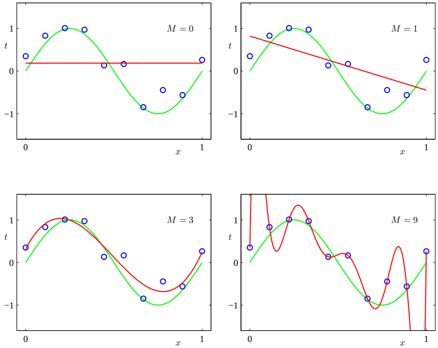

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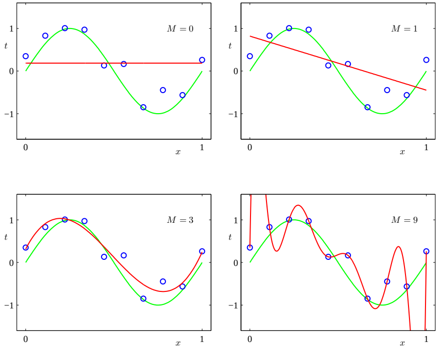

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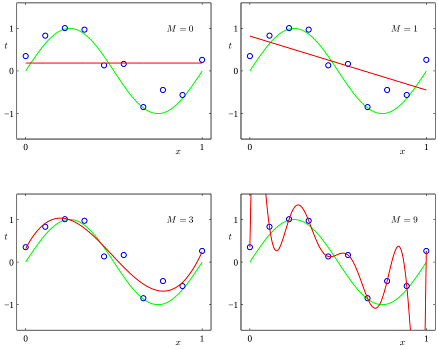

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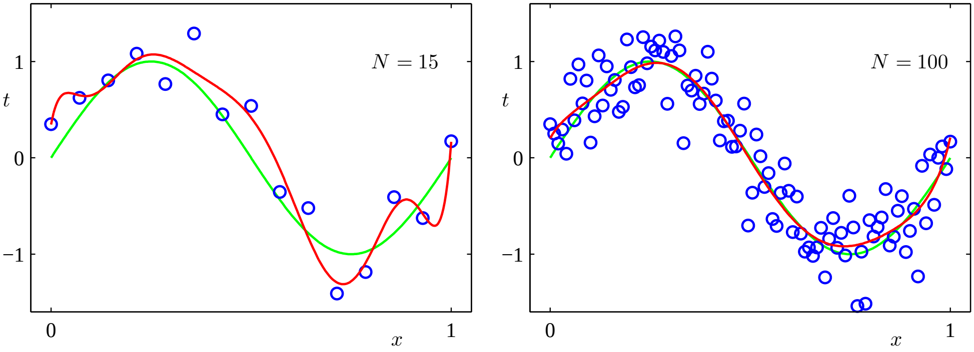
- **Question:** How to avoid over-fitting?



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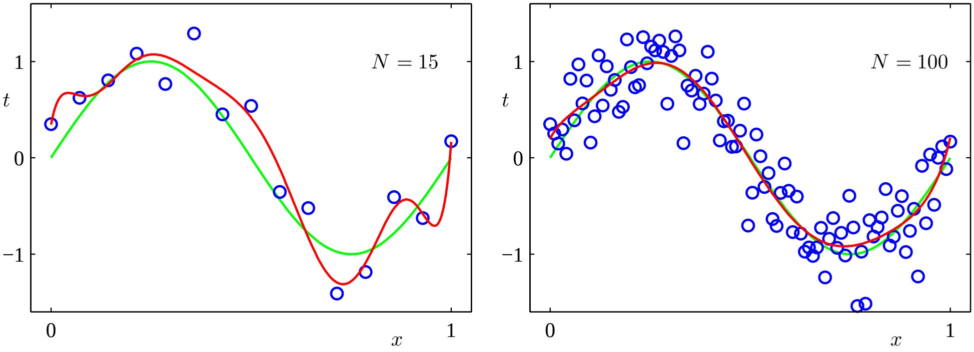

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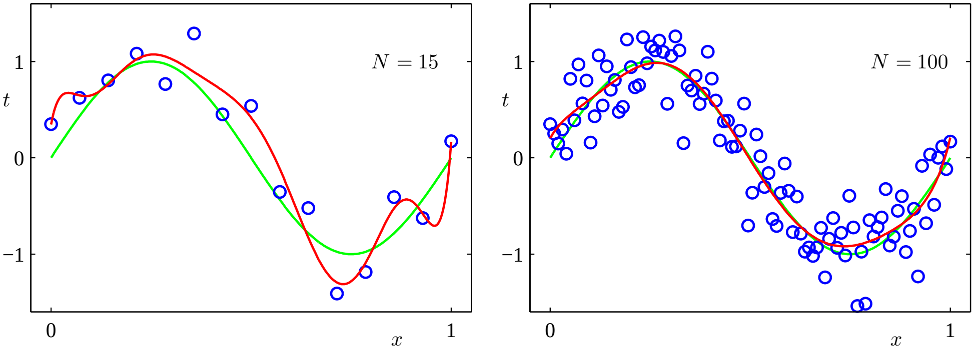

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We will elaborate on this question later!

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Regularization is a way to mitigate this undesirable behavior.

- We will discuss regularization in the context of linear models
- The same principle applies also to more complex models such as neural nets.

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Through regularization, we can penalize complex models and favor simpler ones:

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- Model Complexity $\Longleftrightarrow$ The richness of the model space.

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The most frequently used regularizer is the standard Euclidean norm (L_2-norm), which is

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- *Linear Regression* is a special case of this: by setting $\lambda := 0$.

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$$\mathbf{w}^{\star}_{\text{ridge}} = (\mathbf{X}^{\top}\mathbf{X} + \lambda'\mathbf{I})^{-1}\mathbf{X}^{\top}\mathbf{y} \tag{38}$$

(here for simpler notation $\lambda'/2N = \lambda$)

Ridge Regression to fight ill-conditioning

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Write the Eigenvalue decomposition of $\mathbf{X}^\top\mathbf{X}$ as $\mathbf{USU}^\top$.

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We see now that every Eigenvalue is “lifted” by an amount λ'. □

An alternative proof (optional reading).

Recall that for a symmetric matrix $\mathbf{A}$ we can also compute eigenvalues by looking at the so-called Rayleigh ratio,

$$R(\mathbf{A}, \mathbf{v}) = \frac{\mathbf{v}^\top \mathbf{A}\mathbf{v}}{\mathbf{v}^\top \mathbf{v}}. \tag{41}$$

Note that if $\mathbf{v}$ is an eigenvector with eigenvalue λ, then the Rayleigh coefficient indeed gives us λ.

We can find the smallest and largest eigenvalue by minimizing and maximizing this coefficient.

But note that if we apply this to the symmetric matrix $\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I}$, then for any vector $\mathbf{v}$ we have

$$\frac{\mathbf{v}^\top(\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I})\mathbf{v}}{\mathbf{v}^\top\mathbf{v}} \geq \frac{\lambda'\mathbf{v}^\top\mathbf{v}}{\mathbf{v}^\top\mathbf{v}} = \lambda'\,. \tag{42}$$

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- A very important case is the L_1-norm, leading to L_1-regularization.

In combination with the MSE cost function (i.e., L_1-norm), this is known as the Lasso:

$$\min_{\mathbf{w}} \quad \frac{1}{2N}\sum_{n=1}^{N}\left[y_n - \mathbf{x}_n^\top \mathbf{w}\right]^2 + \lambda \left\|\mathbf{w}\right\|_1 \qquad \text{where } \left\|\mathbf{w}\right\|_1 := \sum_i |w_i| \,. \tag{43}$$

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Geometric interpretation for the Ridge Regression

Recall the definition of the Ridge Regression:

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 \;+\; \lambda \|\mathbf{w}\|_2^2 \,. \tag{44}$$

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The Ridge Regression can be reformulated as

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \sum_{n=1}^{N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 \quad \text{such that } \|\mathbf{w}\|_2^2 \leq \lambda \tag{45}$$

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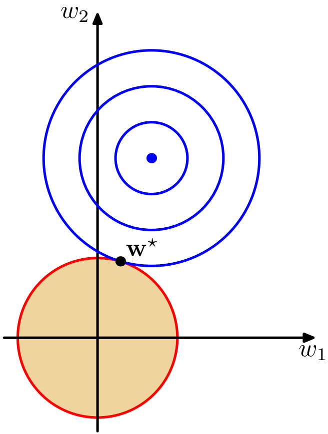

• Blue lines indicate the level sets of the un-regularized MSE.

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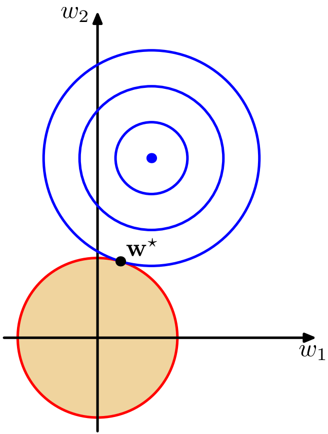

- Blue lines indicate the level sets of the un-regularized MSE.
- The optimum value for $\mathbf{w}$ is $\mathbf{w}^\star$.

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Similarly, the Lasso Regression can be reformulated as

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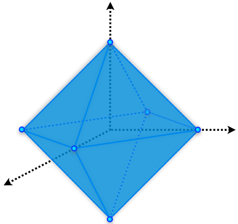

A “ball” of constant L_1 norm

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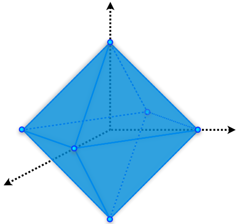

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- The optimal point is somewhere on the surface of this “ball”.

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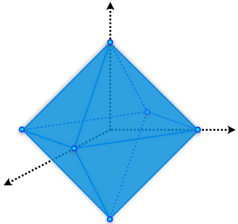

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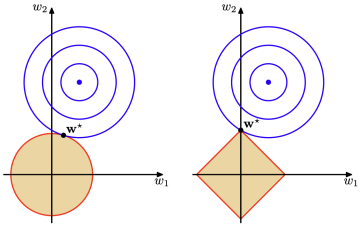

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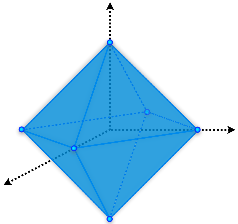

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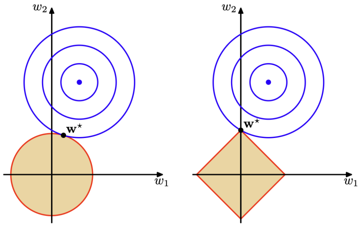

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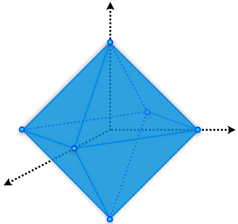

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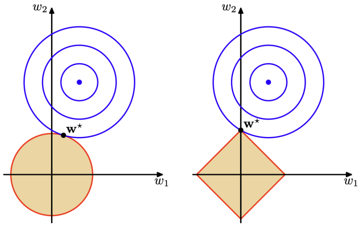

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- This forces some of the elements of $\mathbf{w}$ to be strictly 0.
- As λ is increased, an increasing number of parameters are driven to 0.

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The probabilistic interpretation of least-squares linear regression

Least-Squares linear regression can be interpreted as the Maximum Likelihood Estimator:

$$\mathbf{w}_{\text{lse}} \overset{(a)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y}, \mathbf{X}|\mathbf{w}) \qquad \text{(by the definition of log-likelihood)}$$

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The probabilistic interpretation of Ridge Regression

We start with the posterior $p(\mathbf{w}|\mathbf{X}, \mathbf{y})$ and chose $\mathbf{w}$ to maximize this posterior.

The Maximum-A-Posteriori (MAP) estimate:

$$\mathbf{w}_{\text{ridge}} = \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{w}|\mathbf{X}, \mathbf{y}) \qquad \text{(by the definition of posterior)} \tag{48}$$

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This lecture:

- Normal Equation and Least Squares
- Probabilistic Interpretation of Linear Regression
- Maximum Likelihood Estimation (MLE)
- Over-fitting and Under-fitting
- Polynomial Regression, Ridge Regression, and Lasso

Next lecture:

- Generalization Gap and Model Selection
- Bias-Variance Decomposition