

Linear Least-Squares

Numerical Methods for Deep Learning

Learning Objective: Linear Least-Squares

In this module we review computational methods for linear least-squares problems, which play a role in almost any learning tasks (including deep learning).

Learning tasks:

- ▶ image classification (supervised)
- ▶ image inpainting (semi-supervised)
- ▶ ...

Numerical methods:

- ▶ singular value decomposition
- ▶ steepest descent
- ▶ conjugate gradient method

Reminder: Supervised Learning Problem

Given examples (inputs)

$$\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n] \in \mathbb{R}^{n_f \times n}$$

and labels (outputs)

$$\mathbf{C} = [\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n] \in \mathbb{R}^{n_c \times n},$$

find a classification/prediction function $f(\cdot, \boldsymbol{\theta})$, i.e.,

$$f(\mathbf{y}_j, \boldsymbol{\theta}) \approx \mathbf{c}_j, \quad j = 1, \dots, n.$$

Regression and Least-Squares

Simplest option, a linear model with $\theta = (\mathbf{W}, \mathbf{b})$ and

$$f(\mathbf{Y}, \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{Y} + \mathbf{b}\mathbf{e}_n^\top \approx \mathbf{C}$$

- ▶ $\mathbf{W} \in \mathbb{R}^{n_c \times n_f}$ are *weights*
- ▶ $\mathbf{b} \in \mathbb{R}^{n_c}$ are *biases*
- ▶ $\mathbf{e}_n \in \mathbb{R}^n$ is a vector of ones

Equivalent notation:

$$f(\mathbf{Y}, \mathbf{W}, \mathbf{b}) = (\mathbf{W} \quad \mathbf{b}) \begin{pmatrix} \mathbf{Y} \\ \mathbf{e}_n^\top \end{pmatrix} \approx \mathbf{C}$$

Problem may not have a solution, or may have infinite solutions (when?). Solve through optimization

$$\min_{\mathbf{W}} \frac{1}{2} \|\mathbf{W}\mathbf{Y} - \mathbf{C}\|_F^2$$

(Frobenius norm: $\|\mathbf{A}\|_F^2 = \text{trace}(\mathbf{A}^\top \mathbf{A}) = \sum_{i,j} \mathbf{A}_{i,j}^2$.)

Remark: Relation to Least-Squares

Consider the regression problem

$$\min_{\mathbf{W}} \frac{1}{2} \|\mathbf{W}\mathbf{Y} - \mathbf{C}\|_F^2.$$

It is easy to see that this is equivalent to

$$\min_{\mathbf{W}} \frac{1}{2} \|\mathbf{Y}^\top \mathbf{W}^\top - \mathbf{C}^\top\|_F^2,$$

which can be solved separately for each row in \mathbf{W}

$$\mathbf{W}(j, :)^{\top} = \arg \min_{\mathbf{w}} \frac{1}{2} \|\mathbf{Y}^{\top} \mathbf{w} - \mathbf{C}(j, :)^{\top}\|_F^2.$$

Notation: Let $\mathbf{A} = \mathbf{Y}^\top$ and $\mathbf{X} = \mathbf{W}^\top$ (easy to add bias here), we solve

$$\min_{\mathbf{X}} \frac{1}{2} \|\mathbf{A}\mathbf{X} - \mathbf{C}^\top\|_F^2$$

Detour: Image Inpainting (Semi-Supervised)

Image inpainting: Estimate an image function $f : [0, 1]^2 \rightarrow \mathbb{R}$ from partial observations.

First: Discretize the image on a grid with $n = n_x \cdot n_y$ pixels.

We obtain $\mathbf{f} \in \mathbb{R}^n$.

The input data is given by $\mathbf{c} \in \mathbb{R}^k$ with $k < n$ where

$$\mathbf{d}_i = f(\mathbf{x}_i) + \epsilon_i, \quad i = 1, \dots, k,$$

where \mathbf{x}_i are points in $[0, 1]^2$, and $\epsilon \sim \mathcal{N}(0, \sigma \mathbf{I})$.

Write the inpainting problem as a linear least-squares problem

$$\min_{\mathbf{f}} \frac{1}{2\sigma} \|\mathbf{A}\mathbf{f} - \mathbf{c}\|^2.$$

Question: What is \mathbf{A} ? How good will this approach be?

Optimality Conditions for Least-Squares

To minimize a function need to differentiate and equate to 0

$$\frac{\partial \left(\frac{1}{2} \|\mathbf{AX} - \mathbf{C}^\top\|_F^2 \right)}{\partial \mathbf{X}} = 0$$

Compute the derivatives in three steps

1.

$$\frac{\partial \left(\frac{1}{2} \|\mathbf{R}\|_F^2 \right)}{\partial \mathbf{R}} = ???$$

2.

$$\frac{\partial (\mathbf{AX})}{\partial \mathbf{X}} = ???$$

3. Use chain rule

Least-Squares: Normal Equations

The necessary and sufficient optimality conditions for the least-squares problem are

$$\frac{\partial \left(\frac{1}{2} \|\mathbf{A}\mathbf{X} - \mathbf{C}^\top\|_F^2 \right)}{\partial \mathbf{X}} = \mathbf{A}^\top (\mathbf{A}\mathbf{X} - \mathbf{C}^\top) = 0$$

Reorganize to obtain the **normal equations**

$$\mathbf{X} = (\mathbf{A}^\top \mathbf{A})^{-1} (\mathbf{A}^\top \mathbf{C}^\top).$$

Here, $\mathbf{A}^\top \mathbf{A} \in \mathbb{R}^{n_f \times n_f}$ must be invertible, i.e.,

- ▶ sufficient amount of data ($n > n_f$)
- ▶ data is linearly independent

Coding: Least-Squares for Classification

1. Write a code for solving

$$\min_{\mathbf{W}, \mathbf{b}} \frac{1}{2} \|\mathbf{W}\mathbf{Y} + \mathbf{b}\mathbf{e}_n^\top - \mathbf{C}\|^2$$

and apply it to the MNIST test data from

<http://yann.lecun.com/exdb/mnist/>

2. Solve the problem using the normal equations derived above.
3. Use optimal weights to predict labels for test data. How well does your solution generalize?
4. Visualize the rows of \mathbf{W} as images.

Ill-posedness and the SVD

If the data is linearly dependent or close to be linearly dependent, least-squares problem gives no good solution [2, 6, 3].

Understanding can be gained by the *Singular Value Decomposition* (SVD) (e.g., [1, Ch. 8])

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

where $\mathbf{U} \in \mathbb{R}^{n_f \times n_f}$, $\mathbf{V} \in \mathbb{R}^{n_f \times n}$ satisfy

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I}, \quad \text{and} \quad \mathbf{V}^\top \mathbf{V} = \mathbf{I}$$

Diagonal of $\mathbf{\Sigma}$ contains the singular values $\sigma_1 \geq \dots \sigma_{n_f} \geq 0$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n_f} \end{pmatrix}$$

Ill-posedness and Regularization

Important is the *effective rank*: If $\sigma_j \ll \sigma_k$ for all $j \geq k$, then the effective rank of the problem is k .

If $k < n_f$, the least squares problem is ill-posed, i.e., solution does not exist or is unstable.

Small perturbations in \mathbf{C} or \mathbf{A} yield large perturbations in \mathbf{X}

Solve regularized problem: For some $\lambda > 0$ and matrix \mathbf{G}

$$\min_{\mathbf{X}} \frac{1}{2} \|\mathbf{AX} - \mathbf{C}^\top\|_F^2 + \frac{\lambda}{2} \|\mathbf{GX}\|_F^2$$

Exercise: solve the regularized least-squares problem

$$\mathbf{X} = (\mathbf{A}^\top \mathbf{A} + \lambda \mathbf{G}^\top \mathbf{G})^{-1} \mathbf{A}^\top \mathbf{C}^\top$$

The Bias-Variance Decomposition

Assume $\mathbf{C}^\top = \mathbf{A}\mathbf{X}_{\text{true}} + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma\mathbf{I})$, $\lambda > 0$ fixed, $\mathbf{G} = \mathbf{I}$.

Then setting $\mathbf{A}_\lambda^\dagger = (\mathbf{A}^\top \mathbf{A} + \lambda \mathbf{I})^{-1}$

$$\begin{aligned}\mathbf{X} - \mathbf{X}_{\text{true}} &= \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \mathbf{C}^\top - \mathbf{X}_{\text{true}} \\ &= \left(\mathbf{A}_\lambda^\dagger \mathbf{A}^\top \mathbf{A} - \mathbf{I} \right) \mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \boldsymbol{\epsilon} \\ &= -\lambda \mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \boldsymbol{\epsilon}\end{aligned}$$

Error depends on $\boldsymbol{\epsilon} \rightsquigarrow$ take expectation

$$\begin{aligned}\mathbb{E} \|\mathbf{X} - \mathbf{X}_{\text{true}}\|_F^2 &= \mathbb{E} \|\underbrace{\mathbf{A}_\lambda^\dagger \mathbf{A}^\top \boldsymbol{\epsilon}}_{\text{variance}} - \underbrace{\lambda \mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}}}_{\|\text{bias}\|_F^2}\|_F^2 \\ &= \overbrace{\lambda^2 \|\mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}}\|_F^2}^{\|\text{bias}\|_F^2} + \overbrace{\sigma^2 \text{trace} \left(\mathbf{A} \mathbf{A}_\lambda^{\dagger \top} \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \right)}^{\text{variance}}\end{aligned}$$

Take home: No such thing as exact recovery!

Iterative Solvers for Least-Squares Regression

So far: Given $\mathbf{Y} \in \mathbb{R}^{n_f \times n}$ and $\mathbf{C} \in \mathbb{R}^{n_c \times n}$, solve

$$\min_{\mathbf{X}} \frac{1}{2} \|\mathbf{A}\mathbf{X} - \mathbf{C}^\top\|_F^2$$

directly using $\mathbf{X}^* = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{C}^\top$. Here

$$\mathbf{A} = \begin{pmatrix} \mathbf{Y}^\top & \mathbf{e}_n \end{pmatrix}, \quad \text{and} \quad \mathbf{X} = \mathbf{W}^\top \in \mathbb{R}^{(n_f+1) \times n_c}.$$

Problems:

1. Generating $\mathbf{A}^\top \mathbf{A}$ and solving normal equations is too costly for large-scale problems.
2. Exact solution not useful when problem is ill-posed \leadsto add explicit regularization or do so implicitly by early stopping.

Iterative methods that avoid working with $\mathbf{A}^\top \mathbf{A}$

- ▶ Steepest descent
- ▶ Conjugate gradient for least-squares (CGLS)

Excellent references: Numerical Optimization [4], iterative linear algebra [5], general introduction [1]

Iterative Methods

General idea - obtain a sequence $\mathbf{X}_1, \dots, \mathbf{X}_j, \dots$ that converges to least-squares solution \mathbf{X}^*

$$\mathbf{X}_j \longrightarrow \mathbf{X}^*, \quad \text{for } j \rightarrow \infty.$$

How fast does the sequence converge? Assume

$$\|\mathbf{X}_{j+1} - \mathbf{X}^*\| < \gamma_j \|\mathbf{X}_j - \mathbf{X}^*\|$$

where all $\gamma_j < 1$. Then

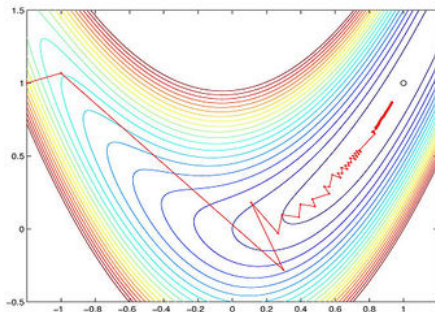
- ▶ If γ_j is bounded away from 0 and 1 the convergence is linear
- ▶ If $\gamma_j \rightarrow 0$ the convergence is superlinear
- ▶ If $\gamma_j \rightarrow 1$ the convergence is sublinear

The sequence converges quadratically if γ_j is bounded away from 0 and 1 and

$$\|\mathbf{X}_{j+1} - \mathbf{X}^*\| < \gamma_j \|\mathbf{X}_j - \mathbf{X}^*\|^2$$

Steepest Descent

Most basic iterative technique for solving $\min_{\mathbf{x}} \phi(\mathbf{x})$



$$\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}_j \quad \text{with} \quad \mathbf{d}_j = -\nabla \phi(\mathbf{x}_j).$$

Interpretation 1: \mathbf{d}_{j+1} maximizes local descent, i.e., solves

$$\min_{\mathbf{s}} \phi(\mathbf{x}_j) + \mathbf{d}^\top \nabla \phi(\mathbf{x}_j) \quad \text{subject to} \quad \|\mathbf{d}\|_2 = 1.$$

Interpretation 2: \mathbf{d}_j is orthogonal to level sets of ϕ at \mathbf{x}_j .

Steepest Descent for Least-Squares

Consider now

$$\phi(\mathbf{x}) = \frac{1}{2} \|\mathbf{Ax} - \mathbf{c}\|^2 \quad \text{with} \quad \nabla_{\mathbf{x}} \phi(\mathbf{x}) = \mathbf{A}^\top (\mathbf{Ax} - \mathbf{c}).$$

Steepest descent direction is $\mathbf{d}_j = \mathbf{A}^\top (\mathbf{c} - \mathbf{Ax}_j)$ and

$$\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}_j$$

How to choose α_j ? Idea: Minimize ϕ along direction \mathbf{d}_j

$$\alpha_j = \arg \min_{\alpha} \phi(\mathbf{x}_j + \alpha \mathbf{d}_j) = \arg \min_{\alpha} \frac{1}{2} \|\alpha \mathbf{Ad}_j - \mathbf{r}_j\|^2$$

with residual $\mathbf{r}_j = \mathbf{c} - \mathbf{Ax}_j$.

This leads to simple quadratic equation in 1D whose solution is

$$\alpha_j = \frac{\mathbf{r}_j^\top \mathbf{Ad}_j}{\|\mathbf{Ad}_j\|^2}$$

Algorithm: Steepest Descent for Least-Squares

for $j = 1, \dots$

- ▶ Compute residual $\mathbf{r}_j = \mathbf{c} - \mathbf{A}\mathbf{x}_j$
- ▶ Compute the SD direction $\mathbf{d}_j = \mathbf{A}^\top \mathbf{r}_j$
- ▶ Compute step size $\alpha_j = \frac{\mathbf{r}_j^\top \mathbf{A} \mathbf{d}_j}{\|\mathbf{A} \mathbf{d}_j\|^2}$
- ▶ Take the step $\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{d}_j$

Converges linearly, i.e.,

$$\|\mathbf{X}_{j+1} - \mathbf{X}^*\| < \gamma \|\mathbf{X}_j - \mathbf{X}^*\| \quad \text{with} \quad \gamma \approx \left| \frac{\kappa - 1}{\kappa + 1} \right|$$

Here, κ depends on condition number of \mathbf{A} , i.e.,

$$\kappa \approx \frac{\sigma_{\max}^2}{\sigma_{\min}^2}$$

Can be painfully slow for ill-conditioned problems

Accelerating Steepest Descent: Post-Conditioning

Idea: Improve convergence by transforming the problem

$$\phi(\mathbf{x}) = \frac{1}{2} \|\mathbf{A}\mathbf{S}\mathbf{S}^{-1}\mathbf{x} - \mathbf{c}\|^2$$

Here: \mathbf{S} is invertible

Solve in two steps:

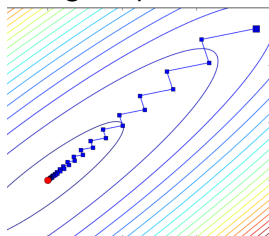
1. Set $\mathbf{z} = \mathbf{S}^{-1}\mathbf{x}$ and compute

$$\mathbf{z}^* = \arg \min_{\mathbf{z}} \frac{1}{2} \|\mathbf{A}\mathbf{S}\mathbf{z} - \mathbf{c}\|^2$$

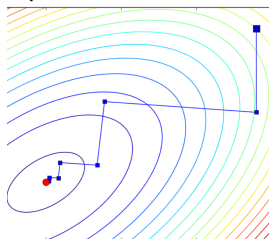
2. Then $\mathbf{x} = \mathbf{S}\mathbf{z}$.

Pick \mathbf{S} such that $\mathbf{A}\mathbf{S}$ is better conditioned.

original problem:



post-conditioned:



Exercise: Steepest Descent for Least-Squares

Goal: Program steepest descent and solve a simple problem.

To verify your code generate data using

$$\mathbf{c} = \mathbf{A}\mathbf{x}_{\text{true}} + \boldsymbol{\epsilon}.$$

where $\boldsymbol{\epsilon}$ is random with zero mean and standard deviation 0.1 and

$$\mathbf{Y} = \begin{pmatrix} 1 & 1+a \\ 1 & 1+2a \\ 1 & 1+3a \end{pmatrix} \quad \text{and} \quad \mathbf{x}_{\text{true}} = \begin{pmatrix} 1 \\ 1.2 \end{pmatrix}.$$

Plot errors $\|\mathbf{x}_j - \mathbf{x}_{\text{true}}\|$ for $j = 1, \dots$ and $a \in \{1, 10^{-2}, 10^{-5}\}$.

Conjugate Gradient Method for Least-Squares

CG is designed to solve quadratic optimization problems

$$\min_{\mathbf{x}} \frac{1}{2} \mathbf{x}^\top \mathbf{H} \mathbf{x} - \mathbf{b}^\top \mathbf{x}$$

with \mathbf{H} symmetric positive definite. In our case

$$\arg \min_{\mathbf{x}} \frac{1}{2} \|\mathbf{A} \mathbf{x} - \mathbf{c}\|^2 = \arg \min_{\mathbf{x}} \frac{1}{2} \mathbf{x}^\top \underbrace{\mathbf{A}^\top \mathbf{A}}_{=\mathbf{H}} \mathbf{x} - \underbrace{\mathbf{c}^\top \mathbf{A}}_{=\mathbf{b}^\top} \mathbf{x}$$

CG improves over SD by using previous step (not a memory-less method) and constructing a basis for the solution.

Facts:

- ▶ terminates after at most n steps (in exact arithmetic)
- ▶ good solutions for $j \ll n$
- ▶ convergence $\gamma_j \approx \left| \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \right|^j$

CGLS: Conjugate Gradient Least-Squares

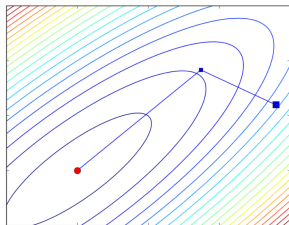
```
function x = mycglsl(A,c,k,tol)
n = size(A,2);
x = zeros(n,1);
d = A'*c;    r = c;
normr2 = d'*d;
for j=1:k
    Ad = A*d; alpha = normr2/(Ad'*Ad);
    x =x+alpha*d;
    r = r - alpha*Ad;
    s = A'*r;
    normr2New = d'*d;
    if normr2New<tol;return; end
    beta = normr2New/normr2;
    normr2 = normr2New;
    d = s + beta*d;
end
```

Conjugate Gradient Least-Squares

- ▶ Uses the structure of the problem to obtain stable implementation
- ▶ Typically converges much faster than SD
- ▶ Accelerate using post conditioning

$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{A}\mathbf{S}\mathbf{S}^{-1}\mathbf{x} - \mathbf{c}\|^2$$

- ▶ Faster convergence when eigenvalues of $\mathbf{S}^\top \mathbf{A}^\top \mathbf{A} \mathbf{S}$ are clustered.



Iterative Regularization

Consider

$$\min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{b}\|^2$$

- ▶ Assume that \mathbf{A} has non-trivial null space
- ▶ The matrix $\mathbf{A}^\top \mathbf{A}$ is not invertible
- ▶ Can we still use iterative methods (CG, CGLS, ...)?

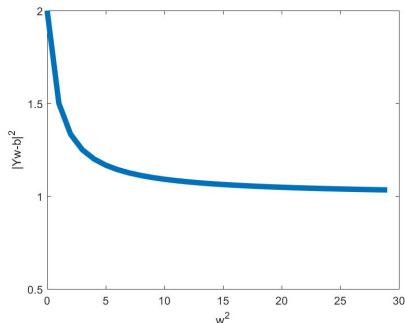
What are the properties of the iterates?

Excellent introduction to computational inverse problems [2, 6, 3]

Iterative Regularization: L-Curve

The CGLS algorithm has the following properties

- ▶ For each iteration $\|\mathbf{Ax}_k - \mathbf{c}\|^2 \leq \|\mathbf{Ax}_{k-1} - \mathbf{c}\|^2$
- ▶ If starting from $\mathbf{x} = 0$ then $\|\mathbf{x}_k\|^2 \geq \|\mathbf{x}_{k-1}\|^2$
- ▶ $\mathbf{x}_1, \mathbf{x}_2, \dots$ converges to the minimum norm solution of the problem
- ▶ Plotting $\|\mathbf{x}_k\|^2$ vs $\|\mathbf{Ax}_k - \mathbf{c}\|^2$ typically has the shape of an L-curve



Cross Validation - 1

Finding good least-squares solution requires good parameter selection.

- ▶ λ when using Tikhonov regularization (weight decay)
- ▶ number of iteration (for SD and CGLS)

Suppose that we have two different “solutions”

$$\mathbf{x}_1 \rightarrow \|\mathbf{x}_1\|^2 = \eta_1 \quad \|\mathbf{A}\mathbf{x}_1 - \mathbf{c}\|^2 = \rho_1.$$

$$\mathbf{x}_2 \rightarrow \|\mathbf{x}_2\|^2 = \eta_2 \quad \|\mathbf{A}\mathbf{x}_2 - \mathbf{c}\|^2 = \rho_2.$$

How to decide which one is better?

Cross Validation - 2

Goal: Gauge how well the model can predict new examples.

Let $\{\mathbf{A}_{CV}, \mathbf{c}_{CV}\}$ be data that is **not used** for the training

Idea: If $\|\mathbf{A}_{CV}\mathbf{x}_1 - \mathbf{c}_{CV}\|^2 \leq \|\mathbf{A}_{CV}\mathbf{x}_2 - \mathbf{c}_{CV}\|^2$, then \mathbf{x}_1 is a better solution than \mathbf{x}_2 .

When the solution depends on some hyper-parameter(s) λ , we can phrase this as bi-level optimization problem

$$\lambda^* = \arg \min_{\lambda} \|\mathbf{A}_{CV}\mathbf{x}(\lambda) - \mathbf{c}_{CV}\|^2,$$

where $\mathbf{x}(\lambda) = \arg \min_{\mathbf{x}} \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2$.

Cross Validation - 3

To assess the final quality of the solution cross validation is not sufficient (why?).

Need a final testing set.

Procedure

- ▶ Divide the data into 3 groups $\{\mathbf{A}_{\text{train}}, \mathbf{A}_{\text{CV}}, \mathbf{A}_{\text{test}}\}$.
- ▶ Use $\mathbf{A}_{\text{train}}$ to estimate $\mathbf{x}(\lambda)$
- ▶ Use \mathbf{A}_{CV} to estimate λ
- ▶ Use \mathbf{A}_{test} to assess the quality of the solution

Important - we are not allowed to use \mathbf{A}_{test} to tune parameters!

Σ : Linear Least-Squares

$$\min_{\mathbf{W}} \frac{1}{2} \|\mathbf{WY} - \mathbf{C}\|_F^2 \quad \rightsquigarrow \quad \min_{\mathbf{x}} \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|_F^2$$

- ▶ optimality conditions: normal equations
- ▶ typically requires regularization
- ▶ direct: Tikhonov weight decay \rightsquigarrow need to choose λ
- ▶ iterative: steepest descent, CG \rightsquigarrow need to choose maximum number of iterations.
- ▶ classification: how to interpret output \mathbf{WY} (not a probability!)
- ▶ image inpainting: effective choice of regularizer and parameter.

References

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- [2] P. C. Hansen. *Rank-deficient and discrete ill-posed problems*. SIAM Monographs on Mathematical Modeling and Computation. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1998.
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