Lecture 8: Optimization-based Approaches

Introduction to Modern Brain-Computer Interface Design

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Outline

1. Introduction
2. Going Beyond CSP
3. Large-Scale Machine Learning
4. Application to the Spectral Model
5. Application to ERPs
6. Learning ERP and Oscillatory Weights Simultaneously
7. Practical Remarks

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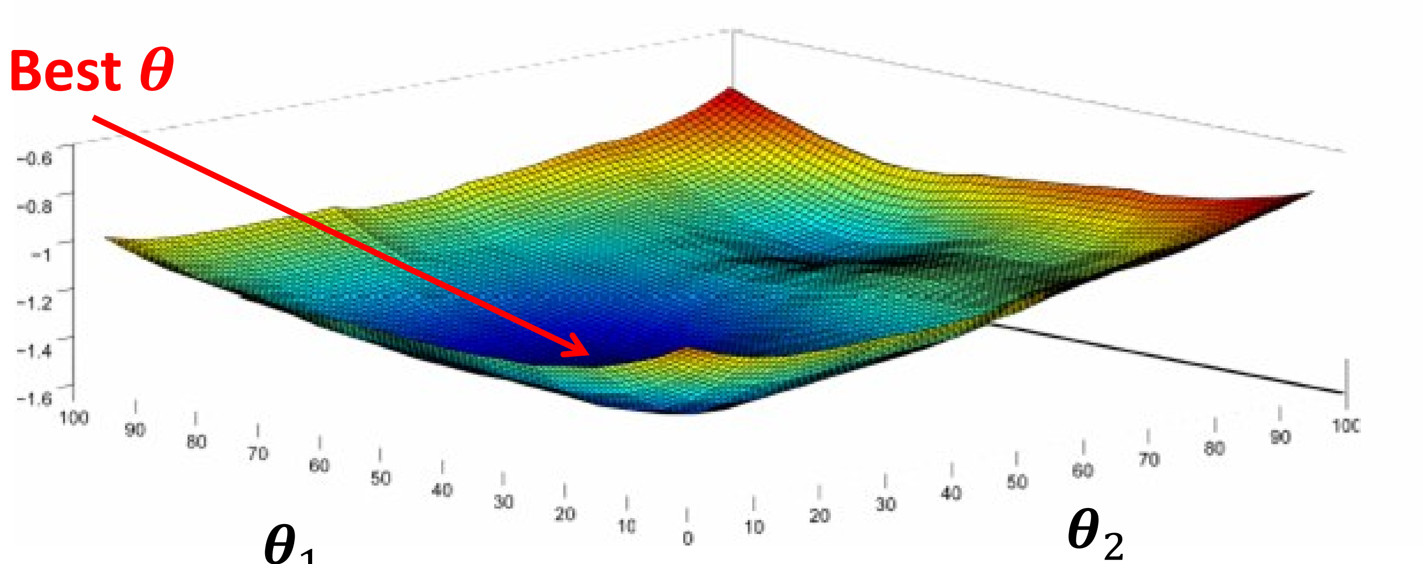
8.1 Introduction

Beyond CSP

- A unified, globally optimal solution to spatial filter estimation has recently been proposed (as an alternative to CSP+LDA)
- The method learns in a single step both the spatial filters and the relative weights for the filtered variance
- This is an *optimization*-based approach

Optimization

- Broad field, concerned with finding assignments to parameters that minimize a *cost function* $\boldsymbol{f}$
- Two branches: *Local optimization* and *Global Optimization*



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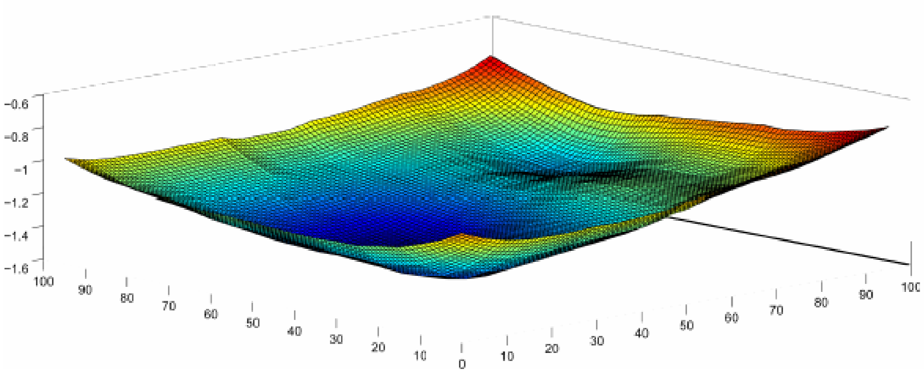
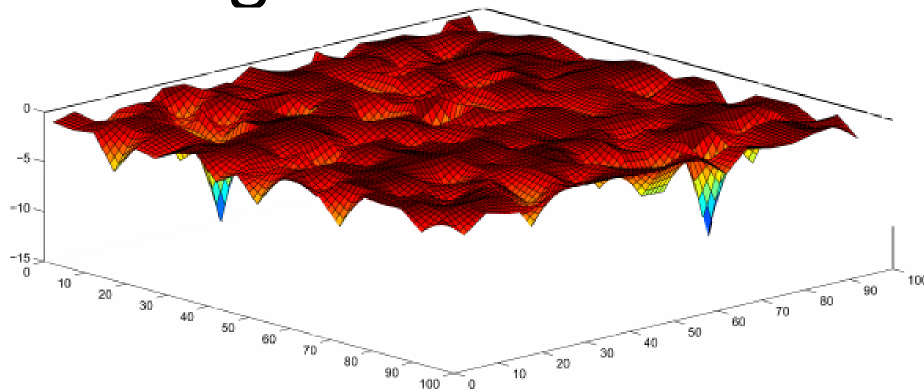
Global Optimization

- Aims to find the global optimum of a function, even if it has multiple local optima
- Can be approximate (e.g., Simulated Annealing) or exact (e.g., Branch-and-Bound)
- **Problem:** Can be *extremely slow*, especially on high-dimensional and pathological data



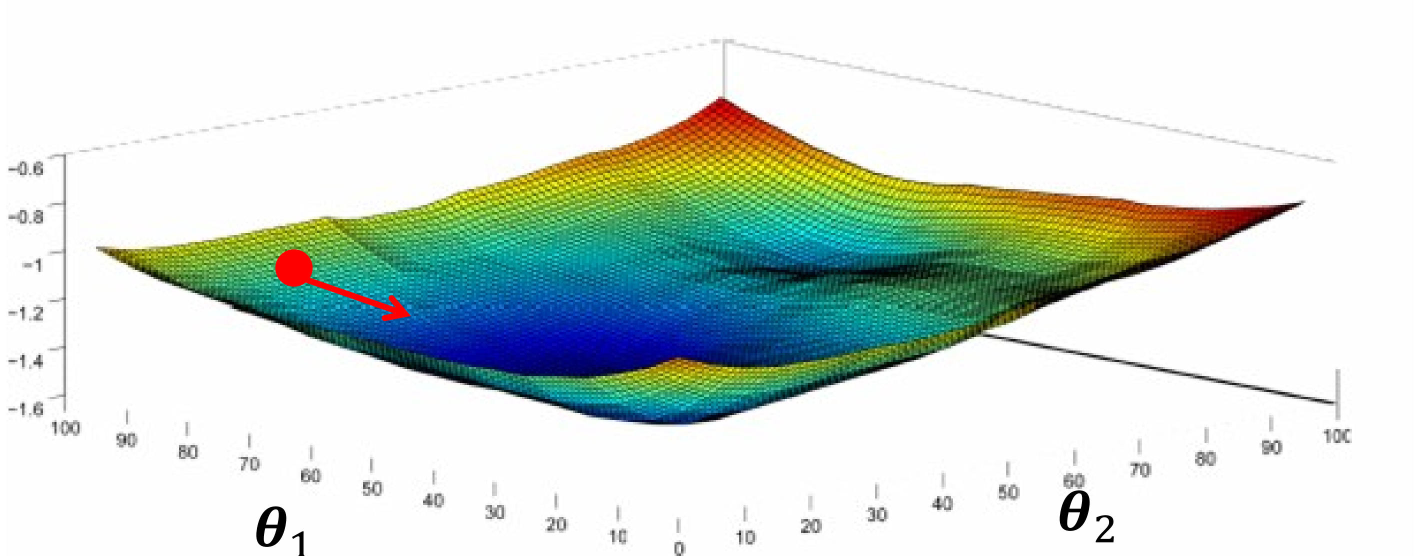
Doable



Problematic

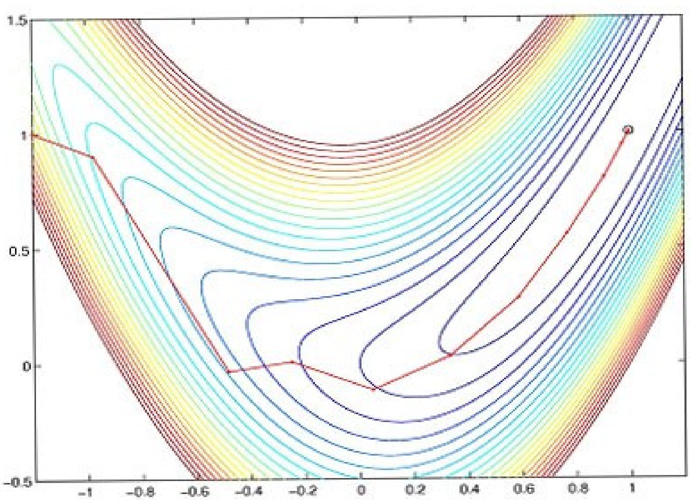
Local Optimization

- Improving an initial guess of a parameter by incremental updates
- **Method 1, Gradient Descent**: walk into the direction of steepest descent, requires 1st derivative $\boldsymbol{g}$ of cost function

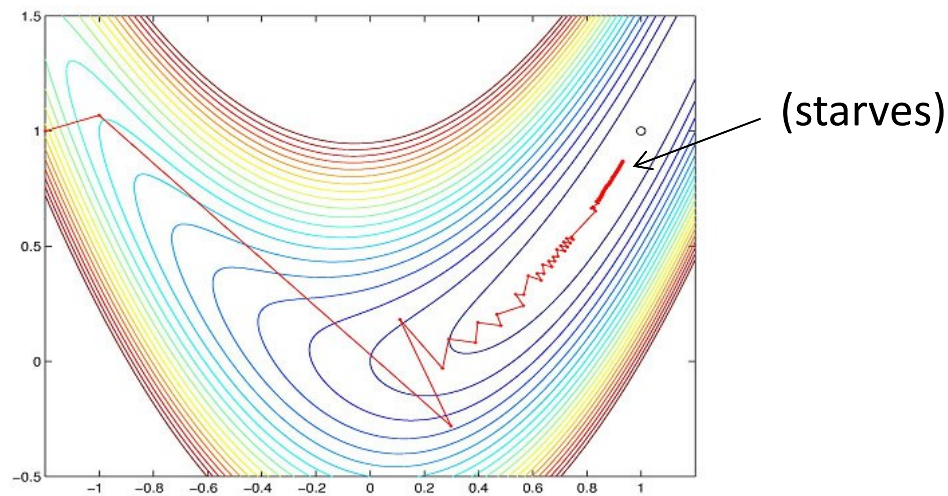


Local Optimization

- **Method 2, Newton Method**: account for local curvature, requires 2nd derivative $\boldsymbol{B}$ of function (Hessian matrix)
- Can be very efficient if $\boldsymbol{g}/\boldsymbol{B}$ is easy to compute (or easy to approximate otherwise)



Newton



Gradient Descent

Local Optimization

- **Method 3, Quasi-Newton**: approximates $\boldsymbol{B}^{-1}$ incrementally from gradients gathered along the way (no second derivatives necessary)
- **Practical variant:** L-BFGS (Limited-Memory Broyden-Fletcher-Goldfarb-Shanno) – one of the best known “off-the-shelf” second-order optimizers, *very easy* to use

Local Optimization

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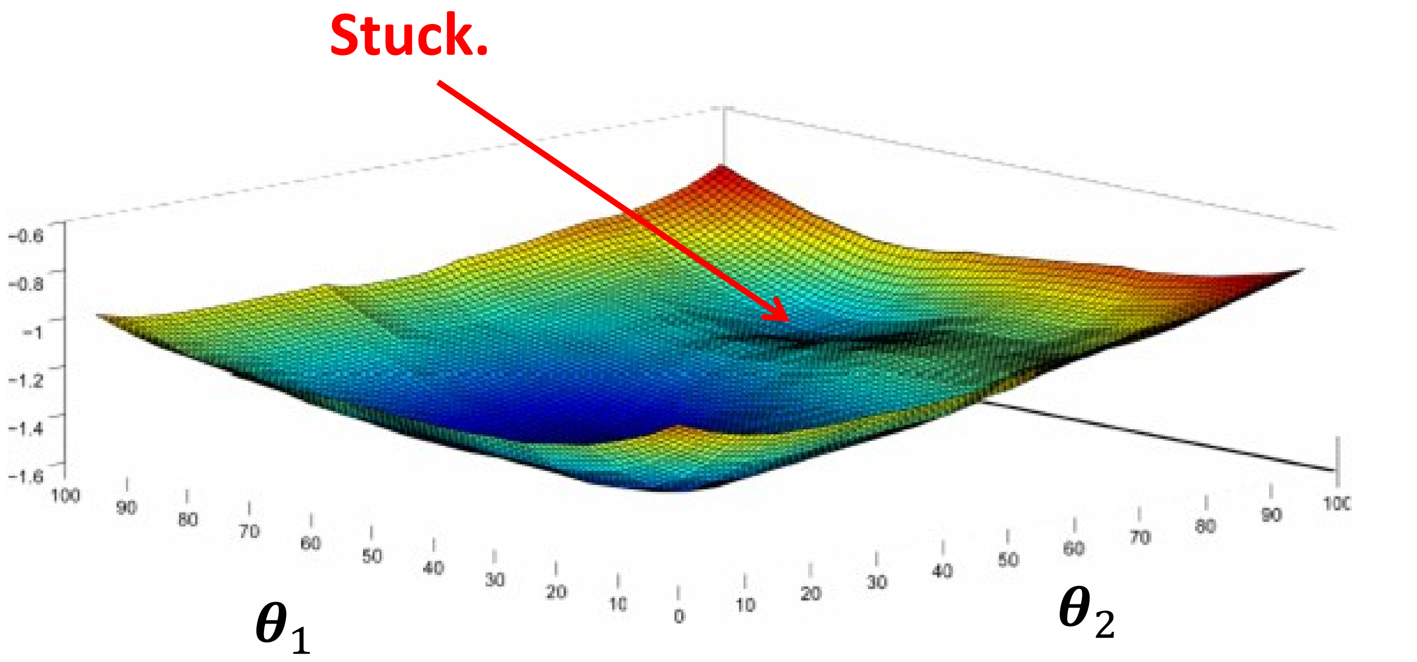
```
>> xopt = liblbfgs(@myfunc,x0)
```

Problems

- Local Optimization can run into *local minima* or *starve on plateaus*, except if the function has some suitable properties…



Convexity

- Convex functions have exactly one local optimum, also for every $\boldsymbol{x}$, $\boldsymbol{y}$ and $t \in [0,1]$ the following holds:

$$f(t\boldsymbol{x} + (1-t)\boldsymbol{y}) \leq tf(\boldsymbol{x}) + (1-t)f(\boldsymbol{y})$$

- This makes them *exactly solvable* by local optimization methods
- Surprisingly many problem types can be formulated as *convex optimization problems*

Smoothness

- Many relevant BCI problems amount to optimization problems with non-differentiable features (e.g., sparse problems), so smooth optimization is not immediately applicable
- **Fixes:** Can use smooth surrogate functions (e.g., *proximal optimization*), or solve an equivalent problem that is smooth (see *convex duality*) or split the non-smooth terms off (see *operator splitting*), or use non-smooth methods (e.g., *subgradient descent*)

8.2 Going Beyond CSP

(and a bit of equation juggling!)

Transforming CSP

- Consideration: Given a zero-mean trial $\boldsymbol{X} \in \mathbb{R}^{C \times T}$ with covariance $\boldsymbol{\Sigma} \in \mathbb{R}^{CxC}$, spatial filters $\boldsymbol{W} \in \mathbb{R}^{SxC}$, linear weights $\boldsymbol{\theta} \in \mathbb{R}^{S}$ and bias b

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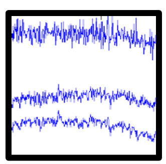
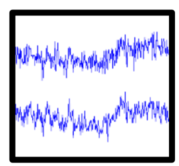
- Omitting the log from CSP, we have:

$$y = b + \boldsymbol{\theta}\text{var}(\boldsymbol{W}\boldsymbol{X})$$

X



WX



var(**WX**) $\begin{bmatrix} 2.3 \\ 4.5 \end{bmatrix}$

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Transforming CSP

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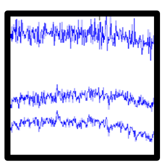
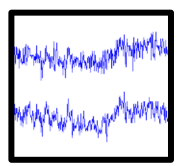
X  **WX**  var(**WX**) $\begin{bmatrix} 2.3 \\ 4.5 \end{bmatrix}$

- Rewriting in terms of individual spatial filters $\boldsymbol{W}_k$:

$$y = b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \,\mathrm{var}(\boldsymbol{W}_k\boldsymbol{X})$$

Transforming CSP

- The variance term can be expressed using the covariance matrix $\boldsymbol{\Sigma}$ of segment $\boldsymbol{X}$:

$$y = b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \operatorname{var}(\boldsymbol{W}_k \boldsymbol{X}) = b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \left(\boldsymbol{W}_k \boldsymbol{\Sigma} \boldsymbol{W}_k{}^{\top}\right)$$

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- And $\boldsymbol{W}_k \mathbf{\Sigma} \boldsymbol{W}_k{}^{\intercal}$ can be replaced by the inner product between two matrices $\left\langle \boldsymbol{W}_k \boldsymbol{W}_k{}^{\intercal}, \mathbf{\Sigma} \right\rangle$

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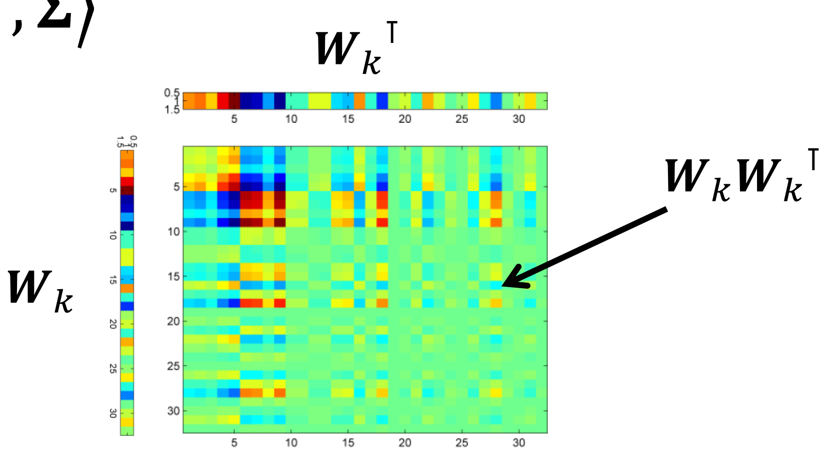
$$b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \langle \boldsymbol{W}_k \boldsymbol{W}_k^{\top}, \boldsymbol{\Sigma} \rangle$$



Transforming CSP

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$$y = b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \operatorname{var}(\boldsymbol{W}_k \boldsymbol{X}) = b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \left(\boldsymbol{W}_k \boldsymbol{\Sigma} \boldsymbol{W}_k^{\top}\right)$$

- And $\boldsymbol{W}_k \boldsymbol{\Sigma} \boldsymbol{W}_k^{\top}$ can be replaced by the inner product between two matrices $\langle \boldsymbol{W}_k \boldsymbol{W}_k^{\top}, \boldsymbol{\Sigma} \rangle$, and regrouped:

$$b + \sum_{k=1}^{S} \boldsymbol{\theta}_k \langle \boldsymbol{W}_k \boldsymbol{W}_k^{\top}, \boldsymbol{\Sigma} \rangle = b + \left\langle \sum_{k=1}^{S} \boldsymbol{\theta}_k \boldsymbol{W}_k \boldsymbol{W}_k^{\top}, \boldsymbol{\Sigma} \right\rangle$$

$$= b + \langle \boldsymbol{\Theta}, \boldsymbol{\Sigma} \rangle$$

Transforming CSP

- Thus this form is *linear in the covariance matrix* of X:

$$y = b + \langle \boldsymbol{\Theta}, \boldsymbol{\Sigma} \rangle = \boldsymbol{b} + \widetilde{\boldsymbol{\theta}}\mathrm{vec}(\boldsymbol{\Sigma})$$

- Could again learn $\widetilde{\boldsymbol{\theta}}$ using a simple linear method (e.g., LDA), but *very* high-dimensional (#parameters=$\mathrm{C}^{2^{2}}$)
- Need a method suitable for large-scale problems

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8.3 Large-Scale Machine Learning

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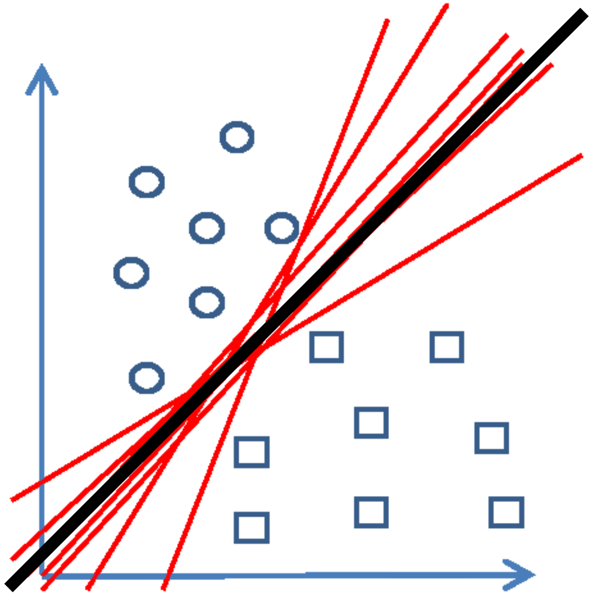
Large-Scale Machine Learning

- *Discriminative* learning approaches like Support Vector Machines (SVMs) and Generalized Linear Models (GLMs) are well-adapted to high-dimensional / large-scale problems
- These directly optimize the parameters $\boldsymbol{\theta}$ given the data



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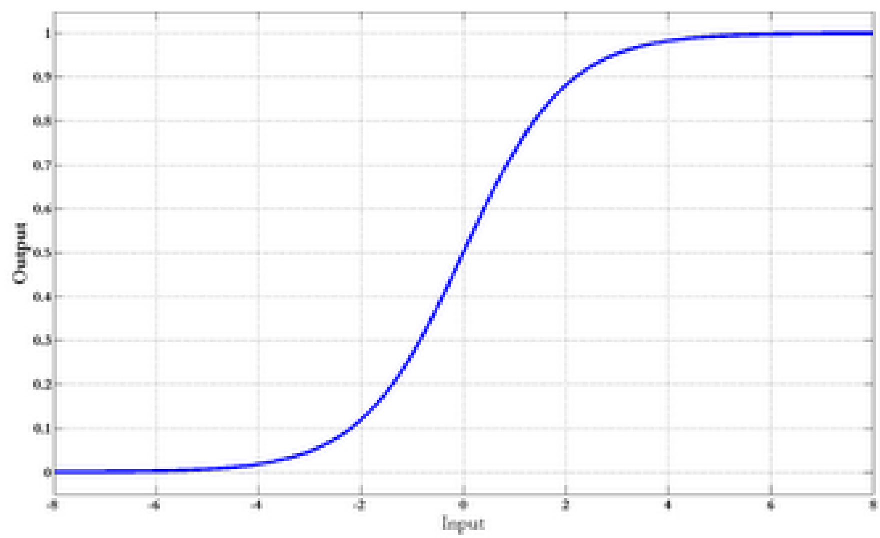
Large-Scale Machine Learning

- Logistic Regression is a GLM that maps X onto binary outputs via a logistic "link function"

$$\frac{1}{1+e^{-y f_\theta(\boldsymbol{X})}}, (y \in \{-1,+1\})$$



$- f_0(\boldsymbol{X}) \rightarrow$

Large-Scale Machine Learning

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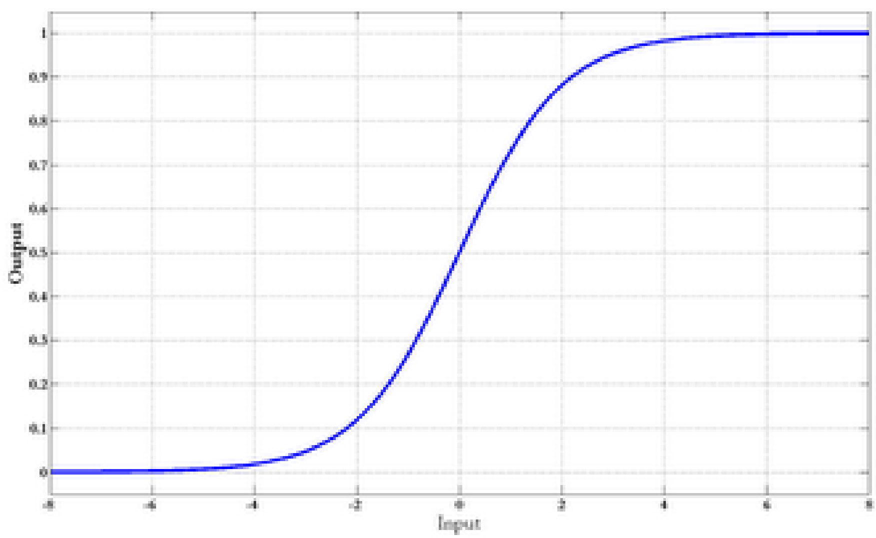
$$q_\theta(Y = y|X) = \frac{1}{1 + e^{-yf_\theta(X)}}, (y \in \{-1, +1\})$$

Interpreted as the probability that Y=1 (or Y=-1)



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- … and linear function $f_\theta(\boldsymbol{X})$

$$f_\theta(\boldsymbol{X}) = \ \boldsymbol{\theta X} + b$$

Large-Scale Machine Learning

- $\boldsymbol{\theta}$ can be obtained via off-the-shelf convex optimization tools (such as CVX) by solving the problem

$$\min_{\boldsymbol{\theta}} \log\left(1 + e^{-\boldsymbol{y} f_{\theta}(\boldsymbol{X})}\right)$$

- The log(…) term is called the *logistic loss* and quantifies the misfit between predicted labels and true labels, for a particular choice of $\boldsymbol{\theta}$

Large-Scale Machine Learning

- For large problems, solution is still prone to *over-fitting* to random noise in the data – need to plug in some *additional assumptions*

$$\min_{\boldsymbol{\theta}} \log\left(1 + e^{-y f_{\theta}(\boldsymbol{X})}\right) + \lambda\Omega(\boldsymbol{\theta})$$

- Many choices for regularization term Ω
  - $\Omega(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|^2$ encourages small weights
  - $\Omega(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1 = |\boldsymbol{\theta}_1| + |\boldsymbol{\theta}_2| + \cdots$ encourages *sparsity*
  - can also get sparsity on groups of weights
  - combinations of these, …

8.4 Application to the Spectral Model

Applying to the Spectral Model

- In the previous supervised oscillatory model $y = b + \langle \boldsymbol{\Theta}, \boldsymbol{\Sigma} \rangle$, the matrix-shaped $\boldsymbol{\Theta}$ allows for a special matrix norm regularization $\Omega(\boldsymbol{\Theta})$:

$$\min_{\boldsymbol{\Theta}} \log\left(1 + e^{-y f_{\boldsymbol{\Theta}}(X)}\right) + \ \ldots$$

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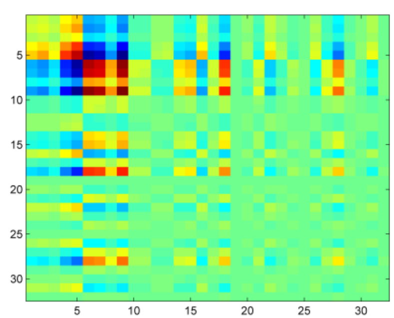
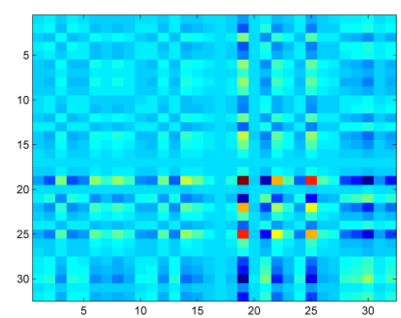
- This encourages a low-rank structure in $\boldsymbol{\Theta}$, i.e.

$\boldsymbol{\Theta}$ =



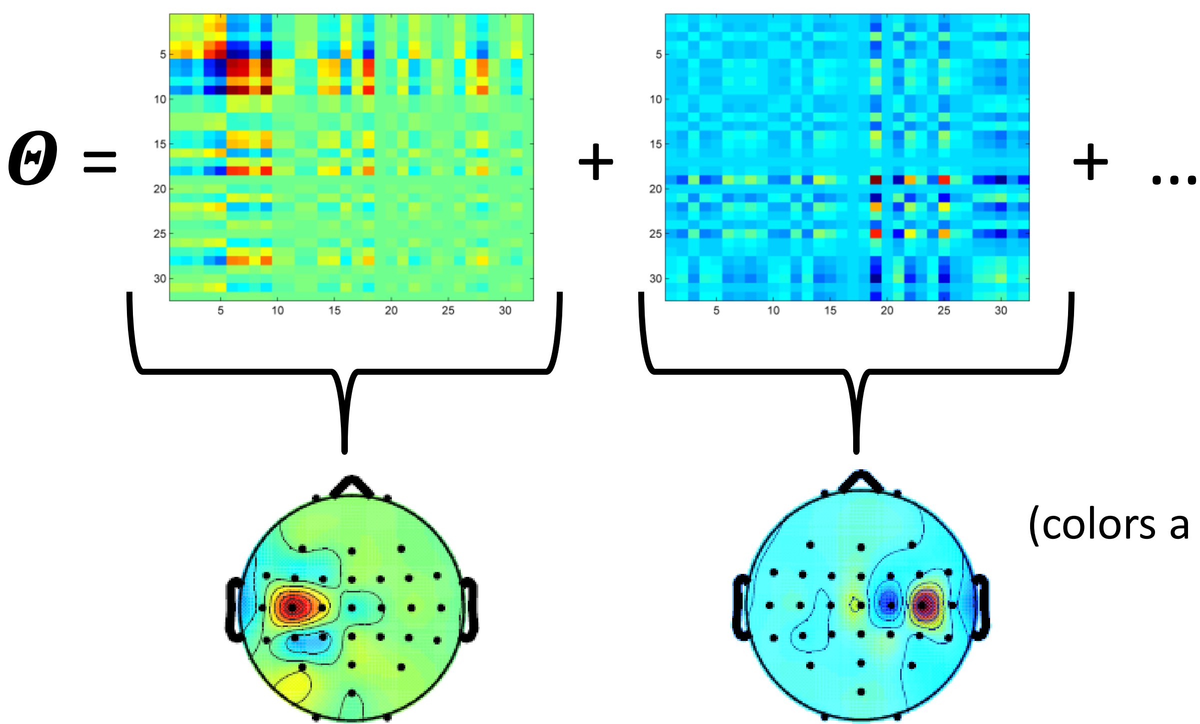
+



+ ...

Applying to the Spectral Model

- Thus, the weight matrix is equivalent to the weighted sum of a small set of spatial filters applied to the covariance matrix of the signal!



(colors a bit off)

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8.5 Application to ERPs

Application to ERPs

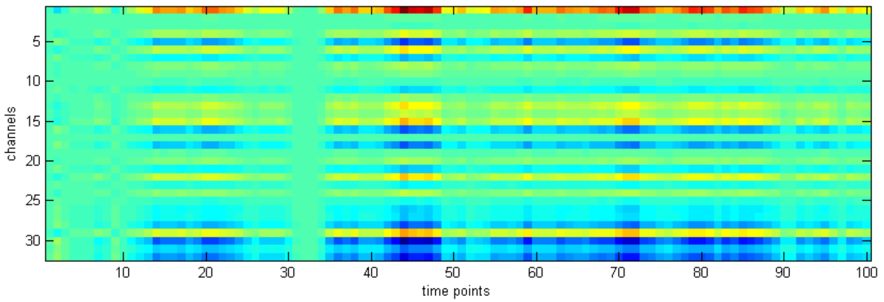
- Same approach can be applied to the raw data epoch **X** instead of its covariance matrix $\boldsymbol{\Sigma}$
- So we optimize for a GLM $y = b + \langle \boldsymbol{\Theta}, \boldsymbol{X} \rangle$

$$\min_{\boldsymbol{\Theta}} \log\left(1 + e^{-y f_{\boldsymbol{\Theta}}(\boldsymbol{X})}\right) + \lambda \sum_{k=1}^{rank(\boldsymbol{\Theta})} \sigma_k(\boldsymbol{\Theta})$$

Application to ERPs

- Same approach can be applied to the raw data epoch **X** instead of its covariance matrix $\boldsymbol{\Sigma}$
- This learns a linear ERP weight matrix with one weight for each channel and time point

$\boldsymbol{\Theta}=$



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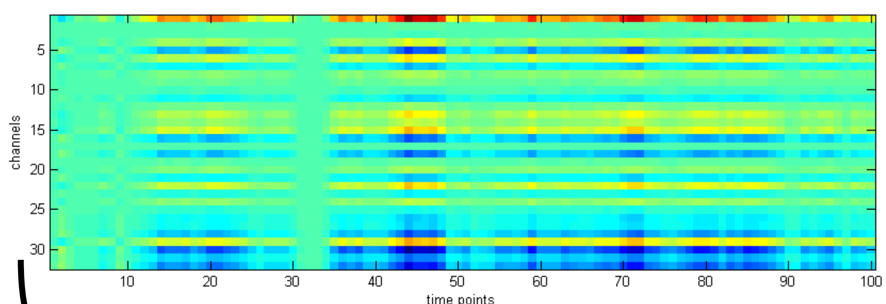
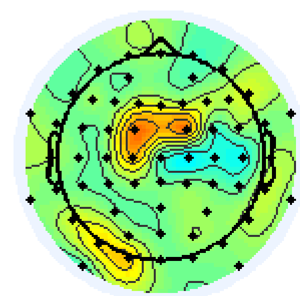
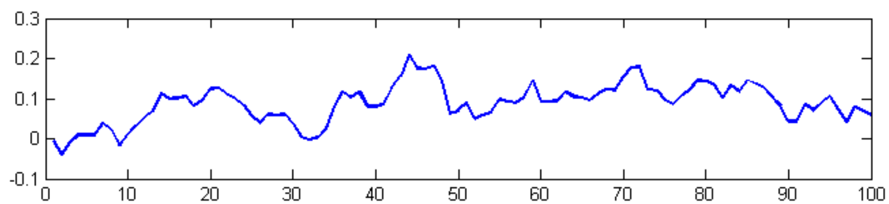




spatial filter



time weights

Application to ERPs

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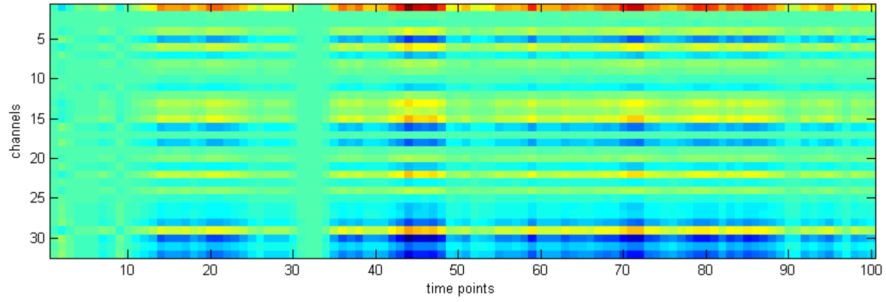
$\boldsymbol{\Theta}$ =



- $\boldsymbol{\Theta}$ is low-rank, so corresponds to a sum of a few spatial filters and their weights over time

Application to ERPs

- Thus, no hand-selected time windows needed
- Also, results are regularized to find / pick up few sources and their relevant time courses

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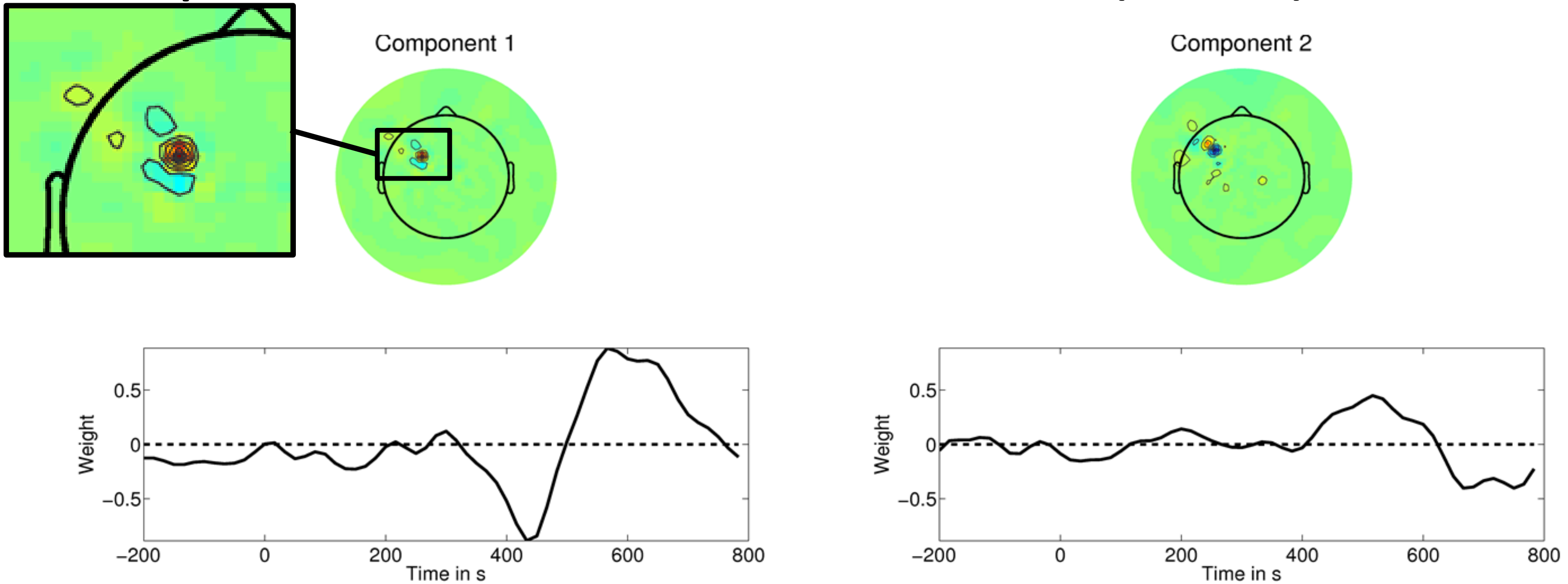
- Also, results are regularized to find / pick up few sources and their relevant time courses
- Rapid Serial Visual Presentation (RSVP) task:



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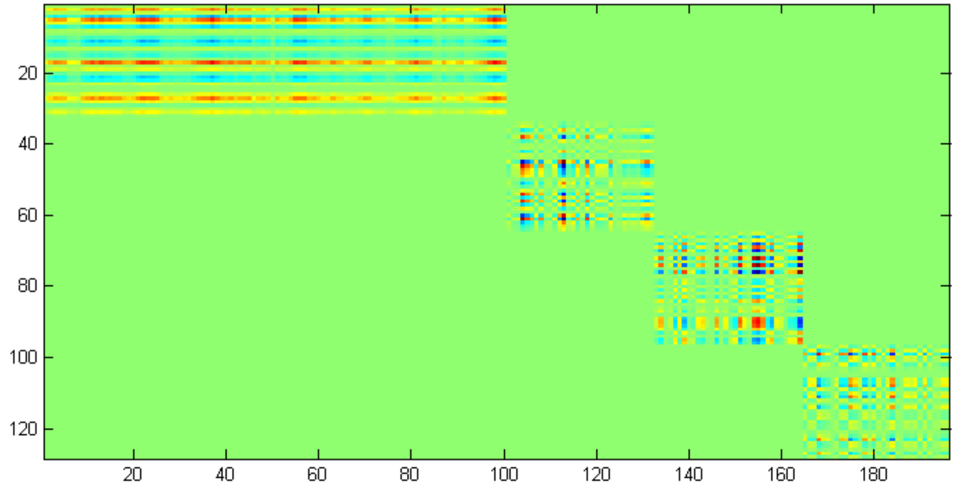
8.6 Learning ERP and Oscillatory Weights Simultaneously

Feature Combination

- If for each trial instead of the covariance matrix or the raw ERP, a *block-diagonal concatenation* of both is used, the method learns a low-rank weight matrix combining both features simultaneously

$\boldsymbol{\Theta}$ =



Feature Combination

- If for each trial instead of the covariance matrix or the raw ERP, a *block-diagonal concatenation* of both is used, the method learns a low-rank weight matrix combining both features simultaneously
- For a block-diagonal weight matrix $\boldsymbol{\Theta}$, it holds that

$$\min_{\boldsymbol{\Theta}} \ldots + \lambda \sum_{k=1}^{rank(\boldsymbol{\Theta})} \sigma_k(\boldsymbol{\Theta})$$

is equivalent to solving for its blocks $\boldsymbol{\Theta}_b$:

$$\min_{\boldsymbol{\Theta}} \ldots + \lambda \sum_{b=1}^{B} \sum_{k=1}^{rank(\boldsymbol{\Theta}_b)} \sigma_k(\boldsymbol{\Theta}_b)$$

Sparsity and Feature Selection

- Also, covariance matrices for multiple frequency bands and time windows can be concatenated
- For regularizers that are a sum of terms (of a certain type), most terms in the sum will be driven to zero and only a *sparse subset* of terms remains non-zero, i.e., the relevant features are selected automatically

$$\min_{\boldsymbol{\Theta}} \ldots + \lambda \sum_{b=1} \ldots$$

- Recovery of the relevant support is statistically extremely efficient – it holds that the number of irrelevant dimensions under which the support can be accurately recovered is *exponential* in the number of observations (i.e., trials) [Ng 1998]

Sparsity and Feature Selection

- Thus, only the relevant subset of frequencies or time windows (for covariance) or ERP sources is typically learned
- Can be taken even further, e.g., could encourage weights for different time/frequency bins to share a small set of spatial filters (again using rank constraints on concatenated matrices) – this is called multi-task learning

Final Prediction Functions

- **Basic oscillatory case** (assuming **X** is band-passed):

$$y = \frac{1}{1 + e^{-\left(b + \langle \boldsymbol{\Theta}, \boldsymbol{X}\boldsymbol{X}^{\top} \rangle\right)}}$$

- **ERP case** (**X** can be band-passed)**:**

$$y = \frac{1}{1 + e^{-\left(b + \langle \boldsymbol{\Theta}, \boldsymbol{X} \rangle\right)}}$$

- **Combined cases** (here for temporal filters $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$):

$$y = \frac{1}{1 + e^{-\left\langle \boldsymbol{\Theta}, \begin{bmatrix} \boldsymbol{X} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{X}\boldsymbol{F}_1\boldsymbol{X}^{\top} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{X}\boldsymbol{F}_2\boldsymbol{X}^{\top} \end{bmatrix} \right\rangle - b}}$$

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8.7 Practical Remarks

Solving It

- Problems of this size are impossible to solve using CVX; need a custom solver
- For a wide range of sparse estimation problems the DAL (Dual-Augmented Lagrangian) solver is applicable and *very fast*
- For an even wider range of problems the ADMM (Alternating Direction Method of Multipliers) framework is applicable and also very fast

ADMM

- Framework for distributed very large scale optimization – leads to parallel algorithms
- Can be done with *very* simple MATLAB code

These are often fairly simple problems

$$
\begin{aligned}
x^{k+1} &:= \operatorname{argmin}_x L_\rho(x, z^k, y^k) \\
z^{k+1} &:= \operatorname{argmin}_z L_\rho(x^{k+1}, z, y^k) \\
y^{k+1} &:= y^k + \rho(Ax^{k+1} + Bz^{k+1} - c)
\end{aligned}
$$

Boyd, 2010

Other Methods in this Framework

- **Support Vector Machines:** use a different loss function (“hinge loss” instead of logistic loss)
- **Multiple Kernel Learning:** using group sparsity on kernel matrices (selecting few kernels)
- **Hierarchical Kernel Learning:** very advanced non-linear feature selection approach using tree-structured sparsity
- **Linear Regression:** Usable for a continuous output space instead of discrete

L8 Questions?