Optimization for Sparse Estimation and Structured Sparsity

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Short Course "Applied Statistics and Machine Learning"

Main topic of the lecture

How do we solve

- sparse estimation problems in machine learning and statistics;
- sparse inverse problems in signal processing.

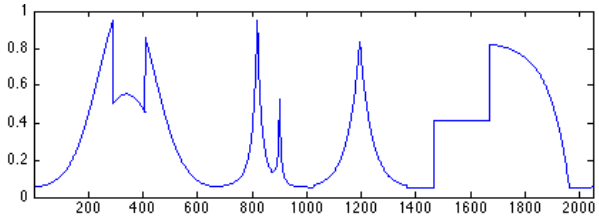
Tools we use

- greedy algorithms;
- "gradient" methods for non-differentiable functions;
- other tricks.

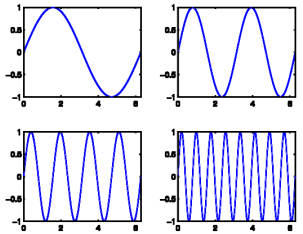
Part I: Short Introduction on Sparsity

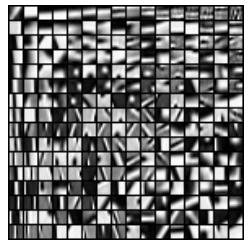
Sparse Linear Models: Signal Processing Point of View

Let $\mathbf{y}$ in $\mathbb{R}^n$ be a signal.



Let $\mathbf{X} = [\mathbf{x}^1, \ldots, \mathbf{x}^p] \in \mathbb{R}^{n \times p}$ be a set of elementary signals.
We call it **dictionary**.



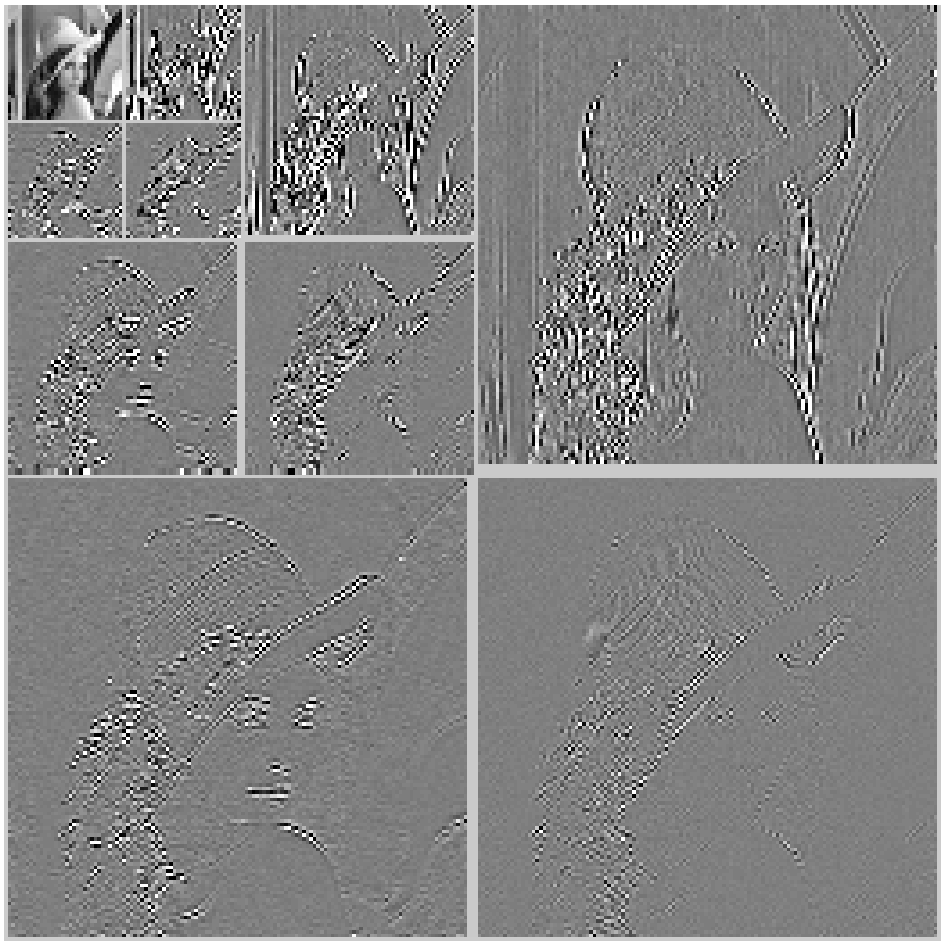


$\mathbf{X}$ is "adapted" to $\mathbf{y}$ if it can represent it with a few elements—that is, there exists a **sparse vector** β in $\mathbb{R}^p$ such that $\mathbf{y} \approx \mathbf{X}\beta$. We call β the **sparse code**.

$$\underbrace{\begin{pmatrix} \mathbf{y} \end{pmatrix}}_{\mathbf{y} \in \mathbb{R}^n} \approx \underbrace{\left(\begin{array}{c|c|c|c} \mathbf{x}^1 & \mathbf{x}^2 & \cdots & \mathbf{x}^p \end{array} \right)}_{\mathbf{X} \in \mathbb{R}^{n \times p}} \underbrace{\begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}}_{\beta \in \mathbb{R}^p, \textbf{sparse}}$$

Sparse Linear Models: Signal Processing Point of View

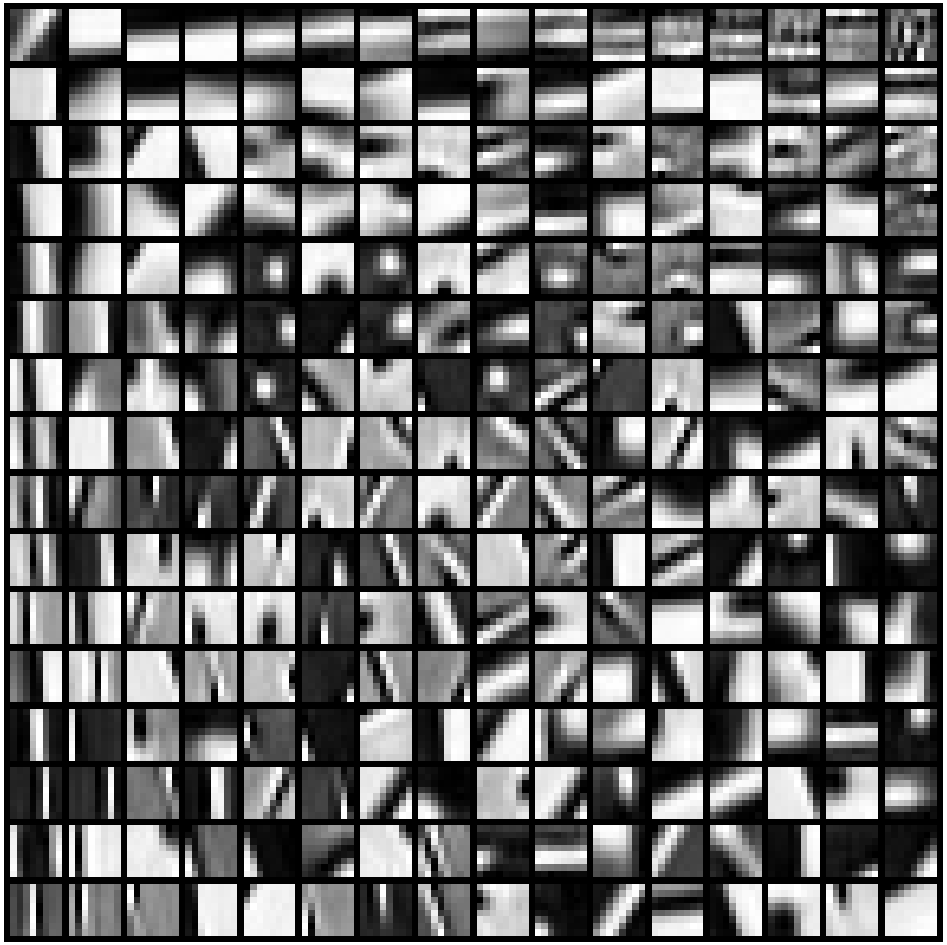
Wavelet Representation [see Mallat, 1999]



$\mathbf{y} = \mathbf{X}\beta$. The coefficients β are represented in a quadtree.

Sparse Linear Models: Signal Processing Point of View

Dictionary for natural image patches [Olshausen and Field, 1997, Elad and Aharon, 2006]



Sparse Linear Models: Machine Learning Point of View

Let $(y^i, \mathbf{x}^i)_{i=1}^n$ be a training set, where the vectors $\mathbf{x}^i$ are in $\mathbb{R}^p$ and are called features. The scalars y^i are in

- $\{-1, +1\}$ for **binary** classification problems.
- $\mathbb{R}$ for **regression** problems.

We assume there is a relation $y \approx \beta^\top \mathbf{x}$, and solve

$$\min_{\beta \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(y^i, \beta^\top \mathbf{x}^i)}_{\text{empirical risk}} + \underbrace{\lambda \Omega(\beta)}_{\text{regularization}} .$$

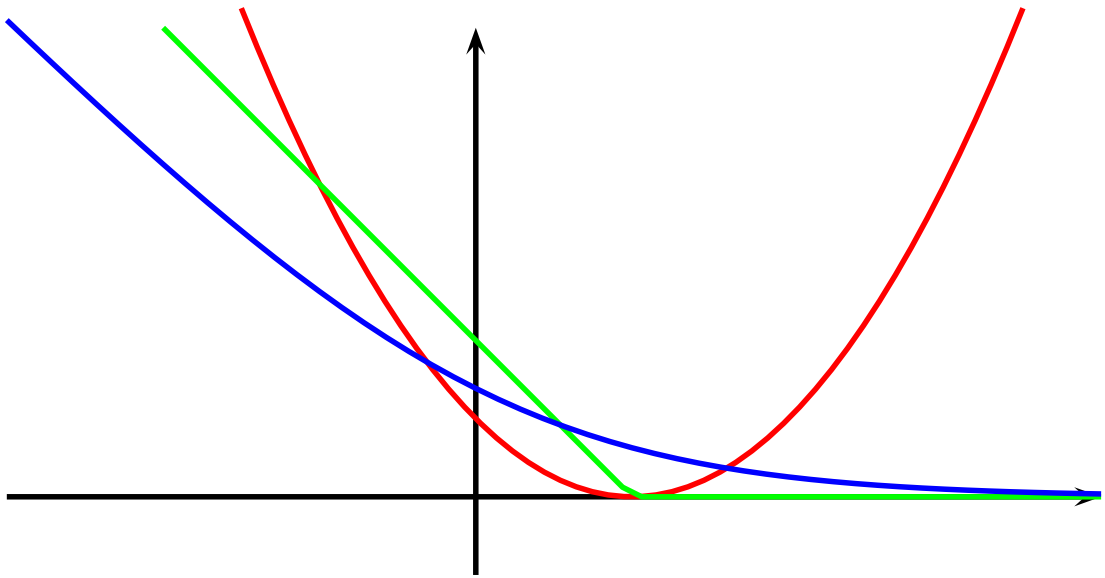
Sparse Linear Models: Machine Learning Point of View

A few examples:

Ridge regression:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2}(y^i - \beta^\top \mathbf{x}^i)^2 + \lambda \|\beta\|_2^2.$$

Linear SVM:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \max(0, 1 - y^i \beta^\top \mathbf{x}^i) + \lambda \|\beta\|_2^2.$$

Logistic regression:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \log\left(1 + e^{-y^i \beta^\top \mathbf{x}^i}\right) + \lambda \|\beta\|_2^2.$$



Sparse Linear Models: Machine Learning Point of View

A few examples:

Ridge regression: $$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2}(y^i - \beta^\top \mathbf{x}^i)^2 + \lambda \|\beta\|_2^2.$$

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Logistic regression: $$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \log\left(1 + e^{-y^i \beta^\top \mathbf{x}^i}\right) + \lambda \|\beta\|_2^2.$$

The **squared ℓ_2-norm** induces "**smoothness**" in β. When one knows in advance that β should be sparse, one should use a **sparsity-inducing** regularization such as the **ℓ_1-norm**. [Chen et al., 1999, Tibshirani, 1996]

Main Topic of the lecture

How do we solve?

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \underbrace{\frac{1}{2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2}_{\text{loss/data-fitting}} + \underbrace{\lambda \Omega(\boldsymbol{\beta})}_{\text{regularization}},$$

$\mathbf{X}$ in $\mathbb{R}^{n \times p}$ is a design matrix, Ω induces sparsity.

- $\|\boldsymbol{\beta}\|_0 \triangleq \#\{i \text{ s.t. } \boldsymbol{\beta}_i \neq 0\}$ (NP-hard)
- $\|\boldsymbol{\beta}\|_1 \triangleq \sum_{i=1}^p |\boldsymbol{\beta}_i|$ (convex),

When Ω is the ℓ_1-norm, the problem is called Lasso [Tibshirani, 1996] or basis pursuit [Chen et al., 1999].

Later in the lecture, extensions to more general smooth loss functions f, other sparsity-inducing penalties.

One Important Question

Why does the ℓ_1-norm induce sparsity?

Can we get some intuition from the simplest isotropic case?

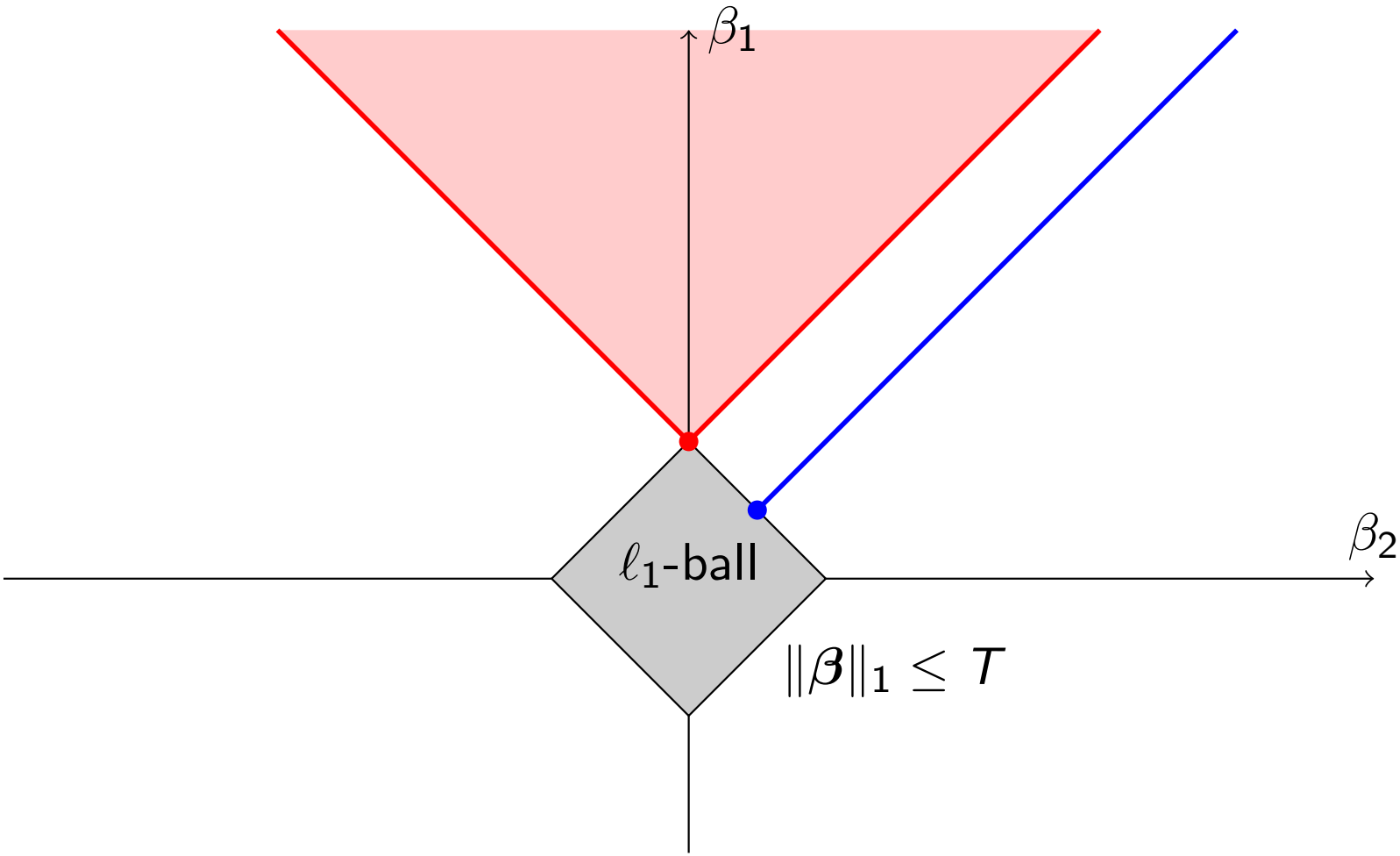
$$\hat{\boldsymbol{\beta}}(\lambda) = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \frac{1}{2}\|\mathbf{y}-\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1,$$

or equivalently the Euclidean projection onto the ℓ_1-ball?

$$\tilde{\boldsymbol{\beta}}(T) = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \frac{1}{2}\|\mathbf{y}-\boldsymbol{\beta}\|_2^2 \quad \text{s.t.} \quad \|\boldsymbol{\beta}\|_1 \leq T.$$

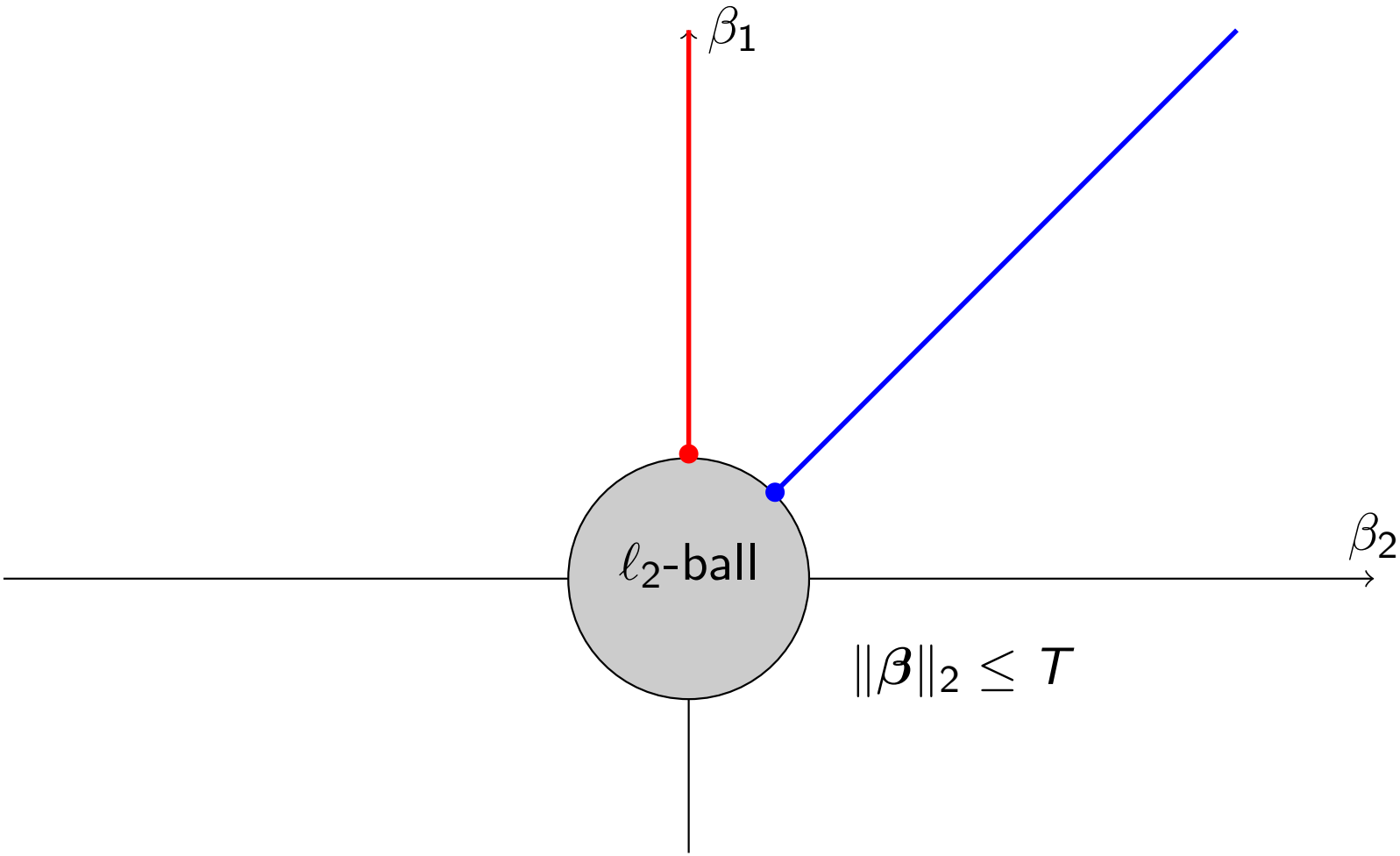
"equivalent" means that $\forall\lambda > 0, \exists T \geq 0$ s.t. $\tilde{\boldsymbol{\beta}}(T) = \hat{\boldsymbol{\beta}}(\lambda)$.

Regularizing with the ℓ_1-norm



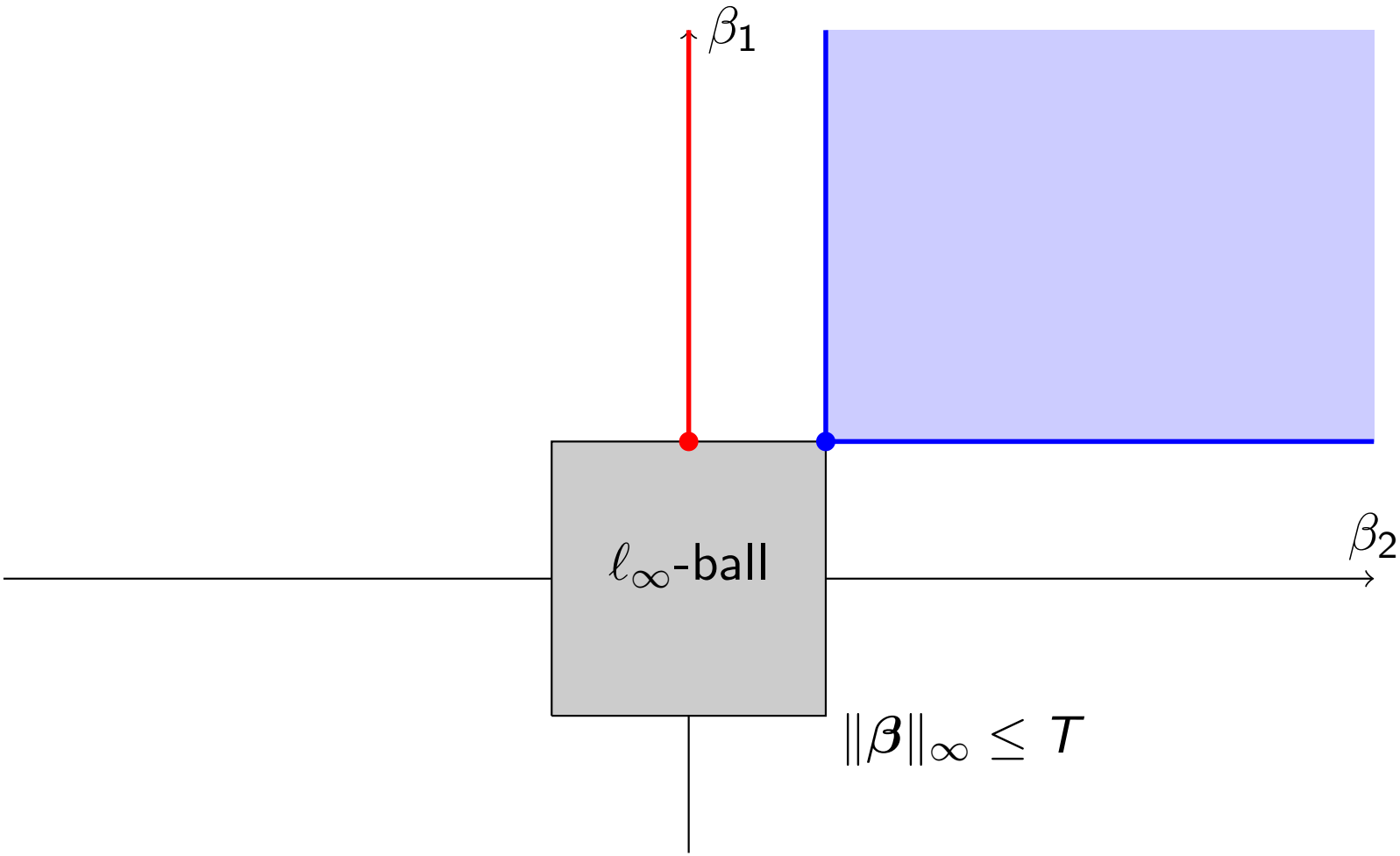
The projection onto a convex set is "biased" towards singularities.

Regularizing with the ℓ_2-norm



The ℓ_2-norm is isotropic.

Regularizing with the ℓ_∞-norm



The ℓ_∞-norm encourages $|\beta_1| = |\beta_2|$.

In 3D.

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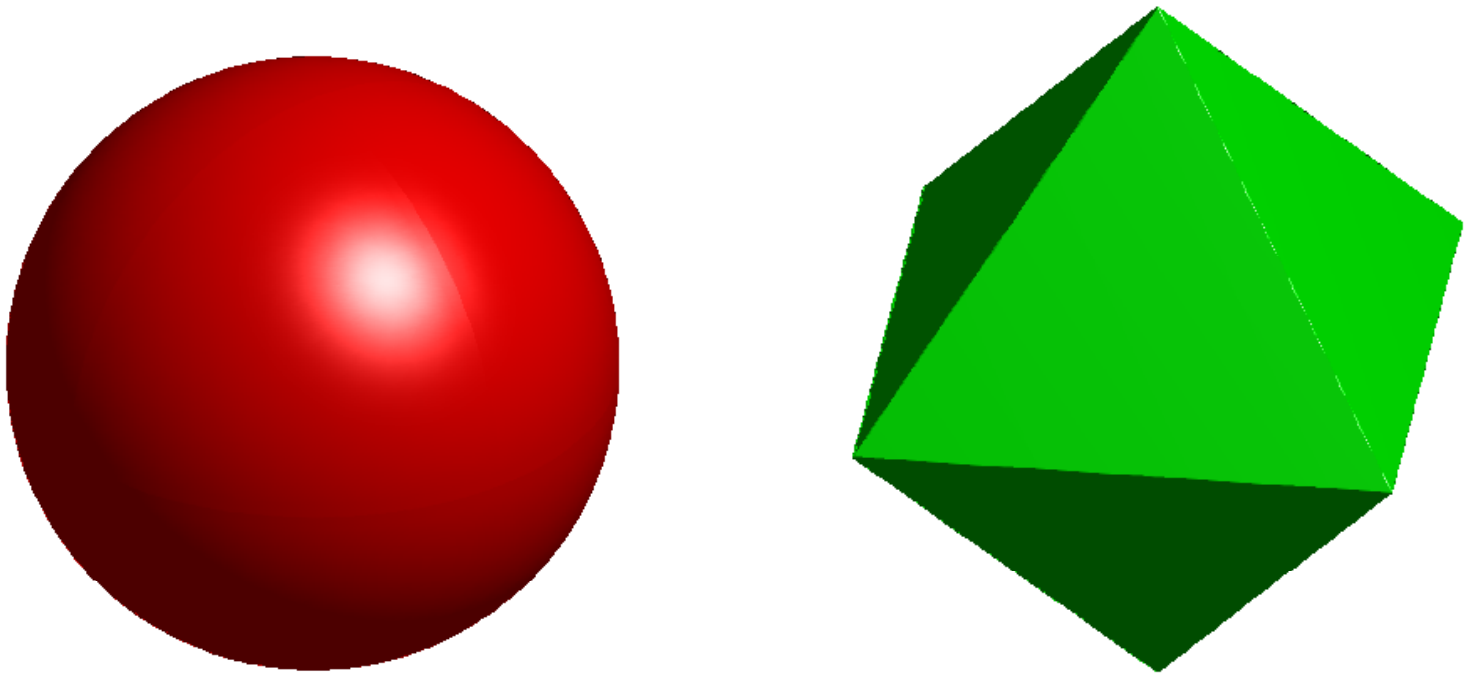


Why does the ℓ_1-norm induce sparsity?

Exemple: quadratic problem in 1D

$$\min_{\beta \in \mathbb{R}} \frac{1}{2}(y-\beta)^2 + \lambda|\beta|$$

Piecewise quadratic function with a kink at zero.

Derivative at 0_+: $g_+ = -y + \lambda$ and 0_-: $g_- = -y - \lambda$.

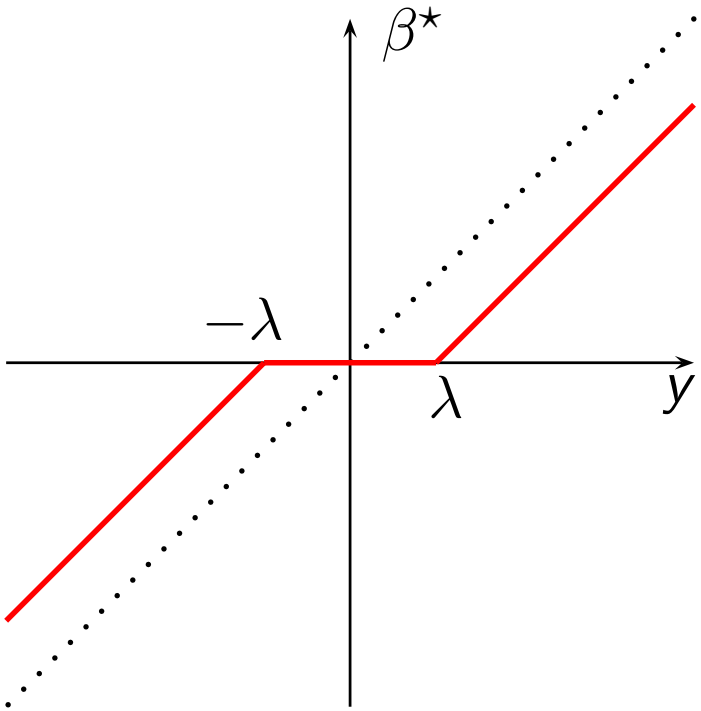
Optimality conditions. β is optimal iff:

- $|\beta| > 0$ and $(y-\beta) + \lambda \operatorname{sign}(\beta) = 0$
- $\beta = 0$ and $g_+ \geq 0$ and $g_- \leq 0$

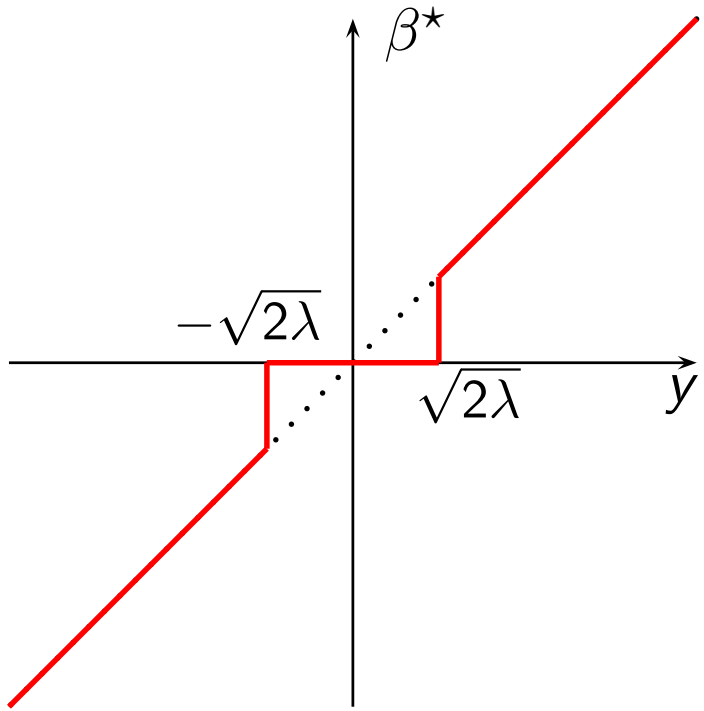
The solution is a **soft-thresholding**:

$$\beta^\star = \operatorname{sign}(y)(|y| - \lambda)^+.$$

Why does the ℓ_1-norm induce sparsity?



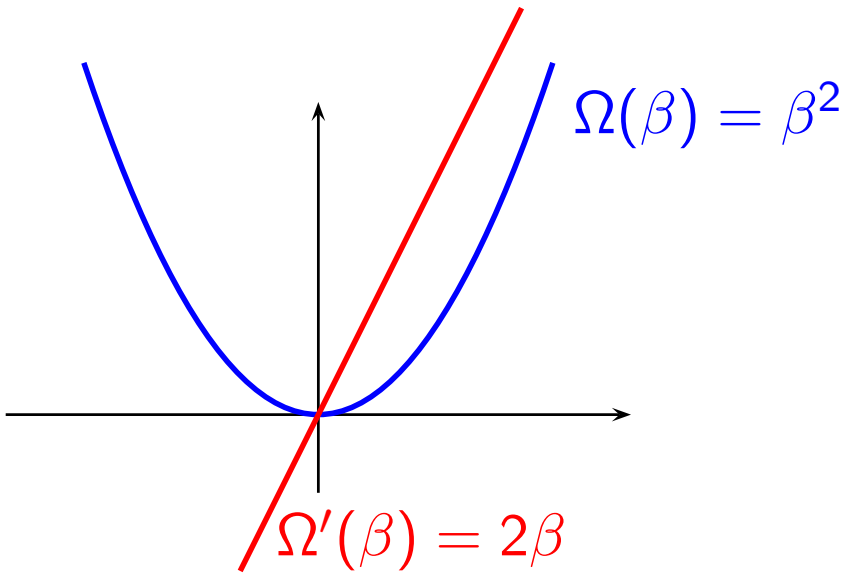
(a) soft-thresholding operator,
$\beta^\star = \text{sign}(y)(|y| - \lambda)^+$,
$\min_\beta \frac{1}{2}(y-\beta)^2 + \lambda|\beta|$

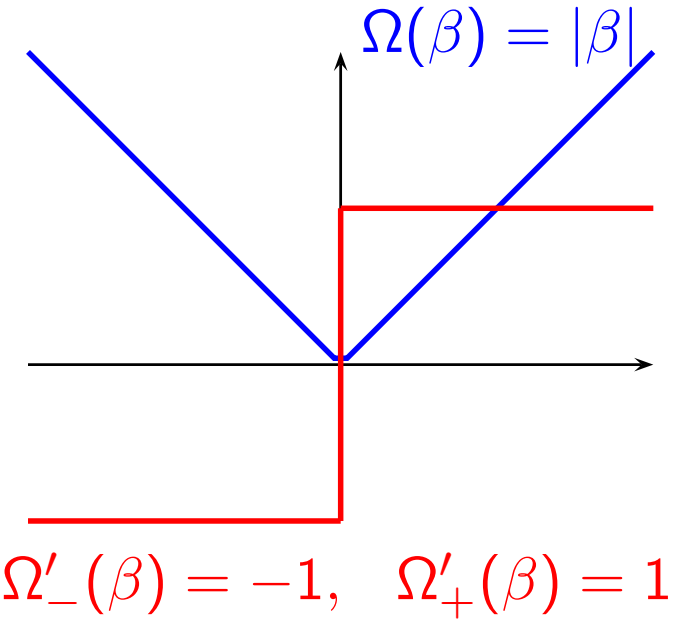


(b) hard-thresholding operator
$\beta^\star = \mathbf{1}_{|u| \geq \sqrt{2\lambda}} y$
$\min_\beta \frac{1}{2}(y-\beta)^2 + \lambda \mathbf{1}_{|\beta|>0}$

Why does the ℓ_1-norm induce sparsity?

Comparison with ℓ_2-regularization in 1D

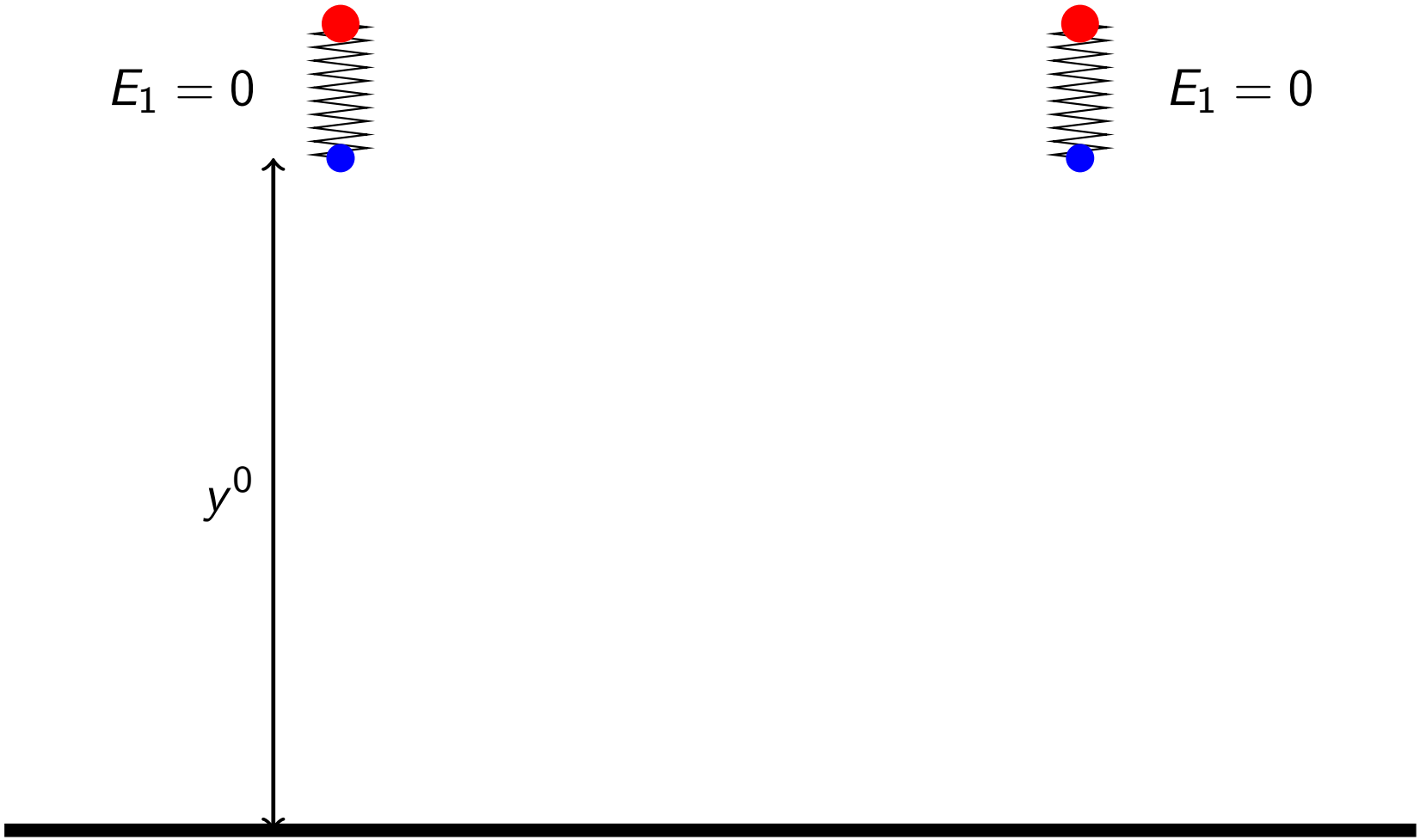




The gradient of the ℓ_2-penalty vanishes when β get close to 0. On its differentiable part, the norm of the gradient of the ℓ_1-norm is constant.

Why does the ℓ_1-norm induce sparsity?

Physical illustration



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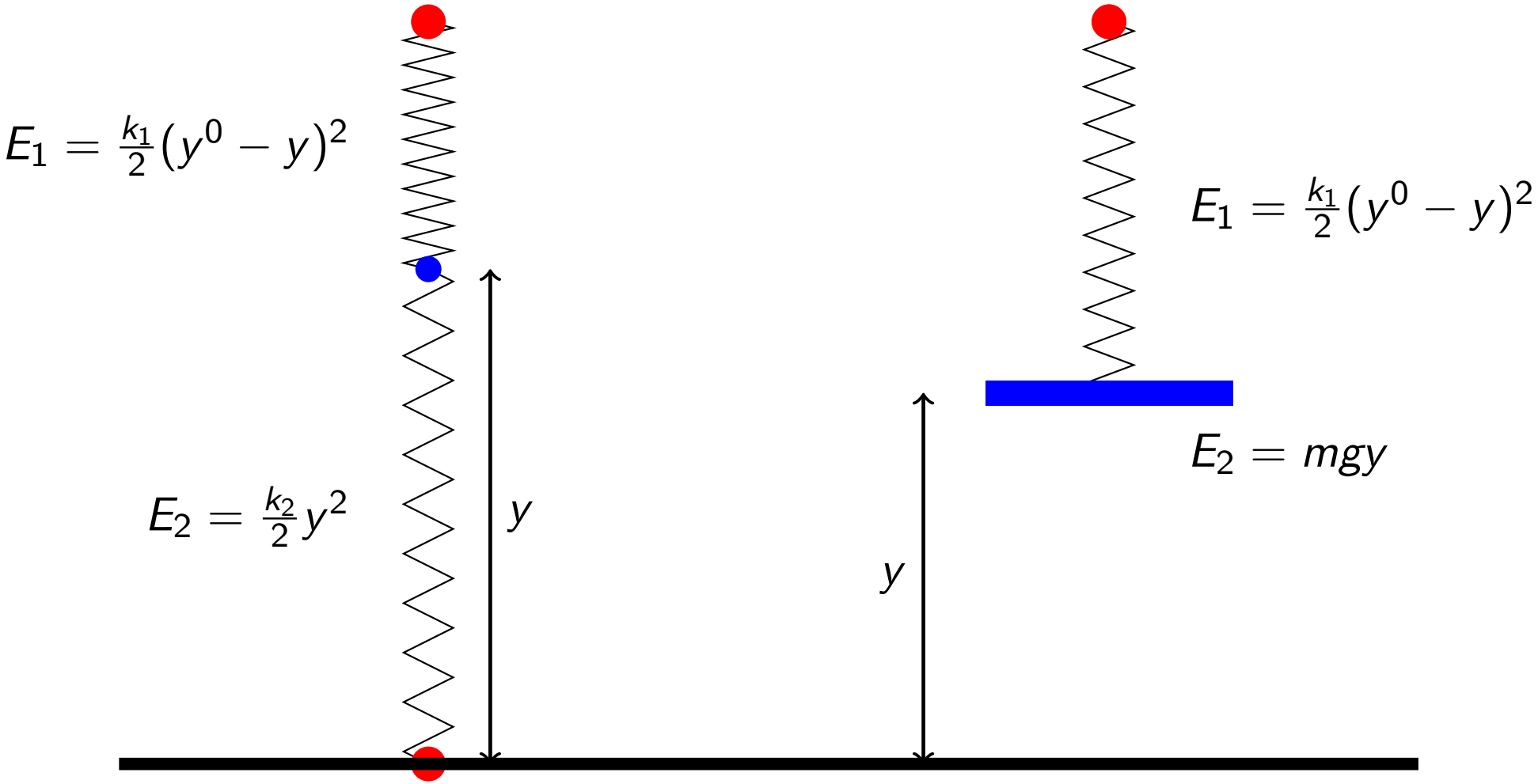
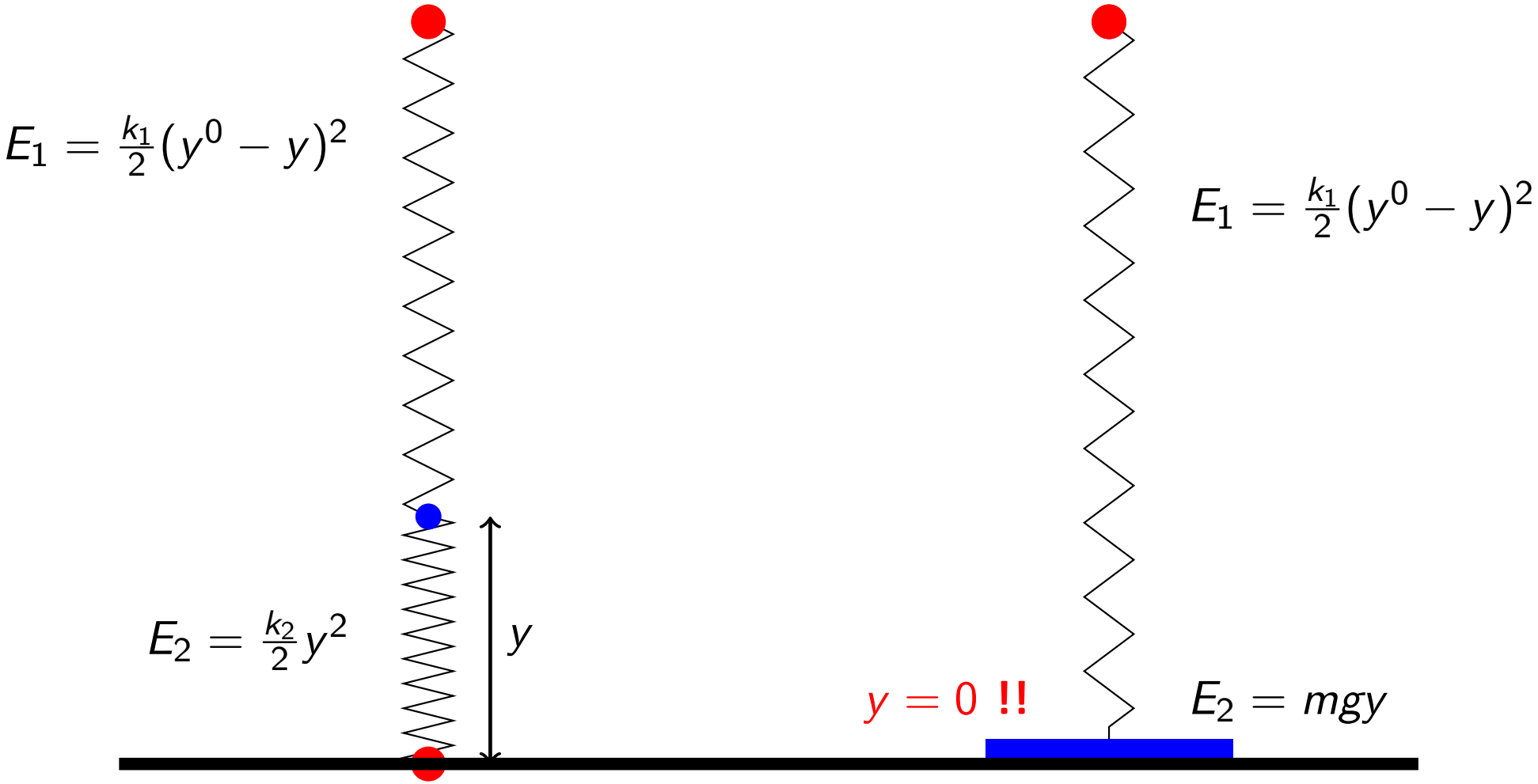
Physical illustration



Why does the ℓ_1-norm induce sparsity?

Physical illustration



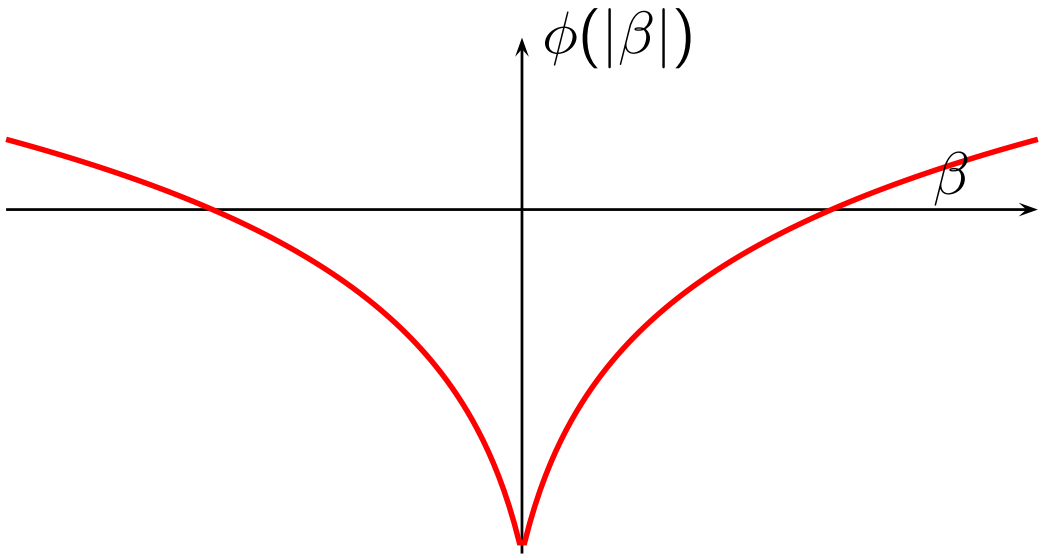
Examples of sparsity-inducing penalties

Exploiting concave functions with a kink at zero

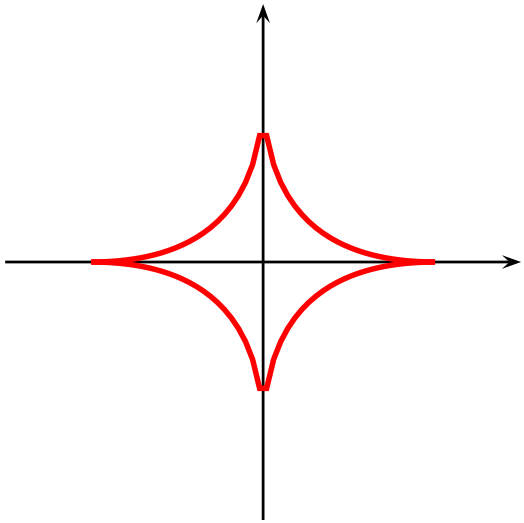
$\Omega(\beta) = \sum_{j=1}^{p} \phi(|\beta_j|)$.

- ℓ_q-"pseudo-norm", with $0 < q < 1$: $\Omega(\beta) \triangleq \sum_{j=1}^{p} |\beta_j|^q$,
- log penalty, $\Omega(\beta) \triangleq \sum_{j=1}^{p} \log(|\beta_j| + \varepsilon)$,

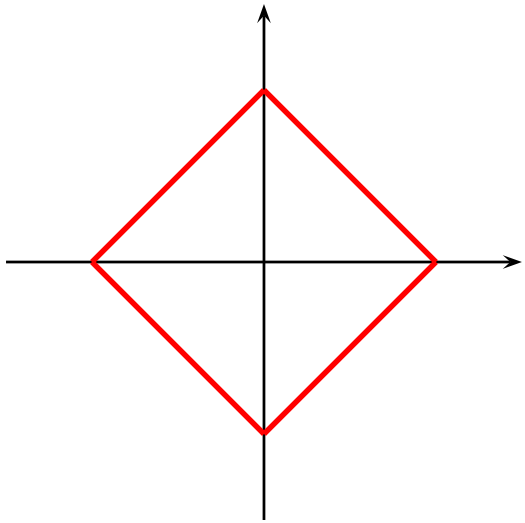
ϕ is any function that looks like this:



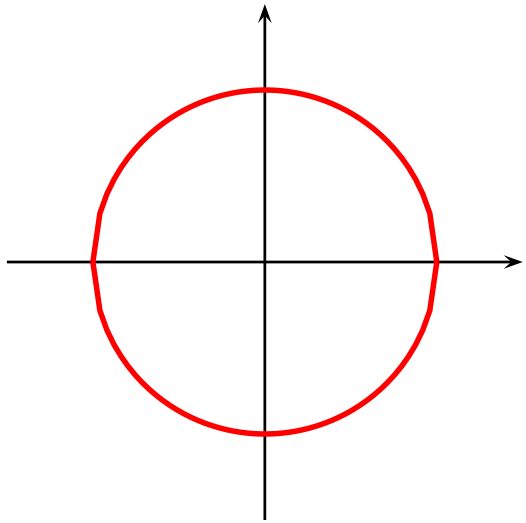
Examples of sparsity-inducing penalties



(c) $\ell_{0.5}$-ball, 2-D



(d) ℓ_1-ball, 2-D



(e) ℓ_2-ball, 2-D

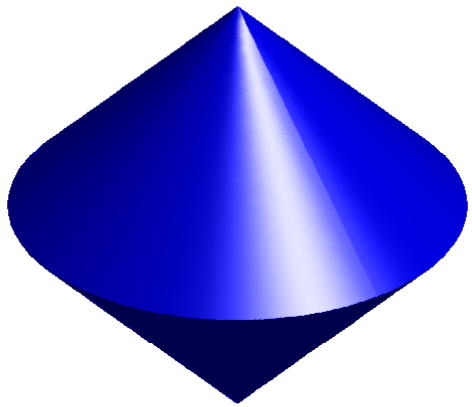
Figure: Open balls in 2-D corresponding to several ℓ_q-norms and pseudo-norms.

Group Lasso

Turlach et al. [2005], Yuan and Lin [2006], Zhao et al. [2009]

$$\text{the } \ell_1/\ell_q\text{-norm}: \qquad \Omega(\beta) = \sum_{g \in \mathcal{G}} \|\beta_g\|_q.$$

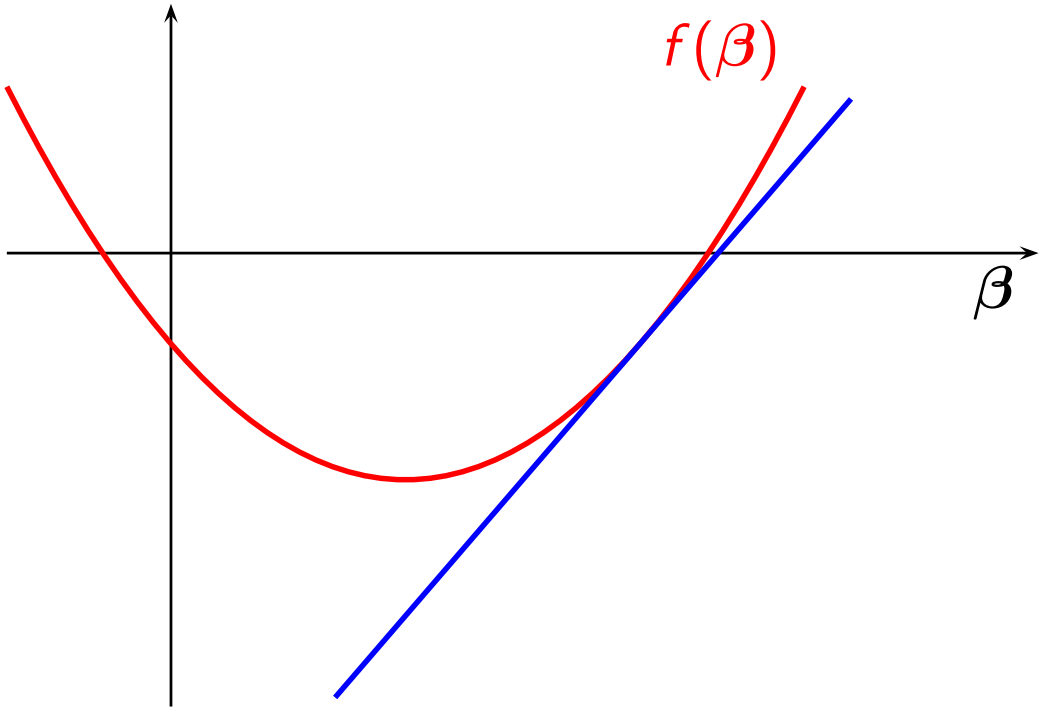
- $\mathcal{G}$ is a **partition** of $\{1, \ldots, p\}$;
- $q = 2$ or $q = \infty$ in practice;
- can be interpreted as the ℓ_1-norm of $[\|\beta_g\|_q]_{g \in \mathcal{G}}$.



$$\Omega(\beta) = \|\beta_{\{1,2\}}\|_2 + |\beta_3|.$$

Part II: Convex Optimization for Sparse Estimation

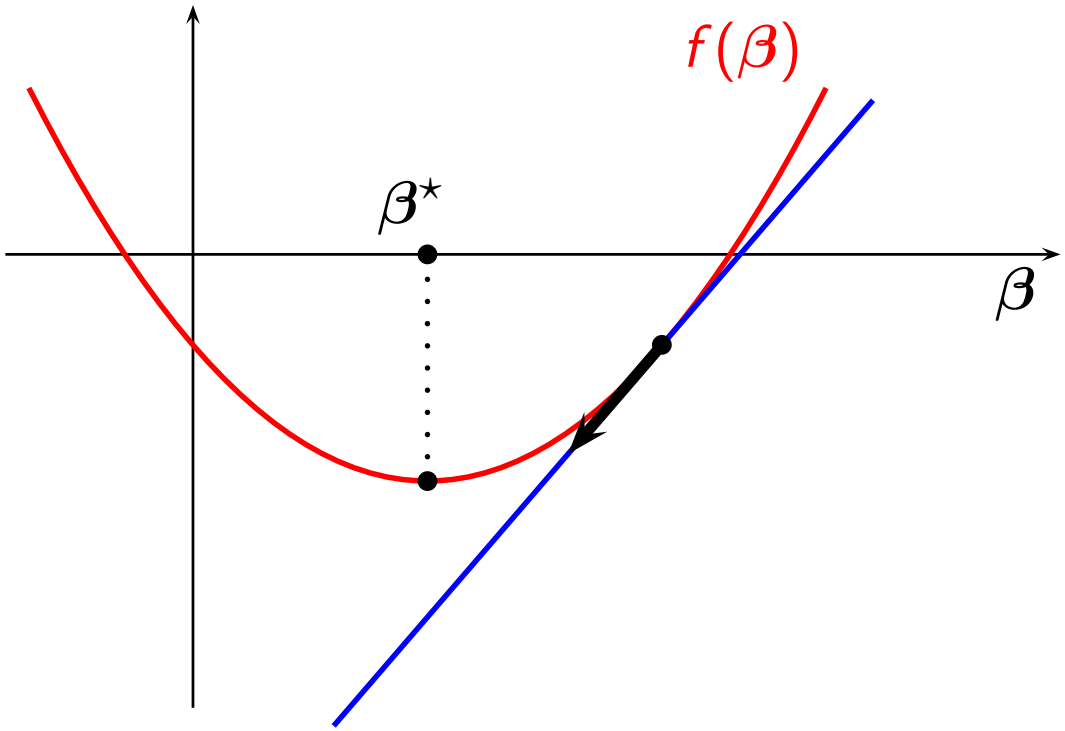
Convex Functions



Why do we care about convexity?

Why do we care about convexity?

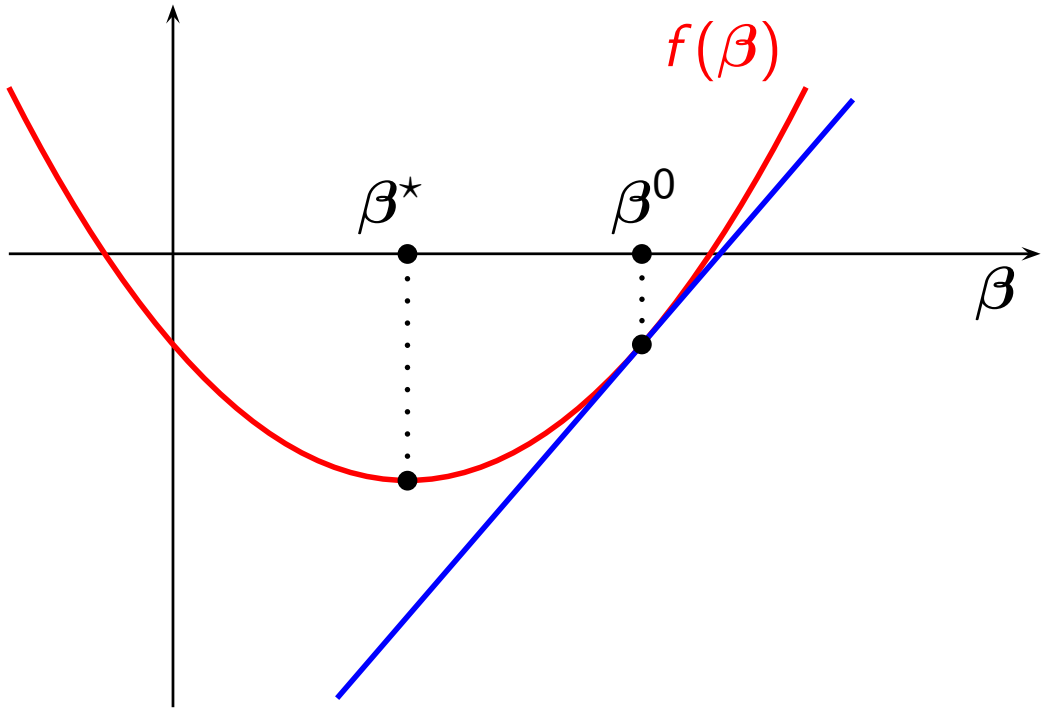
Local observations give some information about the global optimum



- $\nabla f(\beta) = 0$ is a necessary and sufficient optimality condition for differentiable convex functions;
- it is often easy to upper-bound $f(\beta) - f^\star$.

An important inequality for smooth convex functions

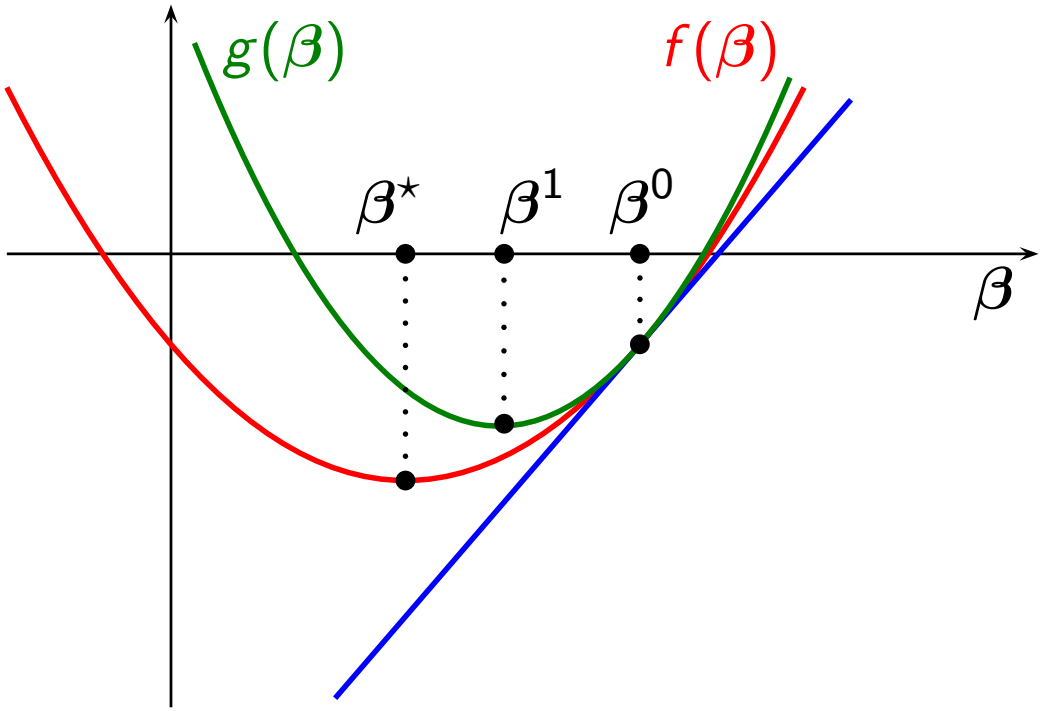
If f is convex



- $f(\beta) \geq \underbrace{f(\beta^0) + \nabla f(\beta^0)^\top (\beta - \beta^0)}_{\text{linear approximation}}$;
- this is an equivalent definition of convexity for smooth functions.

An important inequality for smooth functions

If ∇f is L-Lipschitz continuous



- $f(\beta) \leq g(\beta) = \underbrace{f(\beta^0) + \nabla f(\beta^0)^\top(\beta - \beta^0)}_{\text{linear approximation}} + \frac{L}{2}\|\beta - \beta^0\|_2^2;$
- $\boxed{\beta^1 = \beta^0 - \frac{1}{L}\nabla f(\beta^0). \text{ (gradient descent step).}}$

Gradient Descent Algorithm

Assume that f is convex and differentiable, and that ∇f is L-Lipschitz.

Theorem

Consider the algorithm

$$\boxed{\beta^t \leftarrow \beta^{t-1} - \frac{1}{L}\nabla f(\beta^{t-1}).}$$

Then,

$$f(\beta^t) - f^\star \leq \frac{L\|\beta^0 - \beta^\star\|_2^2}{2t}.$$

Remarks

- the convergence rate improves under additional assumptions on f (strong convexity);
- some variants have a $O(1/t^2)$ convergence rate [Nesterov, 1983].

Proof (1/2)

Proof of the main inequality for smooth functions

We want to show that for all $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$,

$$f(\boldsymbol{\beta}) \leq f(\boldsymbol{\alpha}) + \nabla f(\boldsymbol{\alpha})^\top (\boldsymbol{\beta} - \boldsymbol{\alpha}) + \frac{L}{2}\|\boldsymbol{\beta} - \boldsymbol{\alpha}\|_2^2.$$

By using Taylor's theorem with integral form,

$$f(\boldsymbol{\beta}) - f(\boldsymbol{\alpha}) = \int_0^1 \nabla f(t\boldsymbol{\beta} + (1-t)\boldsymbol{\alpha})^\top (\boldsymbol{\beta} - \boldsymbol{\alpha}) dt.$$

Then,

$$\begin{aligned}
f(\boldsymbol{\beta}) - f(\boldsymbol{\alpha}) - \nabla f(\boldsymbol{\alpha})^\top (\boldsymbol{\beta} - \boldsymbol{\alpha}) &\leq \int_0^1 (\nabla f(t\boldsymbol{\beta} + (1-t)\boldsymbol{\alpha}) - \nabla f(\boldsymbol{\alpha}))^\top (\boldsymbol{\beta} - \boldsymbol{\alpha}) dt \\
&\leq \int_0^1 |(\nabla f(t\boldsymbol{\beta} + (1-t)\boldsymbol{\alpha}) - \nabla f(\boldsymbol{\alpha}))^\top (\boldsymbol{\beta} - \boldsymbol{\alpha})| dt \\
&\leq \int_0^1 \|\nabla f(t\boldsymbol{\beta} + (1-t)\boldsymbol{\alpha}) - \nabla f(\boldsymbol{\alpha})\|_2 \|\boldsymbol{\beta} - \boldsymbol{\alpha}\|_2 dt \quad \text{(C.-S.)} \\
&\leq \int_0^1 Lt\|\boldsymbol{\beta} - \boldsymbol{\alpha}\|_2^2 dt = \frac{L}{2}\|\boldsymbol{\beta} - \boldsymbol{\alpha}\|_2^2.
\end{aligned}$$

Proof (2/2)

Proof of the theorem

We have shown that for all $\boldsymbol{\beta}$,

$$f(\boldsymbol{\beta}) \leq g_t(\boldsymbol{\beta}) = f(\boldsymbol{\beta}^{t-1}) + \nabla f(\boldsymbol{\beta}^{t-1})^\top (\boldsymbol{\beta} - \boldsymbol{\beta}^{t-1}) + \frac{L}{2}\|\boldsymbol{\beta} - \boldsymbol{\beta}^{t-1}\|_2^2.$$

g_t is minimized by $\boldsymbol{\beta}^t$; it can be rewritten $g_t(\boldsymbol{\beta}) = g_t(\boldsymbol{\beta}^t) + \frac{L}{2}\|\boldsymbol{\beta} - \boldsymbol{\beta}^t\|_2^2$. Then,

$$\begin{aligned}
f(\boldsymbol{\beta}^t) \leq g_t(\boldsymbol{\beta}^t) &= g_t(\boldsymbol{\beta}^\star) - \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^t\|_2^2 \\
&= f(\boldsymbol{\beta}^{t-1}) + \nabla f(\boldsymbol{\beta}^{t-1})^\top (\boldsymbol{\beta}^\star - \boldsymbol{\beta}^{t-1}) + \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^{t-1}\|_2^2 - \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^t\|_2^2 \\
&\leq f^\star + \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^{t-1}\|_2^2 - \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^t\|_2^2.
\end{aligned}$$

By summing from $t = 1$ to T, we have a telescopic sum

$$T(f(\boldsymbol{\beta}^T) - f^\star) \leq \sum_{t=1}^{T} f(\boldsymbol{\beta}^t) - f^\star \leq \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^0\|_2^2 - \frac{L}{2}\|\boldsymbol{\beta}^\star - \boldsymbol{\beta}^T\|_2^2.$$

The Proximal Gradient Method

We consider a smooth function f and a non-smooth regularizer Ω.

$$\min_{\beta \in \mathbb{R}^p} f(\beta) + \Omega(\beta)$$

For example,

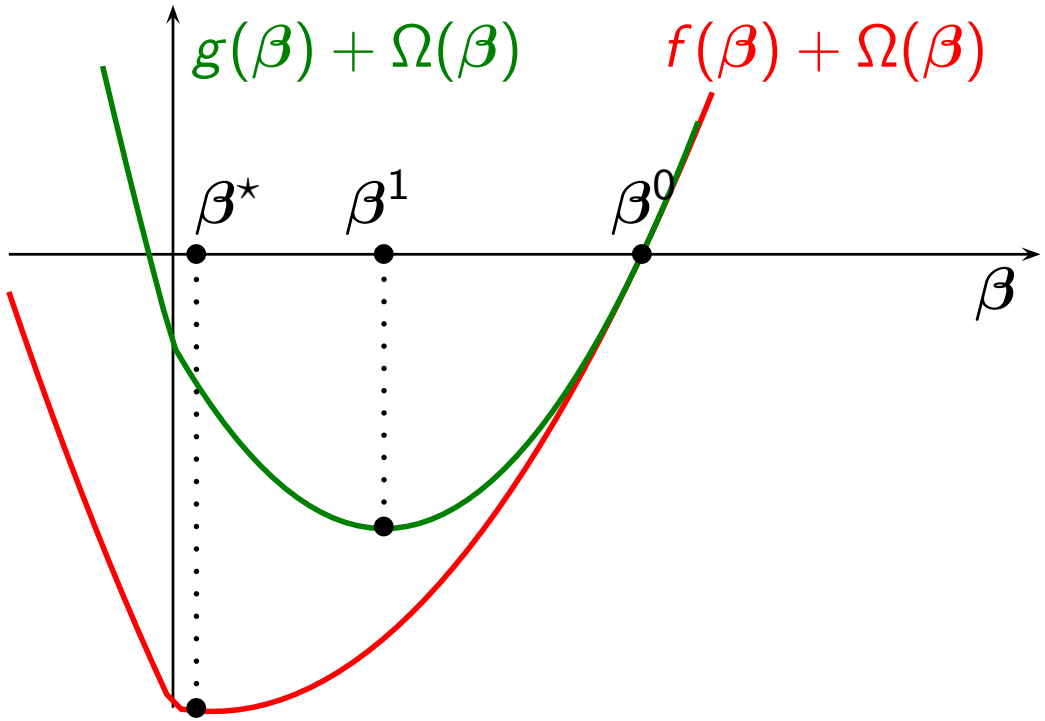
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda\|\beta\|_1.$$

- the objective function is not differentiable.
- an extension of gradient descent for such a problem is called **"proximal gradient descent"**
  [Beck and Teboulle, 2009, Nesterov, 2007].

The Proximal Gradient Method

An important inequality for composite functions

If ∇f is L-Lipschitz continuous



- $f(\beta) + \Omega(\beta) \leq f(\beta^0) + \nabla f(\beta^0)^\top(\beta - \beta^0) + \frac{L}{2}\|\beta - \beta^0\|_2^2 + \Omega(\beta)$;
- β^1 minimizes $g + \Omega$.

The Proximal Gradient Method

Gradient descent for minimizing f consists of

$$\beta^t \leftarrow \arg\min_{\beta \in \mathbb{R}^p} g_t(\beta) \quad \Longleftrightarrow \quad \beta^t \leftarrow \beta^{t-1} - \frac{1}{L}\nabla f(\beta^{t-1}).$$

The proximal gradient method for minimizing $f + \Omega$ consists of

$$\beta^t \leftarrow \arg\min_{\beta \in \mathbb{R}^p} g_t(\beta) + \Omega(\beta),$$

which is equivalent to

$$\boxed{\beta^t \leftarrow \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\left\|\beta^{t-1} - \frac{1}{L}\nabla f(\beta^{t-1}) - \beta\right\|_2^2 + \frac{1}{L}\Omega(\beta).}$$

It requires computing efficiently the **proximal operator** of Ω.

$$\alpha \mapsto \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|\alpha - \beta\|_2^2 + \Omega(\beta).$$

The Proximal Gradient Method

Remarks

- also known as forward-backward algorithm;
- has similar convergence rates as the gradient descent method [Beck and Teboulle, 2009, Nesterov, 2007];
- there exists line search schemes to automatically tune L.

The case of ℓ_1

The proximal operator of $\lambda\|.\|_1$ is the soft-thresholding operator

$$\boldsymbol{\beta}_j^\star = \text{sign}(\boldsymbol{\alpha}_j)(|\boldsymbol{\alpha}_j| - \lambda)^+.$$

The resulting algorithm is called iterative soft-thresholding [Daubechies et al., 2004].

The Proximal Gradient Method for the Group Lasso

The proximal operator for the Group Lasso penalty

$$\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \frac{1}{2}\|\boldsymbol{\alpha}-\boldsymbol{\beta}\|_2^2 + \lambda \sum_{g\in\mathcal{G}} \|\boldsymbol{\beta}_g\|_q.$$

For $q=2$,

$$\boldsymbol{\beta}_g^\star = \frac{\boldsymbol{\alpha}_g}{\|\boldsymbol{\alpha}_g\|_2}(\|\boldsymbol{\alpha}_g\|_2-\lambda)^+, \quad \forall g\in\mathcal{G}.$$

For $q=\infty$,

$$\boldsymbol{\beta}_g^\star = \boldsymbol{\alpha}_g - \Pi_{\|.\|_1\leq\lambda}[\boldsymbol{\alpha}_g], \quad \forall g\in\mathcal{G}.$$

These formula generalize soft-thresholding to groups of variables.

Coordinate Descent for the Lasso

$$\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \frac{1}{2}\|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|_2^2+\lambda\|\boldsymbol{\beta}\|_1.$$

The coordinate descent method consists of iteratively fixing all variables and optimizing with respect to one:

$$\beta_j \leftarrow \arg\min_{\beta\in\mathbb{R}} \frac{1}{2}\| \underbrace{\mathbf{y}-\sum_{i\neq j}\boldsymbol{\beta}_i\mathbf{x}^i}_{\mathbf{r}} -\beta\mathbf{x}^j\|_2^2+\lambda|\beta|,$$

where $\mathbf{X}=[\mathbf{x}^1,\ldots,\mathbf{x}^p]$. Assume the columns of $\mathbf{X}$ to have unit ℓ_2-norm,

$$\boldsymbol{\beta}_j \leftarrow \text{sign}(\mathbf{x}^{j\top}\mathbf{r})(|\mathbf{x}^{j\top}\mathbf{r}|-\lambda)^+$$

This involves again the **soft-thresholding** operator.

Coordinate Descent for the Lasso

Remarks

- no parameter to tune!
- impressive performance with five lines of code.
- coordinate descent + nonsmooth objective is **not convergent in general**. Here, the problem is equivalent to a convex smooth optimization problem with separable constraints

$$\min_{\beta_+,\beta_-} \frac{1}{2}\|\mathbf{y} - \mathbf{X}_+\beta_+ + \mathbf{X}_-\beta_-\|_2^2 + \lambda\beta_+^T\mathbf{1} + \lambda\beta_-^T\mathbf{1} \quad \text{s.t.} \quad \beta_-, \beta_+ \geq 0.$$

  For this specific problem, the algorithm is **convergent** [see Bertsekas, 1999].
- can be extended to group-Lasso, or other loss functions.
- j can be picked up at random, or by cycling (harder to analyze).

Smoothing Techniques: Reweighted ℓ_2

Let us start from something simple

$$a^2 - 2ab + b^2 \geq 0.$$

Smoothing Techniques: Reweighted ℓ_2

Let us start from something simple

$$a^2 - 2ab + b^2 \geq 0.$$

Then

$$a \leq \frac{1}{2}\left(\frac{a^2}{b} + b\right) \quad \text{with equality iff} \quad a = b$$

and

$$\|\beta\|_1 = \min_{\eta_j \geq 0} \frac{1}{2} \sum_{j=1}^{p} \frac{\beta_j^2}{\eta_j} + \eta_j.$$

The formulation becomes

$$\min_{\beta, \eta_j \geq \varepsilon} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \frac{\lambda}{2} \sum_{j=1}^{p} \frac{\beta_j^2}{\eta_j} + \eta_j.$$

The Regularization Path of the Lasso

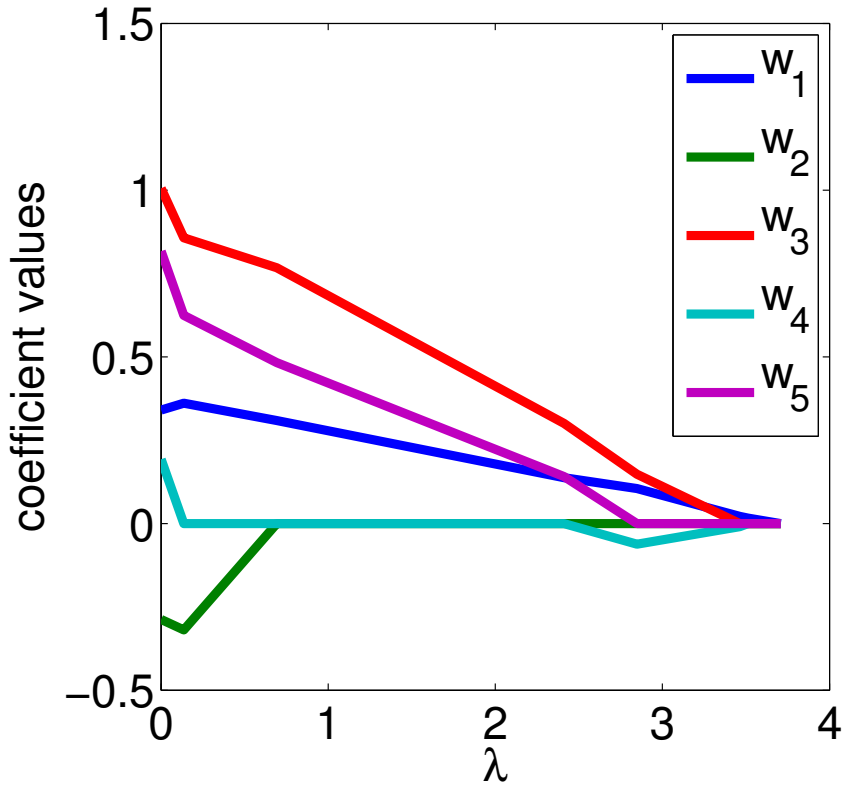


Figure: The regularization path of the Lasso is piecewise linear.

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda\|\beta\|_1.$$

Lasso and optimality conditions

Theorem

β is a solution of the Lasso if and only if

$$\left\{ \begin{array}{rcll} |\mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\beta)| & \leq & \lambda & \text{if } \beta_j = 0 \\ \mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\beta) & = & \lambda \operatorname{sign}(\beta_j) & \text{otherwise.} \end{array} \right.$$

Consequence

$$\beta^\star_\Gamma(\lambda) = (\mathbf{X}_\Gamma^T \mathbf{X}_\Gamma)^{-1}(\mathbf{X}_\Gamma^T \mathbf{y} - \lambda \operatorname{sign}(\beta^\star_\Gamma)) = \mathbf{A} + \lambda \mathbf{B},$$

where $\Gamma = \{j \text{ s.t. } \beta_j \neq 0\}$. If we know Γ and the signs of $\beta^\star$ in advance, we have a closed form solution.

Following the piecewise linear regularization path is called the **homotopy** method [Osborne et al., 2000, Efron et al., 2004].

LARS algorithm (Homotopy)

The regularization path $(\lambda, \beta^\star(\lambda))$ is piecewise linear.

1. Start from the trivial solution $(\lambda = \|\mathbf{X}^T\mathbf{y}\|_\infty, \beta^\star(\lambda) = 0)$.
2. Define $\Gamma = \{j \text{ s.t. } |\mathbf{x}^{j\top}\mathbf{y}| = \lambda\}$,
3. Follow the regularization path: $\beta^\star_\Gamma(\lambda) = \mathbf{A} + \lambda\mathbf{B}$, keeping $\beta^\star_{\Gamma^c} = 0$, decreasing the value of λ, until one of the following event occurs:
   - $\exists j \notin \Gamma$ such that $|\mathbf{x}^{j\top}(\mathbf{y} - \mathbf{X}\beta^\star(\lambda))| = \lambda$, then $\Gamma \leftarrow \Gamma \cup \{j\}$.
   - $\exists j \in \Gamma$ such that $\beta^\star(\lambda) = 0$, then $\Gamma \leftarrow \Gamma \setminus \{j\}$.
4. Update the direction of the path and go back to 3.

Hidden assumptions

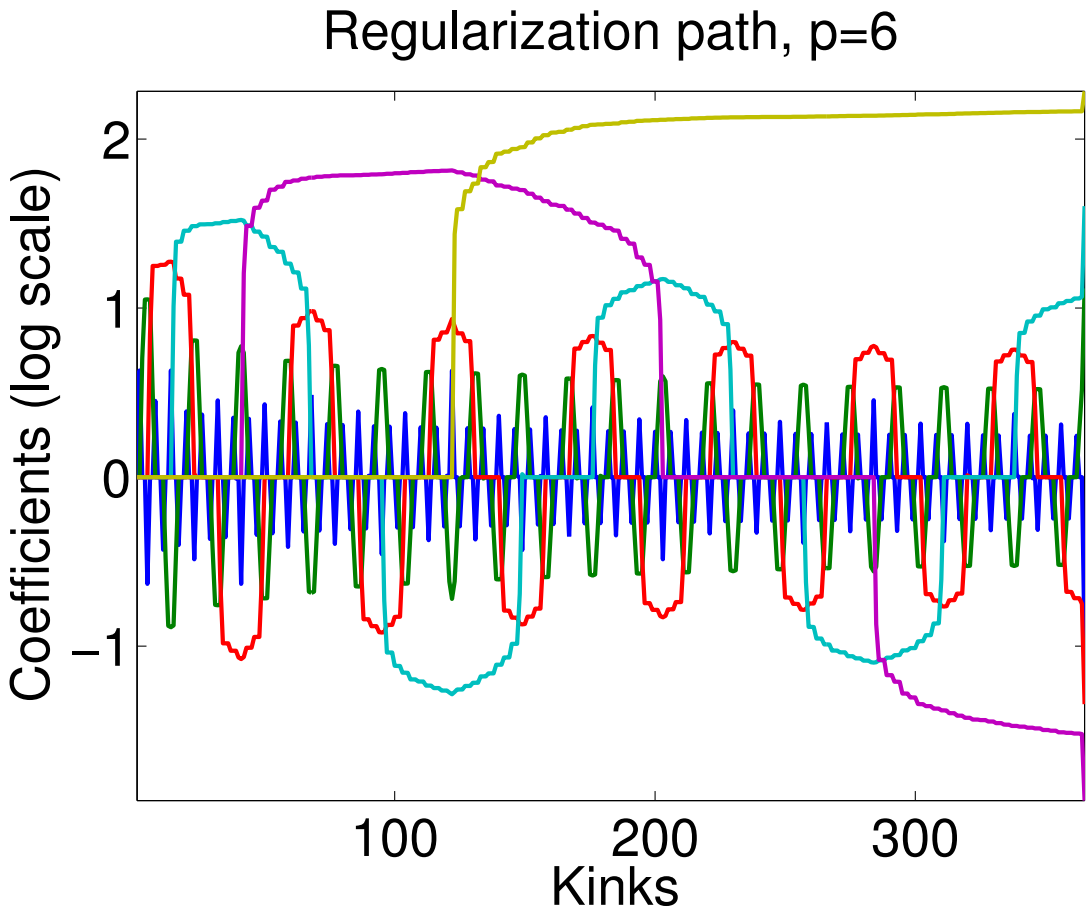
- the regularization path is unique.
- variables enter the path one at a time.

Extremely efficient for **small/medium scale** problems ($p \leq 10\,000$) and/or **very sparse** problems (when implemented correctly). **Robust to correlated features**. Can solve the elastic-net.

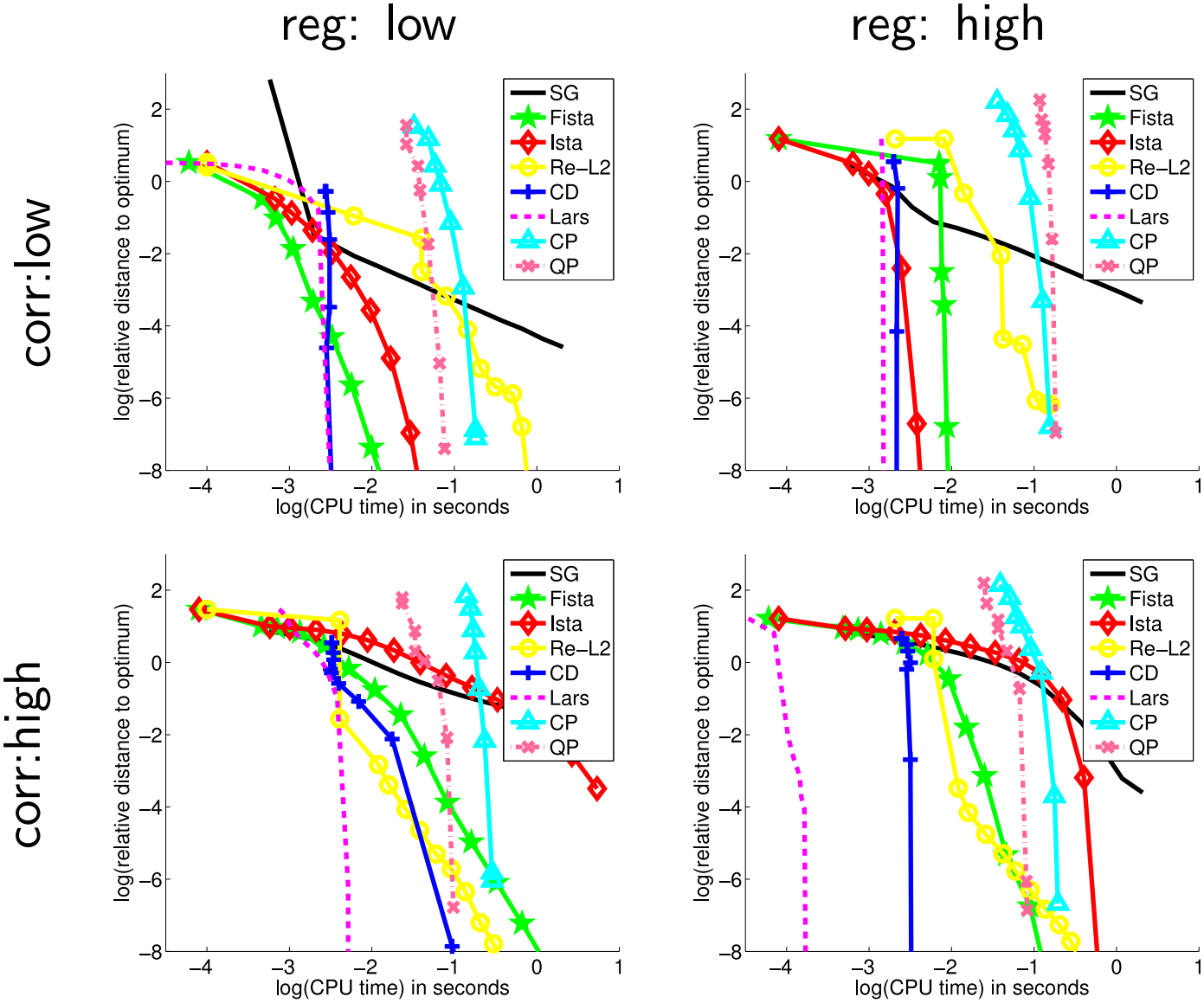
LARS algorithm (Homotopy) - Complexity

Theorem - worst case analysis [Mairal and Yu, 2012]

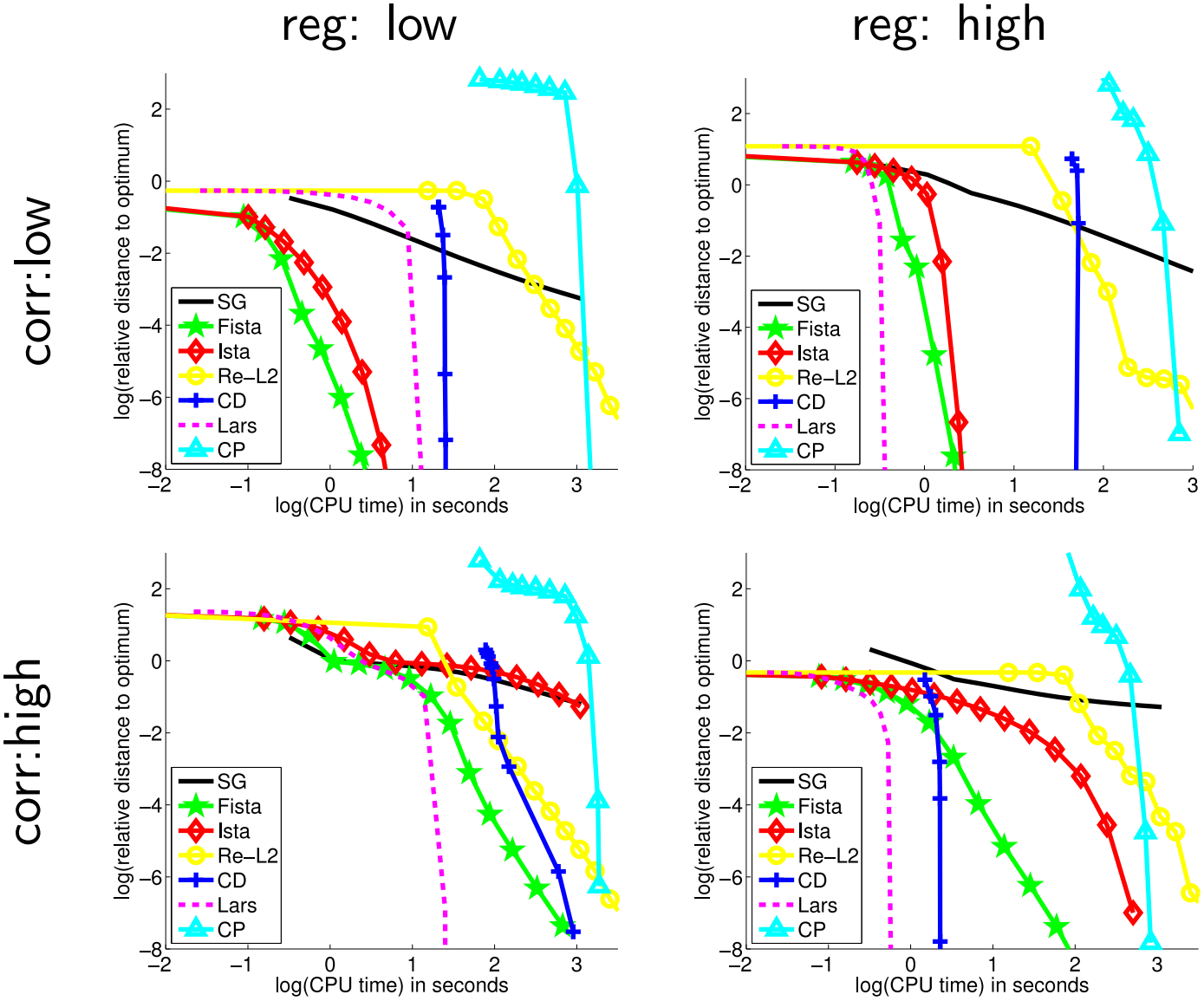
In the worst-case, the regularization path of the Lasso has exactly $(3^p + 1)/2$ *linear segments.*



Lasso Empirical comparison: Lasso, small scale ($n = 200, p = 200$)



Empirical comparison: Lasso, medium scale ($n = 2000, p = 10000$)



Empirical comparison: conclusions

Lasso

- Generic methods (subgradient descent, QP/CP solvers) are slow;
- homotopy fastest in **low dimension** and/or for **high correlation**
- Proximal methods are competitive
  - esp. larger setting and/or weak corr. and/or weak reg. and/or low precision
- Coordinate descent
  - usually dominated by LARS;
  - but much simpler to implement!

Smooth Losses and other regularization

- LARS not available $\rightarrow$ (block) coordinate descent, proximal gradient methods are good candidates.

Conclusion of the part

What was not covered in this part:

- other penalty functions, fused lasso (total variation), hierarchical penalties, structured sparsity with overlapping groups.
- stochastic optimization, Augmented Lagrangian, convergence rates, parallel computing, duality gaps via Fenchel duality...

Software. Try it yourself

`http://www.di.ens.fr/willow/SPAMS/` (Matlab/R/Python/C++).

More reading on optimization

- Bach, Jenatton, Mairal and Obozinski. Optimization with Sparsity-Inducing Penalties. 2012.
- convex optimization: [Boyd and Vandenberghe, 2004, Borwein and Lewis, 2006, Nocedal and Wright, 2006, Bertsekas, 1999, Nesterov, 2004].

Part III: Non-convex Optimization for Sparse Estimation

Greedy Algorithms

Several equivalent non-convex NP-hard problems:

$$\min_{\beta \in \mathbb{R}^p} \underbrace{\frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|_2^2}_{\text{residual } \mathbf{r}} + \underbrace{\lambda\|\beta\|_0}_{\text{regularization}},$$

$$\min_{\beta \in \mathbb{R}^p} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 \quad \text{s.t.} \quad \|\beta\|_0 \leq L,$$

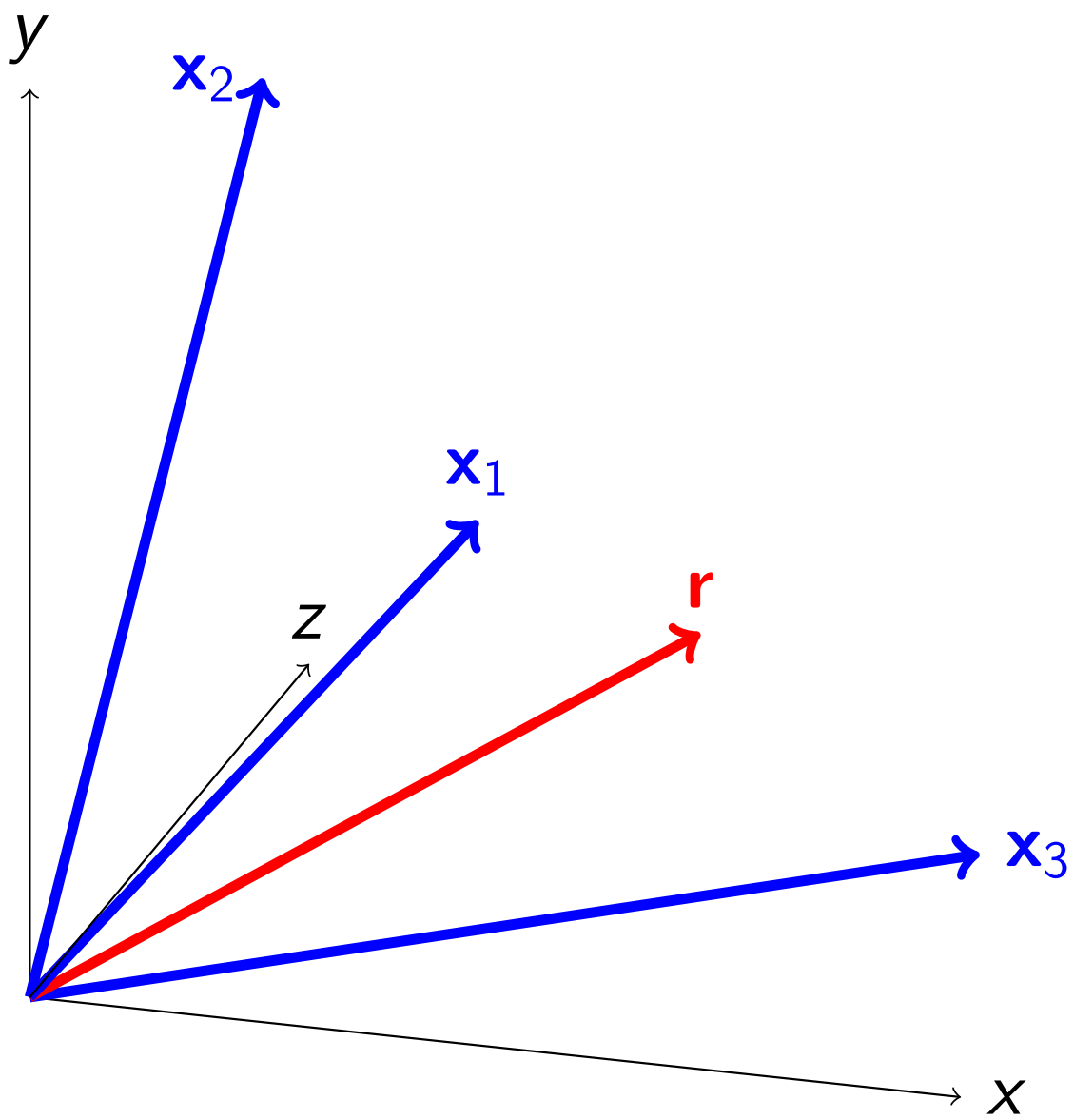
$$\min_{\beta \in \mathbb{R}^p} \|\beta\|_0 \quad \text{s.t.} \quad \|\mathbf{y} - \mathbf{X}\beta\|_2^2 \leq \varepsilon,$$

The solution is often approximated with a **greedy** algorithm.

- **Signal processing**: Matching Pursuit [Mallat and Zhang, 1993], Orthogonal Matching Pursuit [Pati et al., 1993];
- **Statistics**: L2-boosting [Bühlmann and Yu, 2003], forward selection.

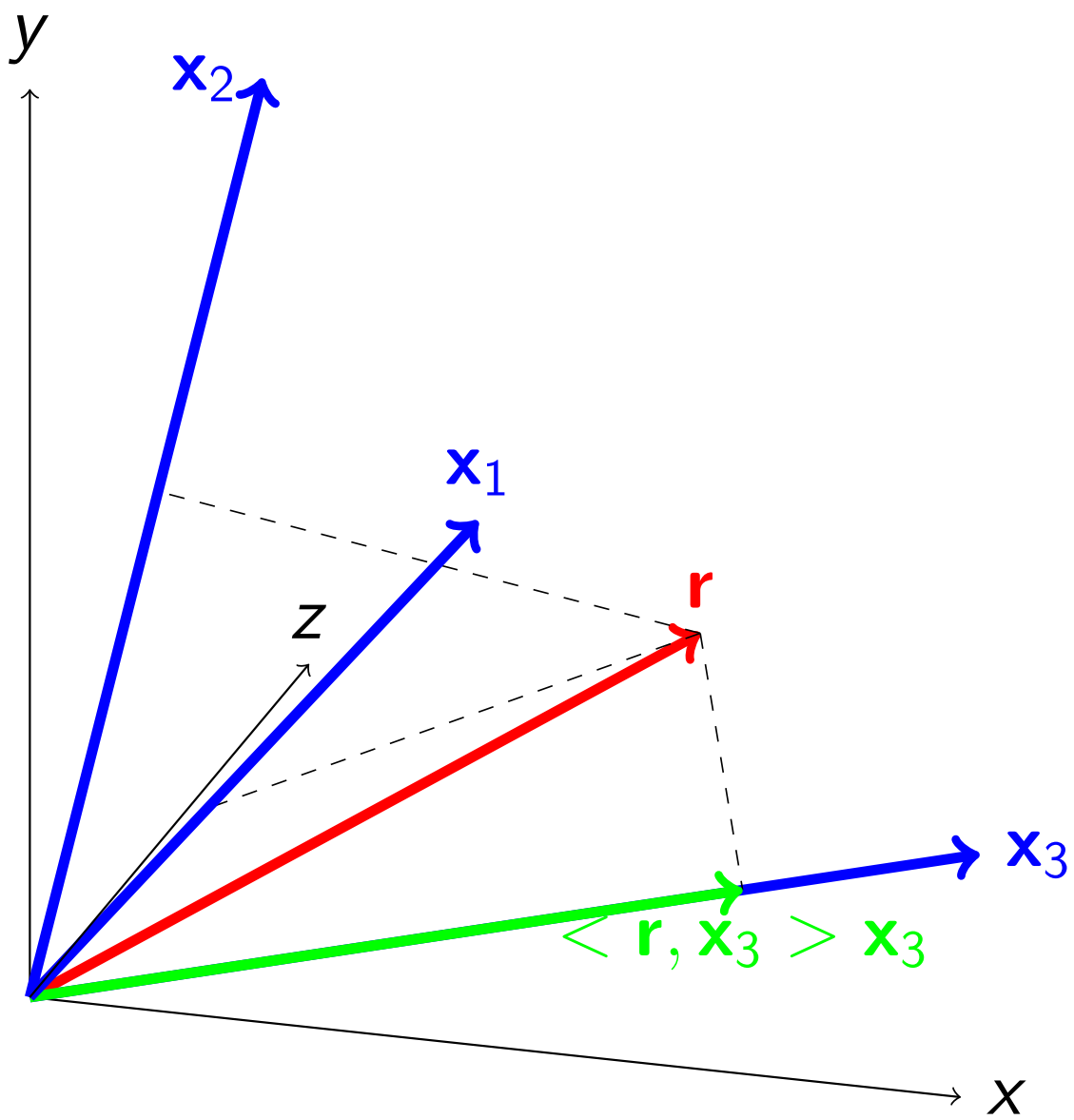
Matching Pursuit

$$\beta = (0, 0, 0)$$



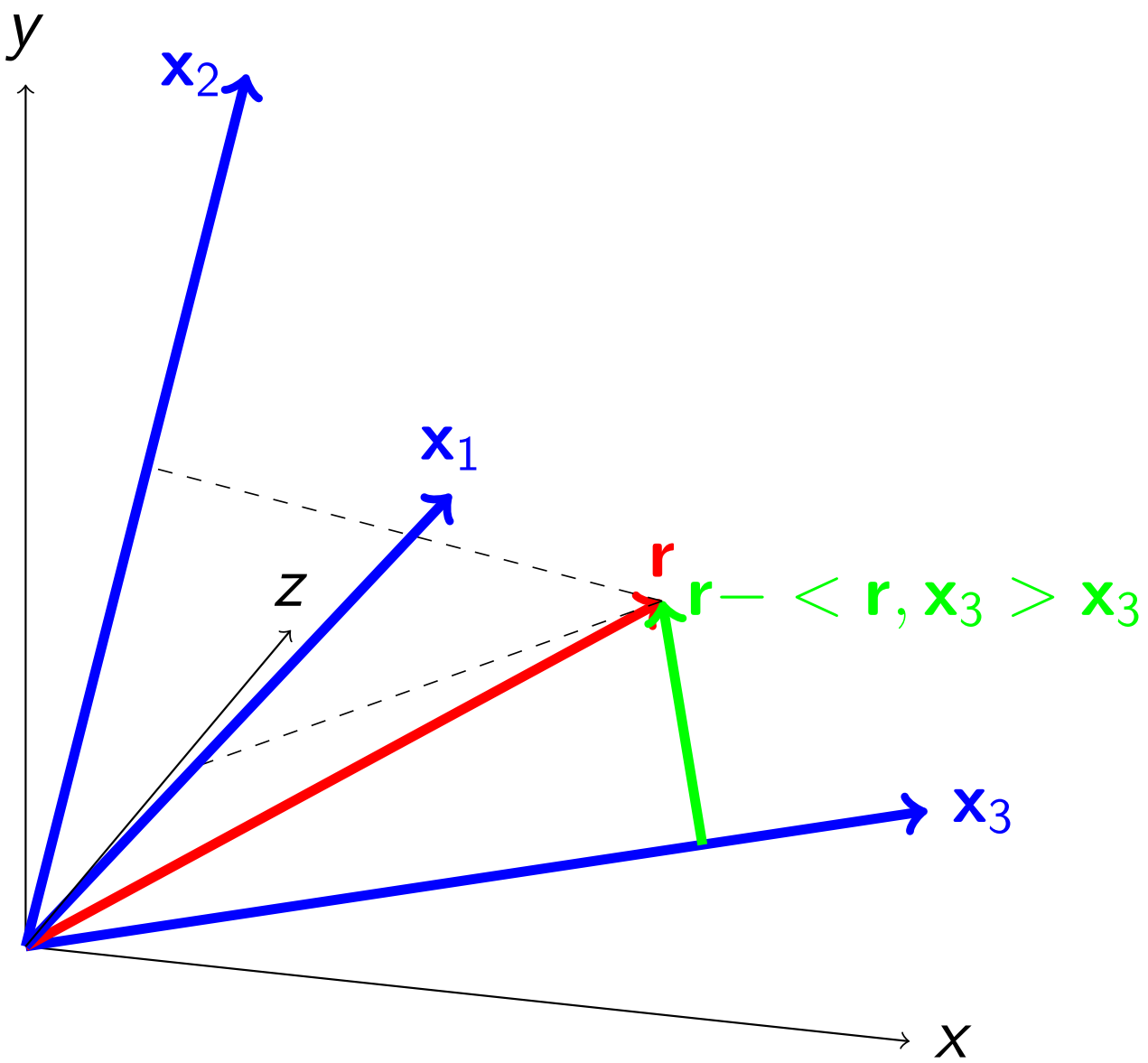
Matching Pursuit

$$\boldsymbol{\beta} = (0, 0, 0)$$



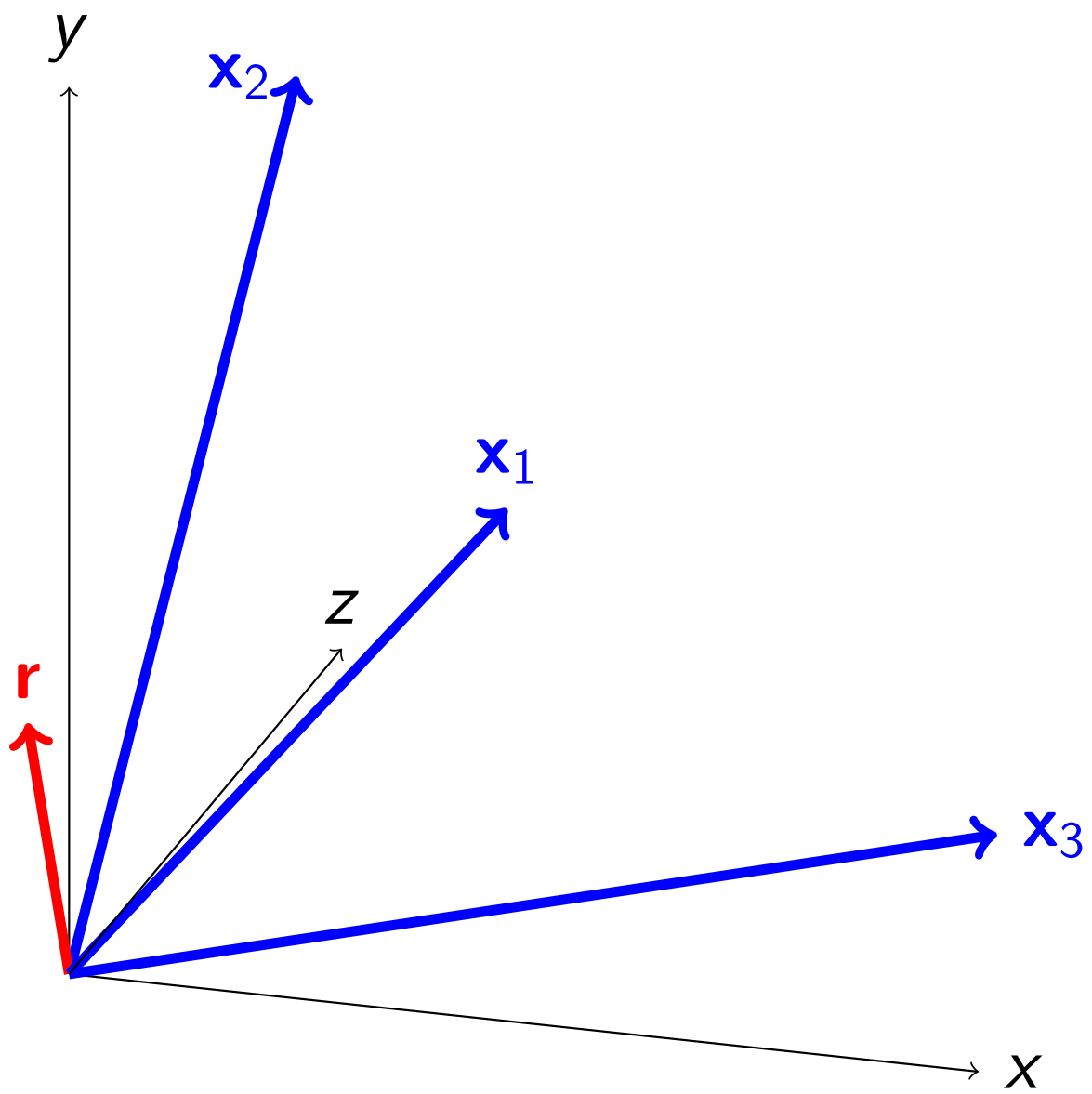
Matching Pursuit

$$\beta = (0, 0, 0)$$



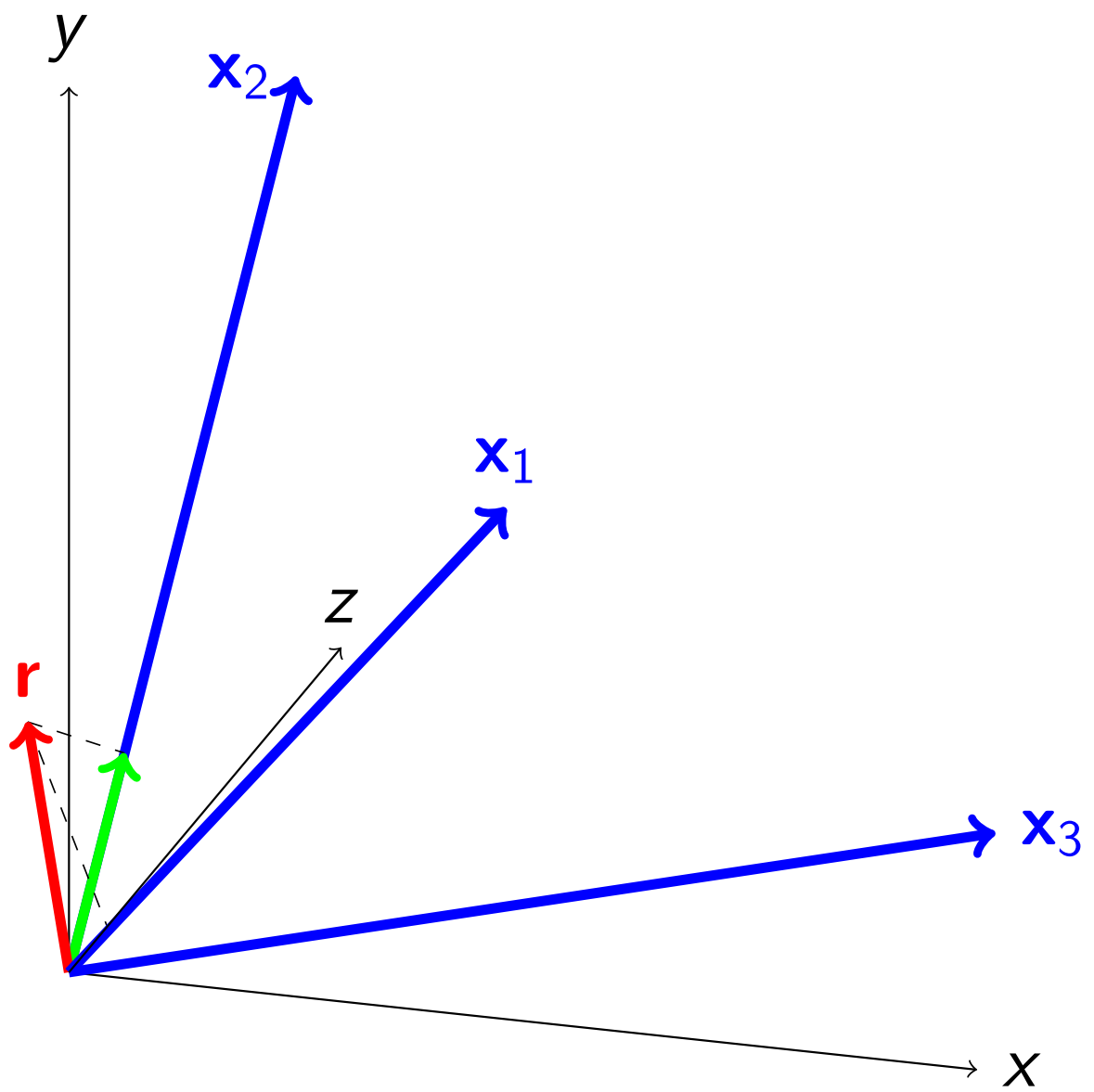
Matching Pursuit

$$\beta = (0, 0, 0.75)$$



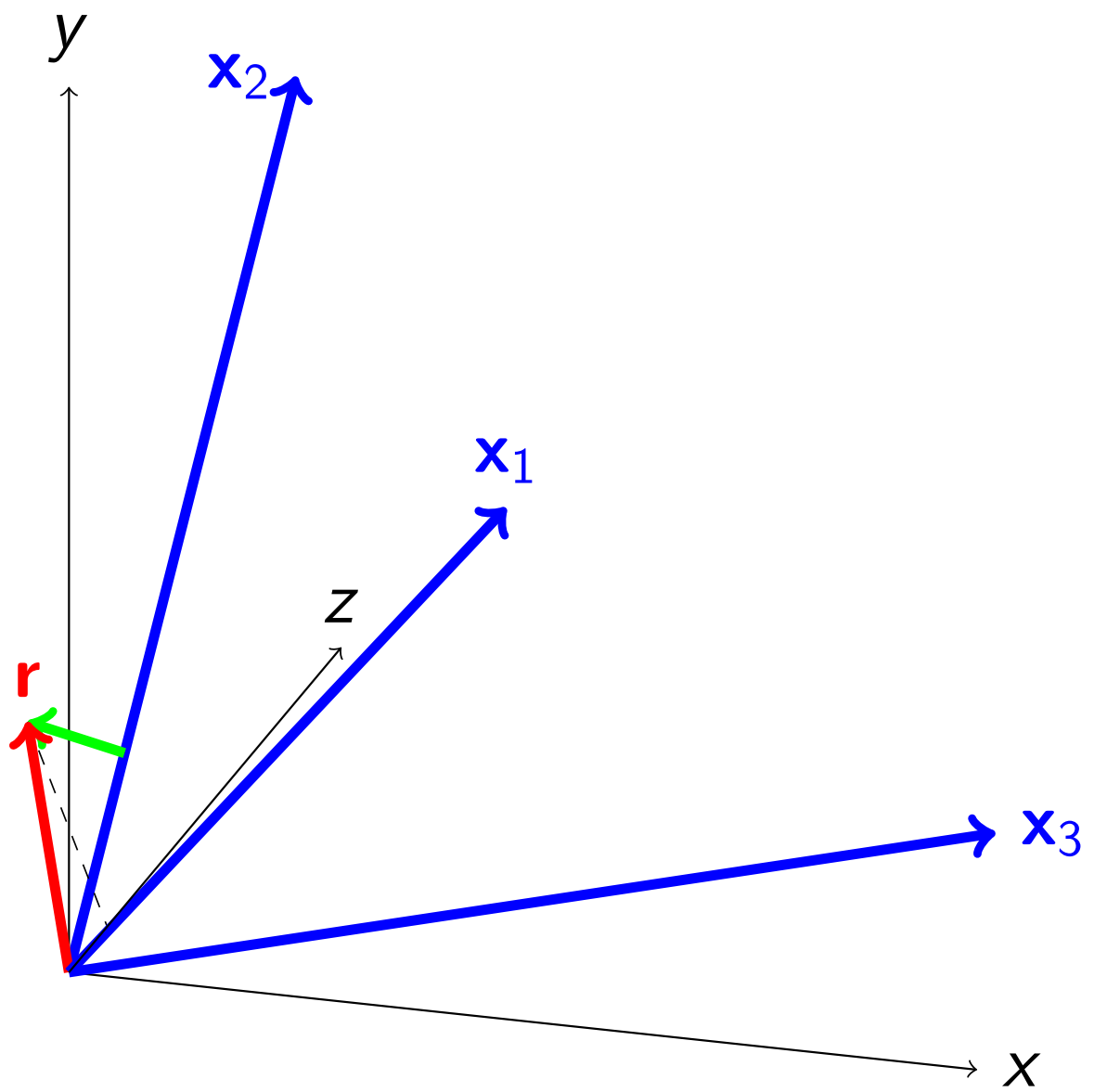
Matching Pursuit

$$\beta = (0, 0, 0.75)$$



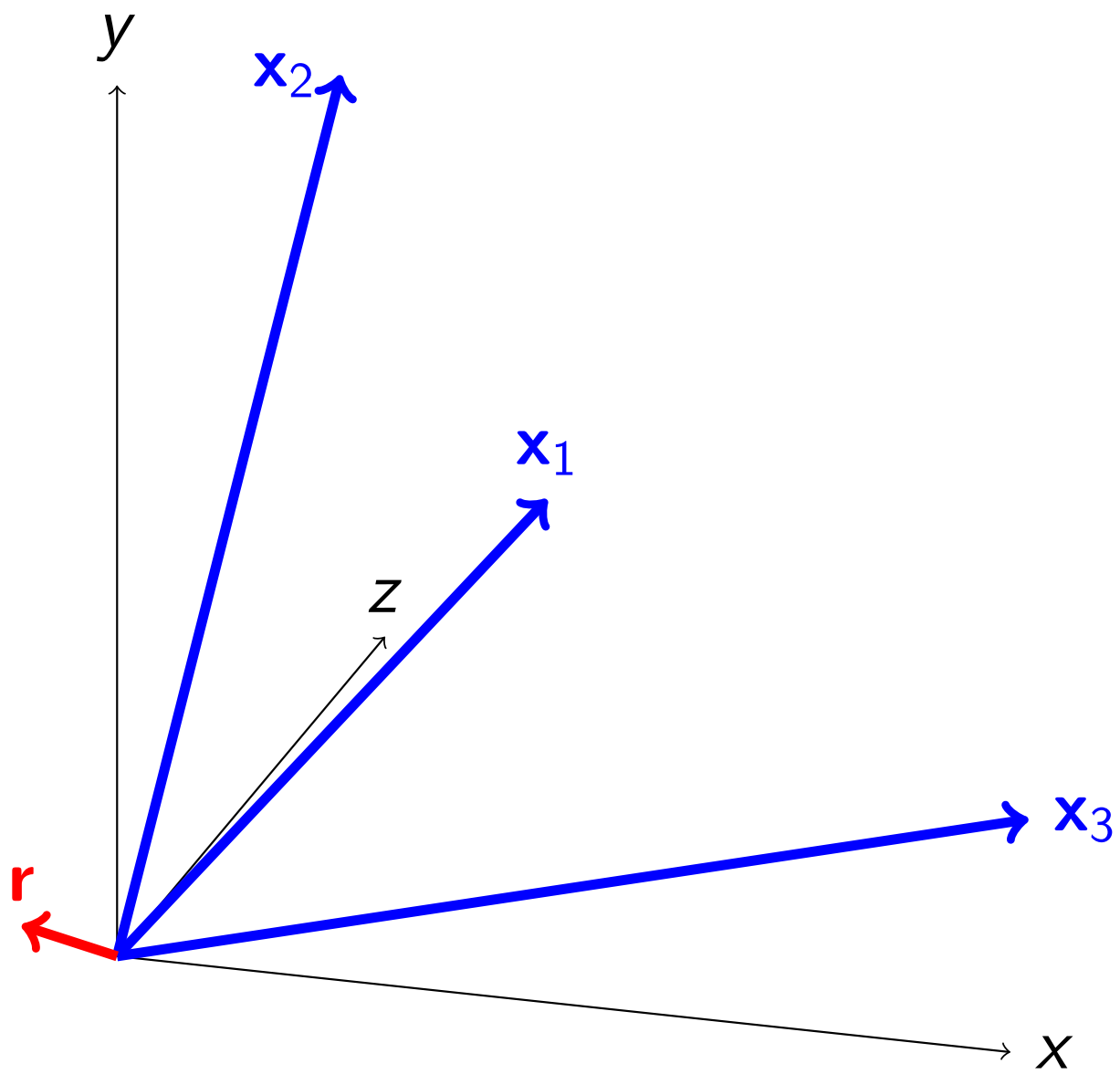
Matching Pursuit

$$\beta = (0, 0, 0.75)$$



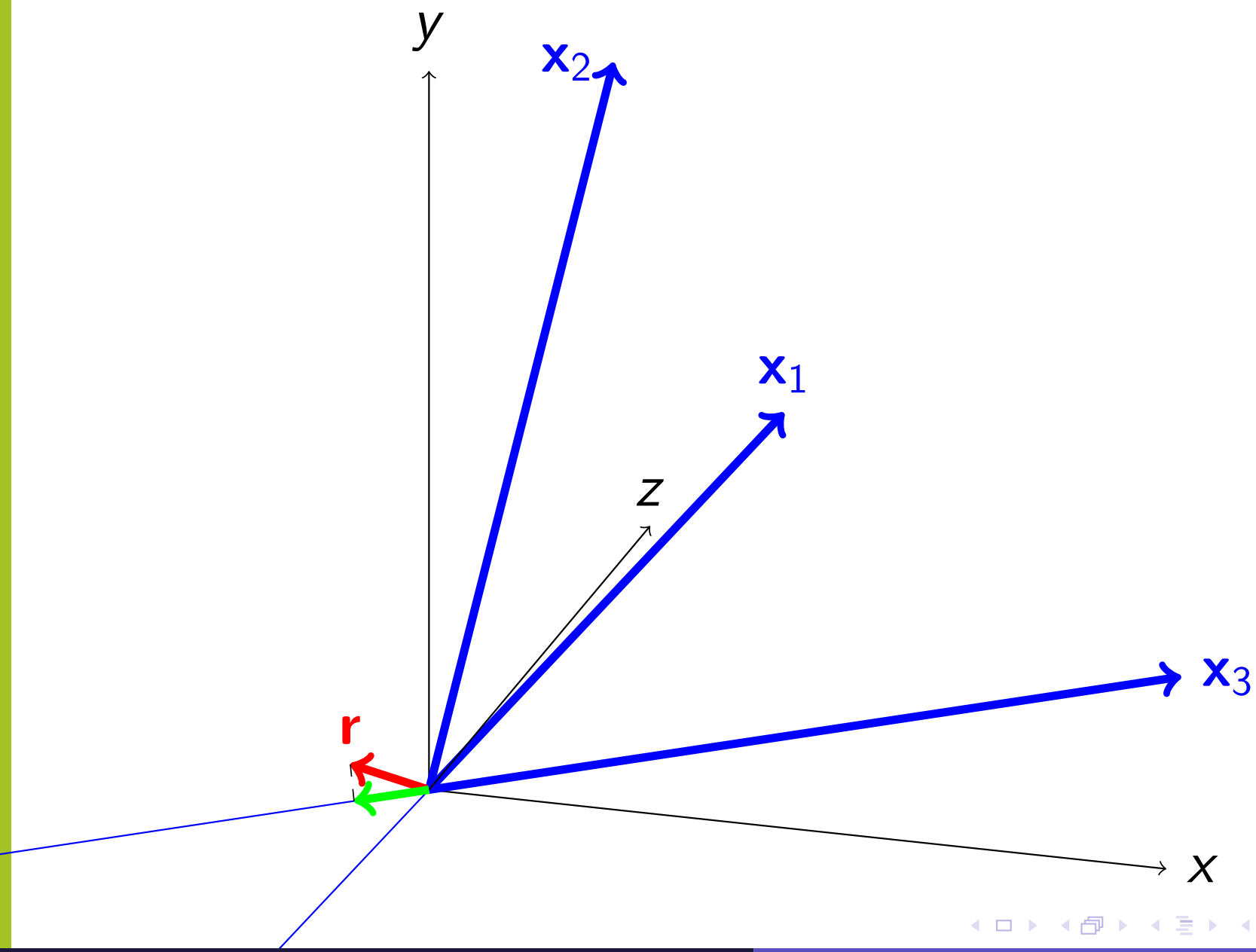
Matching Pursuit

$$\beta = (0, 0.24, 0.75)$$



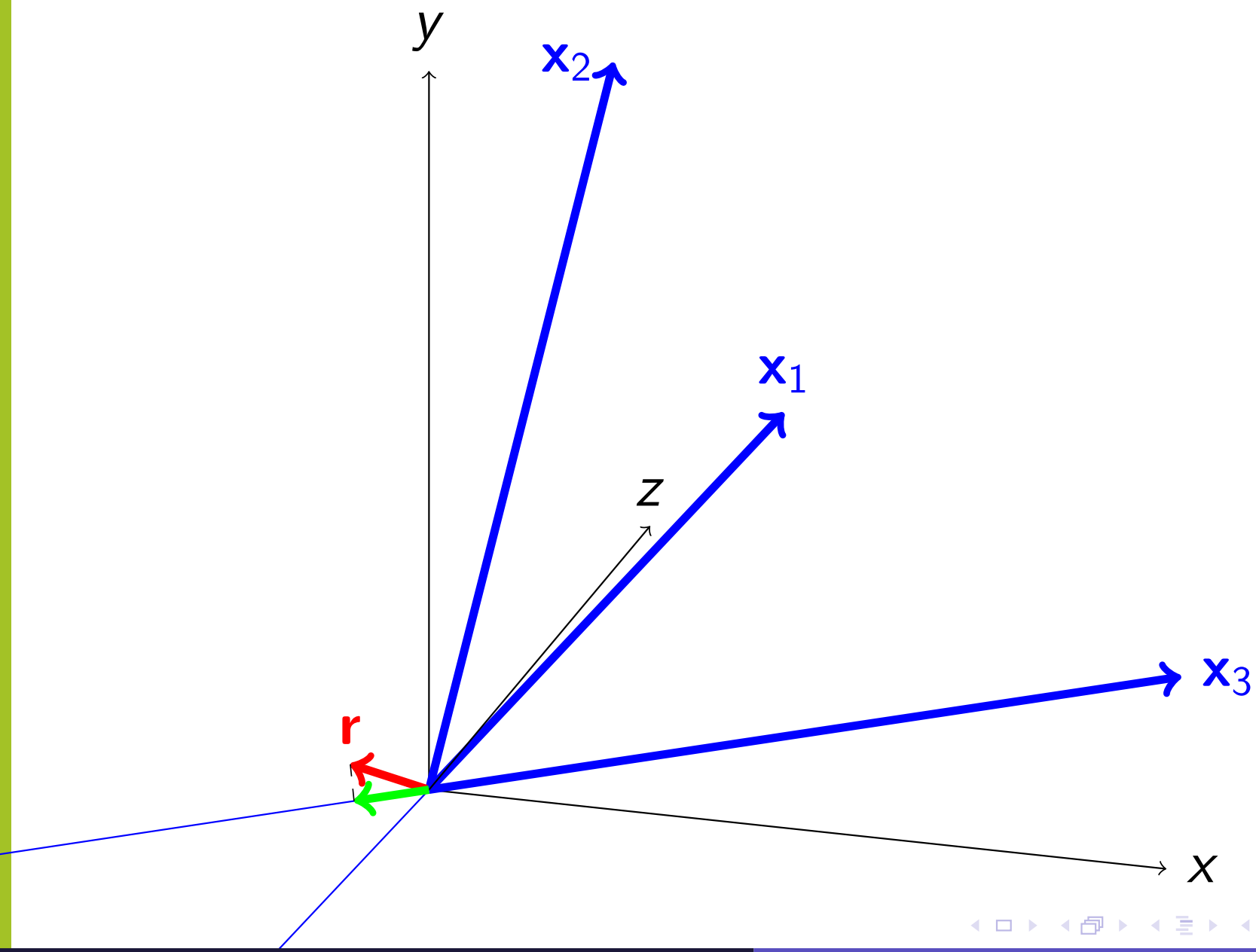
Matching Pursuit

$$\beta = (0, 0.24, 0.75)$$



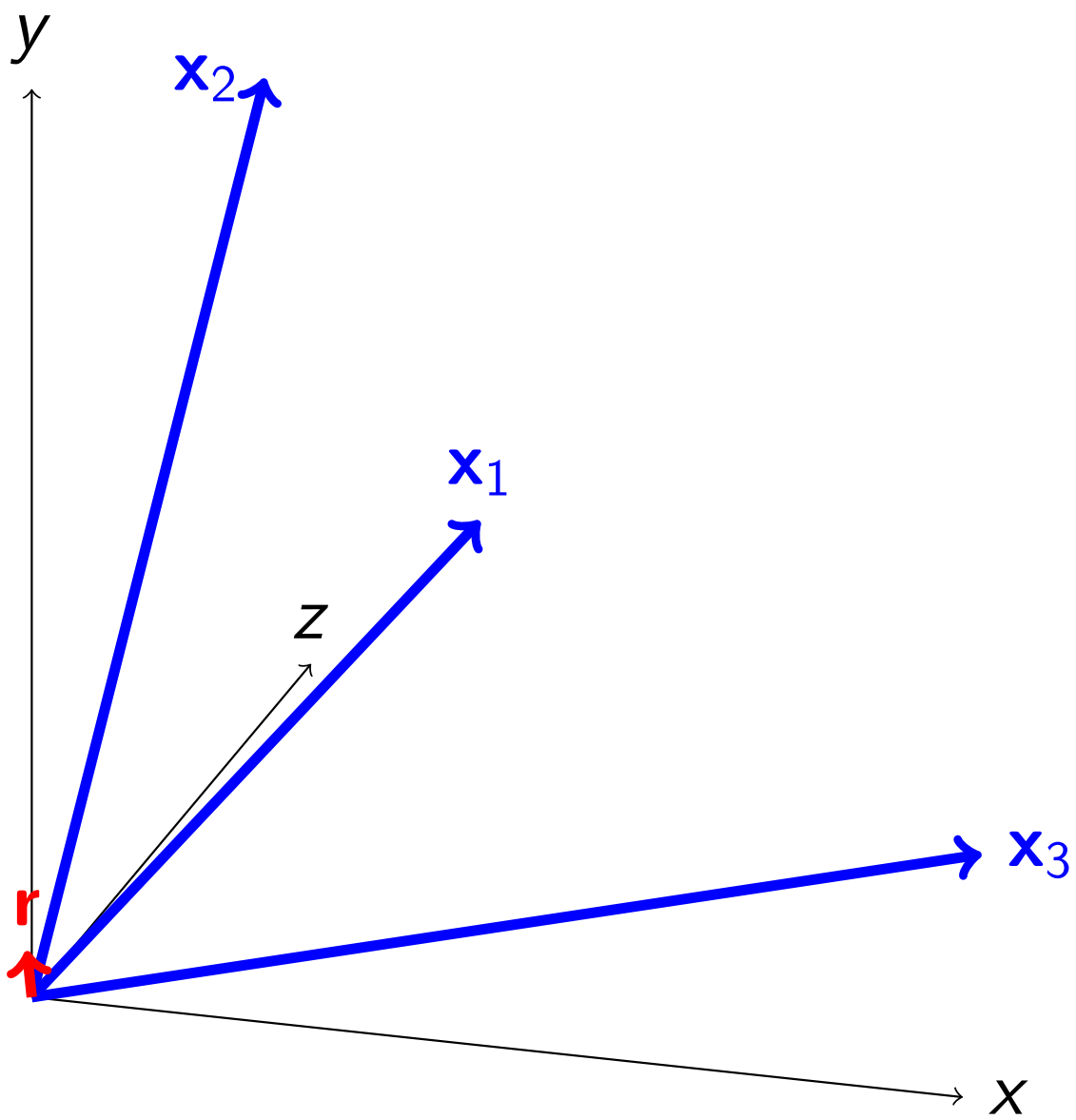
Matching Pursuit

$$\beta = (0, 0.24, 0.75)$$



Matching Pursuit

$$\beta = (0, 0.24, 0.65)$$



Matching Pursuit

$$\min_{\beta \in \mathbb{R}^p} \| \underbrace{\mathbf{y} - \mathbf{X}\beta}_{\mathbf{r}} \|_2^2 \quad \text{s.t.} \quad \|\beta\|_0 \leq L$$

1: $\beta \leftarrow 0$
2: $\mathbf{r} \leftarrow \mathbf{y}$ (residual).
3: **while** $\|\beta\|_0 < L$ **do**
4: Select the predictor with maximum correlation with the residual

$$\hat{\jmath} \leftarrow \arg\max_{j=1,\ldots,p} |\mathbf{x}^{j\top} \mathbf{r}|$$

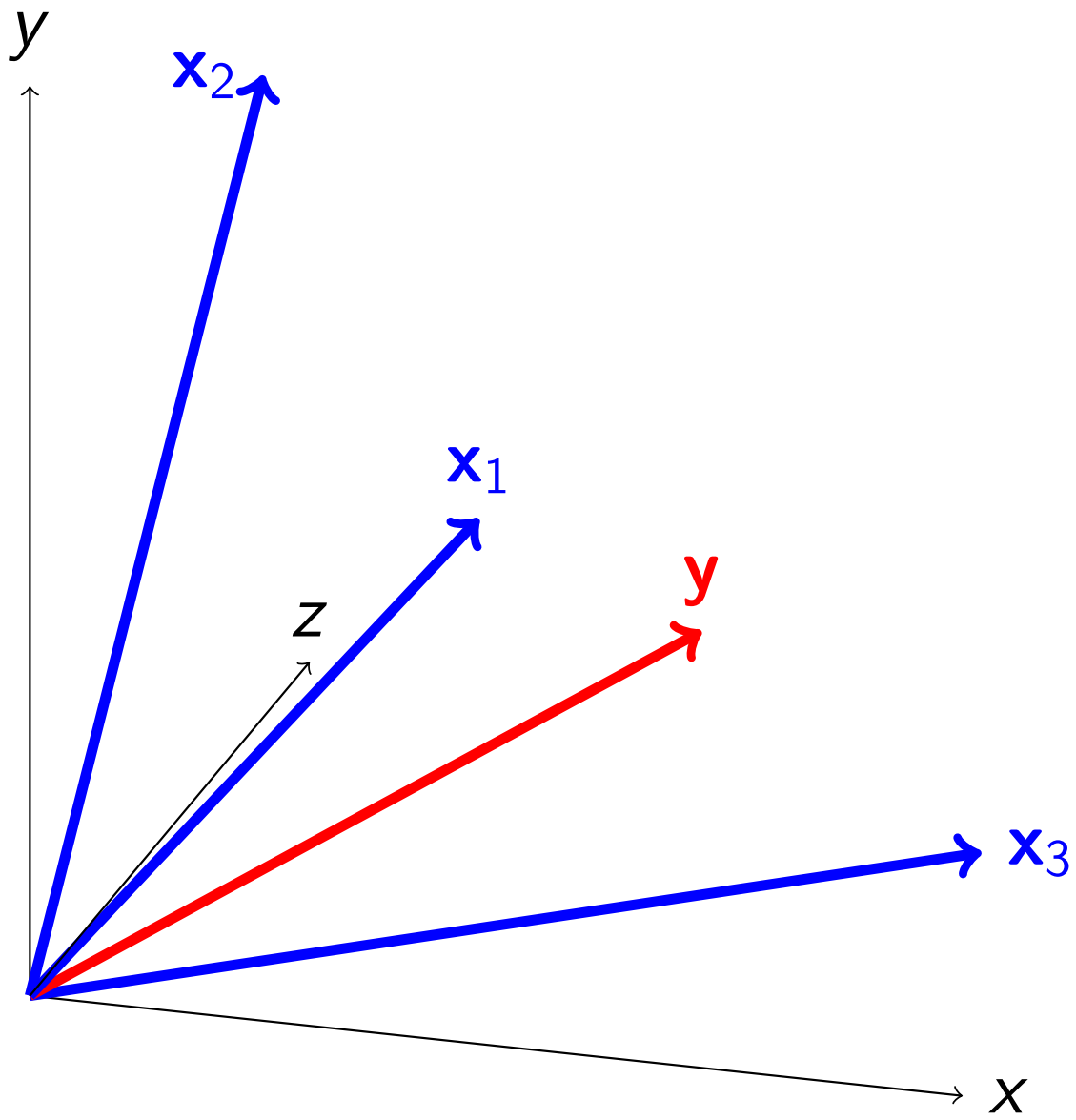
5: Update the residual and the coefficients

$$\begin{aligned} \beta_{\hat{\jmath}} &\leftarrow \beta_{\hat{\jmath}} + \mathbf{x}^{\hat{\jmath}\top} \mathbf{r} \\ \mathbf{r} &\leftarrow \mathbf{r} - (\mathbf{x}^{\hat{\jmath}\top} \mathbf{r}) \mathbf{x}^{\hat{\jmath}} \end{aligned}$$

6: **end while**

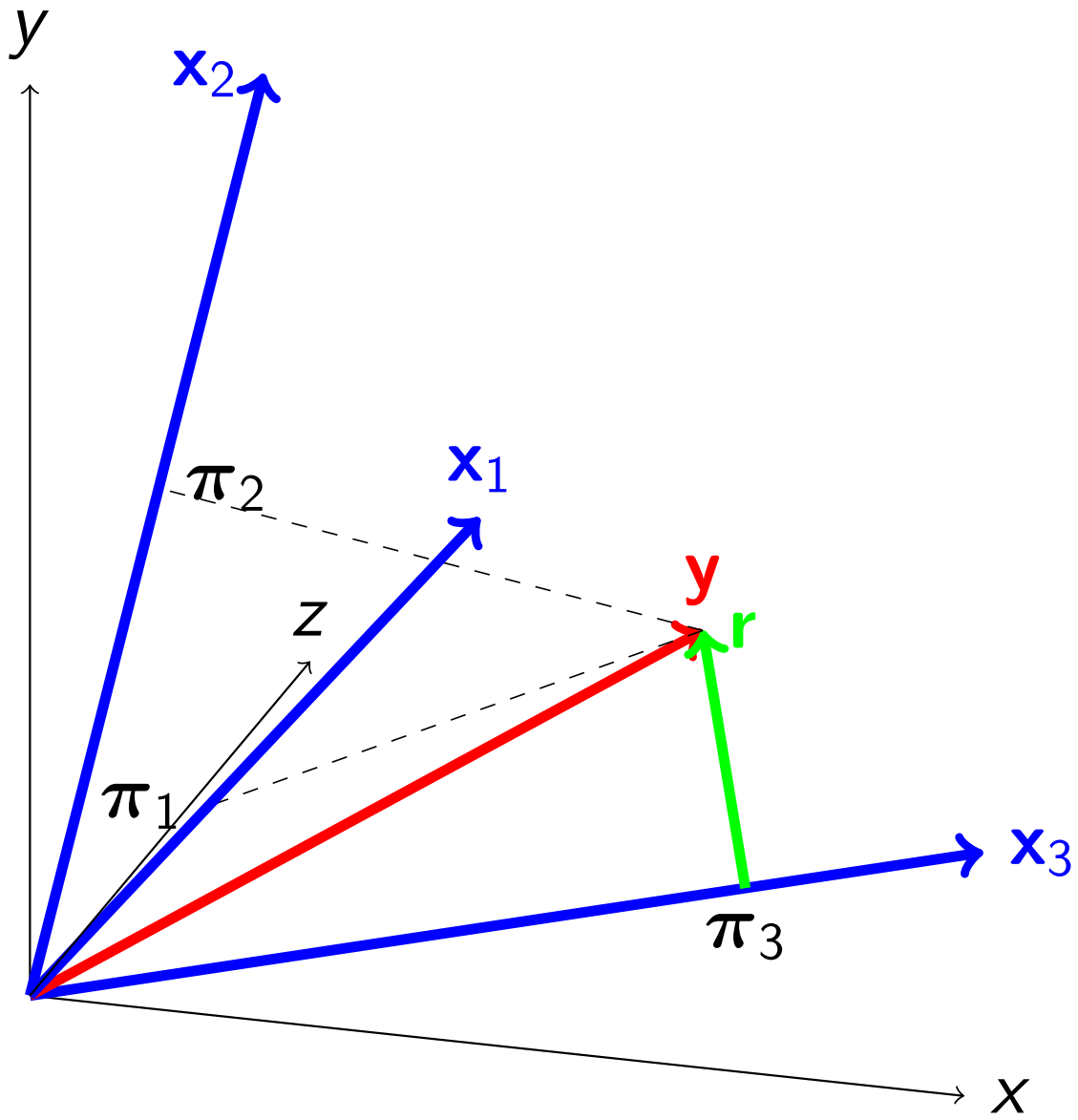
Orthogonal Matching Pursuit

$$\boldsymbol{\beta} = (0, 0, 0)$$
$$\Gamma = \emptyset$$



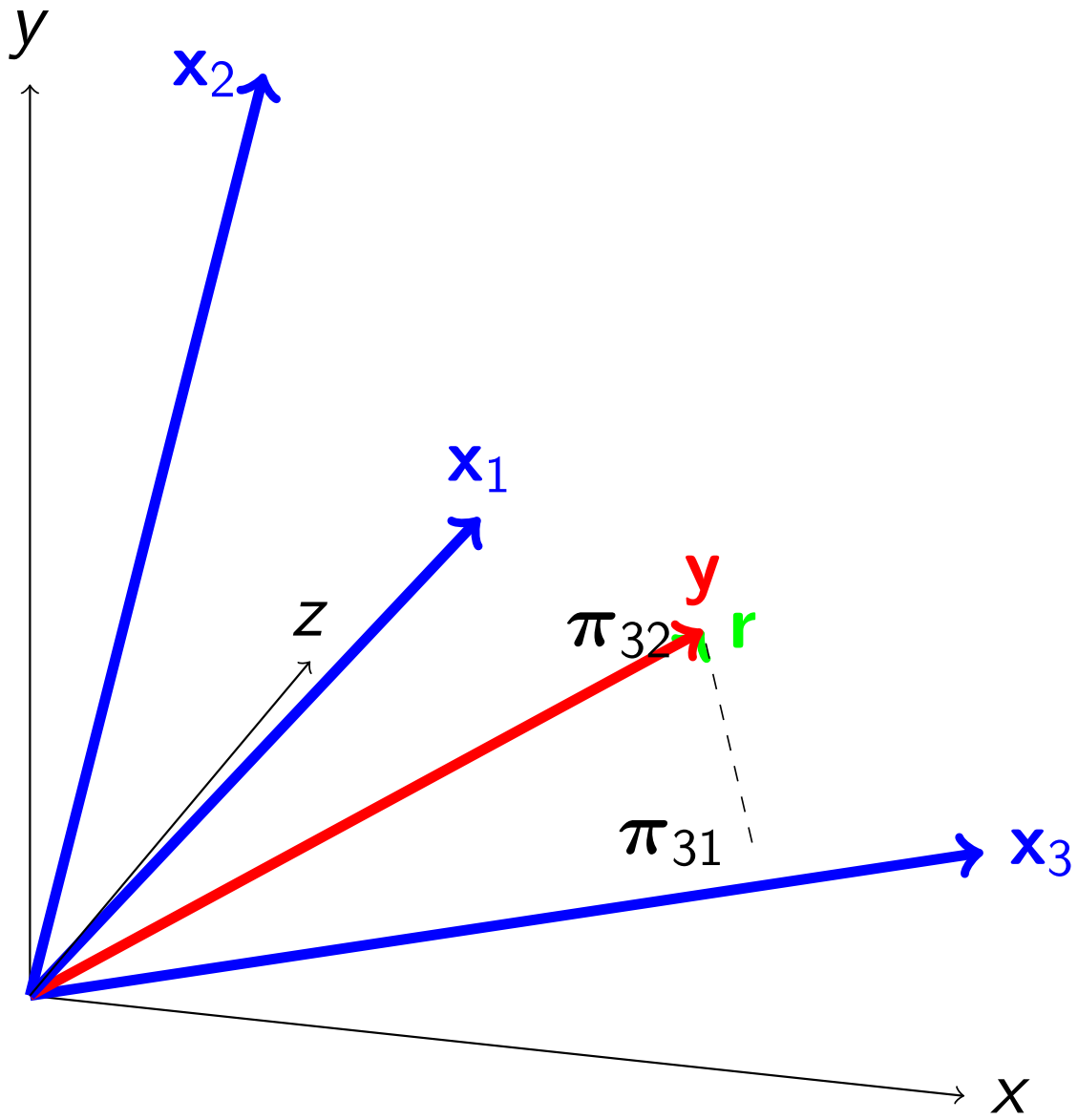
Orthogonal Matching Pursuit

$$\beta = (0, 0, 0.75)$$
$$\Gamma = \{3\}$$



Orthogonal Matching Pursuit

$$\beta = (0, 0.29, 0.63)$$
$$\Gamma = \{3, 2\}$$



Orthogonal Matching Pursuit

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 \quad \text{s.t.} \quad \|\boldsymbol{\beta}\|_0 \leq L$$

1: $\Gamma = \emptyset$.
2: **for** *iter* $= 1, \ldots, L$ **do**
3: Select the predictor which most reduces the objective

$$\hat{\imath} \leftarrow \arg\min_{i \in \Gamma^c} \left\{ \min_{\boldsymbol{\beta}'} \|\mathbf{y} - \mathbf{X}_{\Gamma \cup \{i\}} \boldsymbol{\beta}'\|_2^2 \right\}$$

4: Update the active set: $\Gamma \leftarrow \Gamma \cup \{\hat{\imath}\}$.
5: Update the residual (orthogonal projection)

$$\mathbf{r} \leftarrow (\mathbf{I} - \mathbf{X}_\Gamma (\mathbf{X}_\Gamma^\top \mathbf{X}_\Gamma)^{-1} \mathbf{X}_\Gamma^\top)\mathbf{y}.$$

6: Update the coefficients

$$\boldsymbol{\beta}_\Gamma \leftarrow (\mathbf{X}_\Gamma^\top \mathbf{X}_\Gamma)^{-1} \mathbf{X}_\Gamma^\top \mathbf{y}.$$

7: **end for**

Orthogonal Matching Pursuit

The keys for a good implementation

- If available, use Gram matrix $\mathbf{G} = \mathbf{X}^\top \mathbf{X}$,
- Maintain the computation of $\mathbf{X}^\top \mathbf{r}$ for each signal,
- Maintain a Cholesky decomposition of $(\mathbf{X}_\Gamma^\top \mathbf{X}_\Gamma)^{-1}$ for each signal.

The total complexity for decomposing n L-sparse signals of size m with a dictionary of size p is

$$\underbrace{O(p^2 m)}_{\text{Gram matrix}} + \underbrace{O(nL^3)}_{\text{Cholesky}} + \underbrace{O(n(pm + pL^2))}_{\mathbf{X}^T\mathbf{r}} = O(np(m + L^2))$$

It is also possible to use the matrix inversion lemma instead of a Cholesky decomposition (same complexity, but less numerical stability).

Example with the software SPAMS

Software available at `http://www.di.ens.fr/willow/SPAMS/`

```
>> I=double(imread('data/lena.eps'))/255;
>> %extract all patches of I
>> X=im2col(I,[8 8],'sliding');
>> %load a dictionary of size 64 x 256
>> D=load('dict.mat');
>>
>> %set the sparsity parameter L to 10
>> param.L=10;
>> alpha=mexOMP(X,D,param);
```

On a 4-cores 3.6Ghz machine: **150000 signals processed per second!**

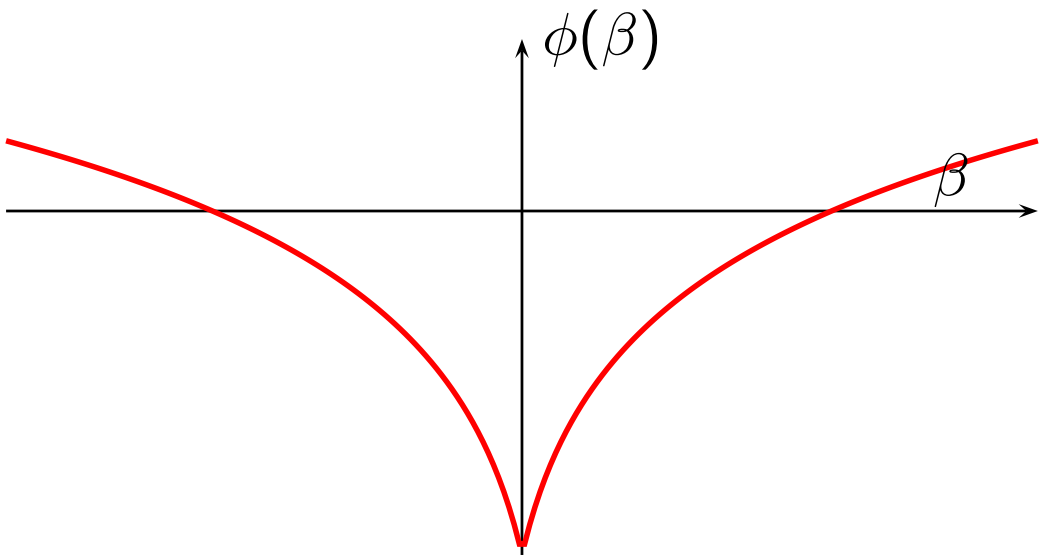
DC (difference of convex) - Programming

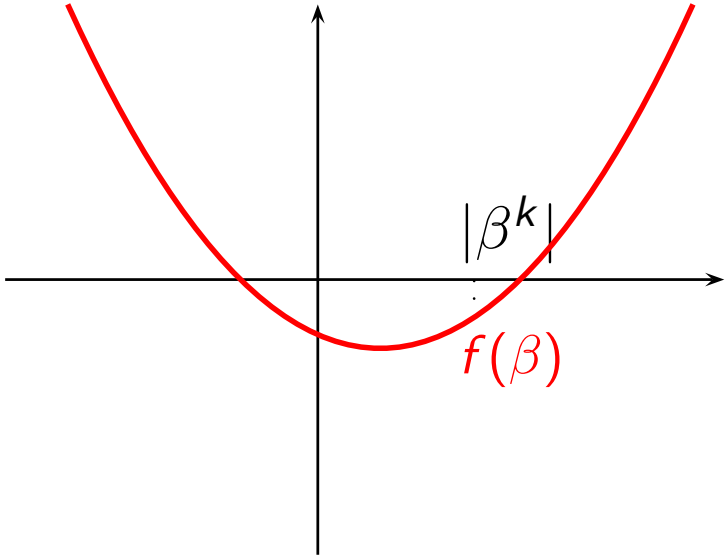
Remember? Concave functions with a kink at zero

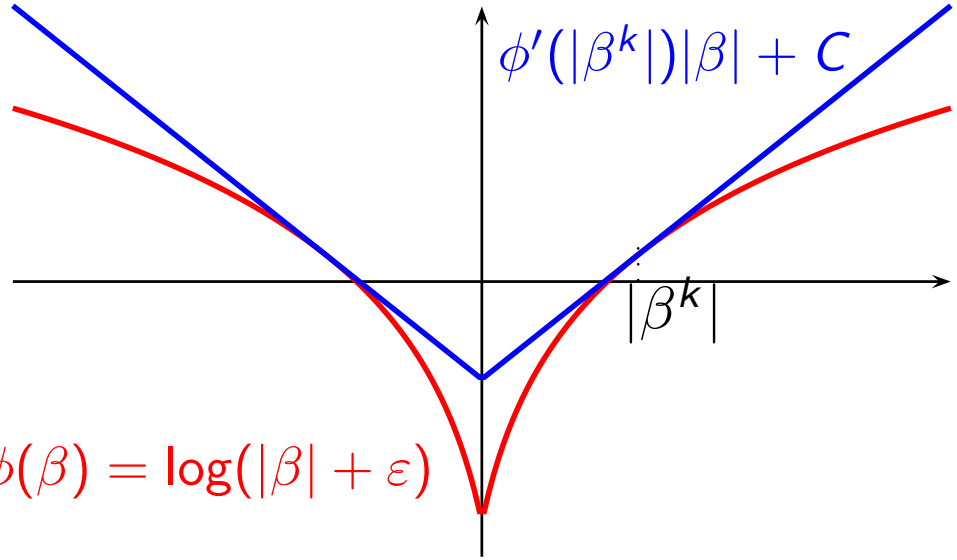
$\Omega(\boldsymbol{\beta}) = \sum_{j=1}^{p} \phi(|\boldsymbol{\beta}_j|)$.

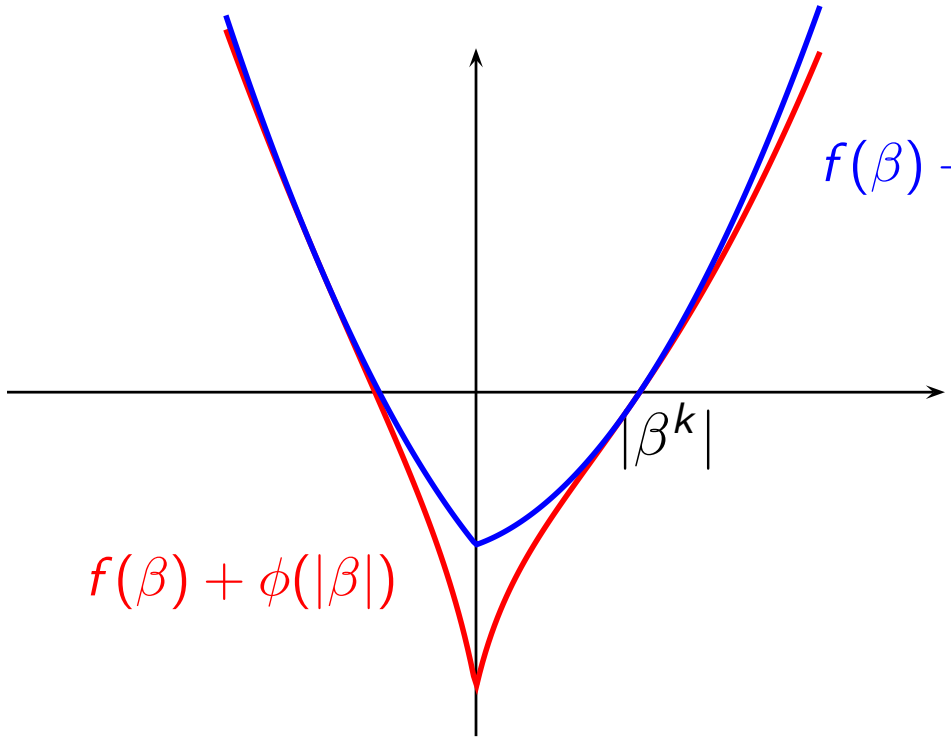
- ℓ_q-"pseudo-norm", with $0 < q < 1$: $\Omega(\boldsymbol{\beta}) \triangleq \sum_{j=1}^{p} (|\boldsymbol{\beta}_j| + \varepsilon)^q$,
- log penalty, $\Omega(\boldsymbol{\beta}) \triangleq \sum_{j=1}^{p} \log(|\boldsymbol{\beta}_j| + \varepsilon)$,

ϕ is any function that looks like this:




$|\beta^k|$
$f(\beta)$


$\phi'(|\beta^k|)|\beta| + C$
$|\beta^k|$
$\phi(\beta) = \log(|\beta| + \varepsilon)$


$f(\beta) + \phi'(|\beta^k|)|\beta| + C$
$|\beta^k|$
$f(\beta) + \phi(|\beta|)$

DC (difference of convex) - Programming

$$\min_{\beta \in \mathbb{R}^p} f(\beta) + \lambda \sum_{j=1}^{p} \phi(|\beta_j|).$$

This problem is non-convex. f is convex, and ϕ is concave on $\mathbb{R}^+$.
if β^k is the current estimate at iteration k, the algorithm solves

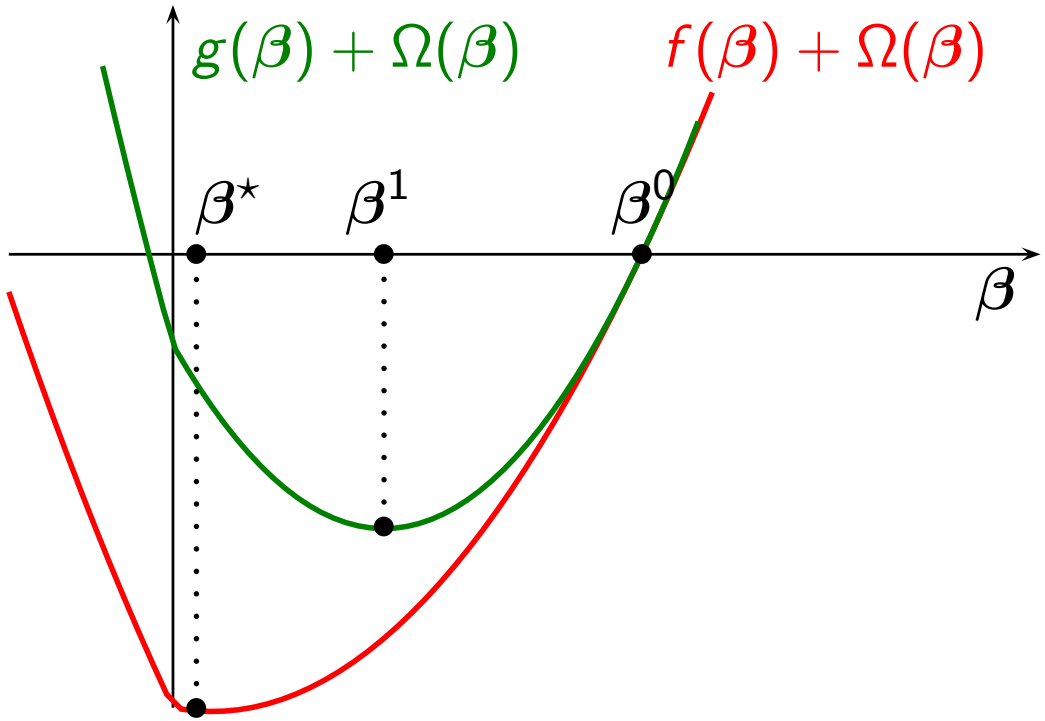
$$\beta^{k+1} \leftarrow \arg\min_{\beta \in \mathbb{R}^p} \left[f(\beta) + \lambda \sum_{j=1}^{p} \psi'(|\beta_j^k|)|\beta_j| \right],$$

which is a **reweighted**-ℓ_1 problem.
Warning: It does not solve the non-convex problem, only provides a stationary point.
In practice, each iteration sets to zero small coefficients. After $2-3$ iterations, the result does not change much.

The Proximal Gradient Method

This inequality is also true for non-convex functions!

If ∇f is L-Lipschitz continuous



- $f(\beta) + \Omega(\beta) \leq f(\beta^0) + \nabla f(\beta^0)^\top(\beta - \beta^0) + \frac{L}{2}\|\beta - \beta^0\|_2^2 + \Omega(\beta)$;

The Proximal Gradient Method

As before, the method consits of the following iteration

$$\boxed{\beta^t \leftarrow \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \left\| \beta^{t-1} - \frac{1}{L} \nabla f(\beta^{t-1}) - \beta \right\|_2^2 + \Omega(\beta).}$$

- It requires computing efficiently the **proximal operator** of Ω.

$$\alpha \mapsto \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \|\alpha - \beta\|_2^2 + \Omega(\beta).$$

- For the ℓ_0-penalty ($\Omega(\beta) = \lambda \|\beta\|_0$), this amounts to a hard-thresholding:

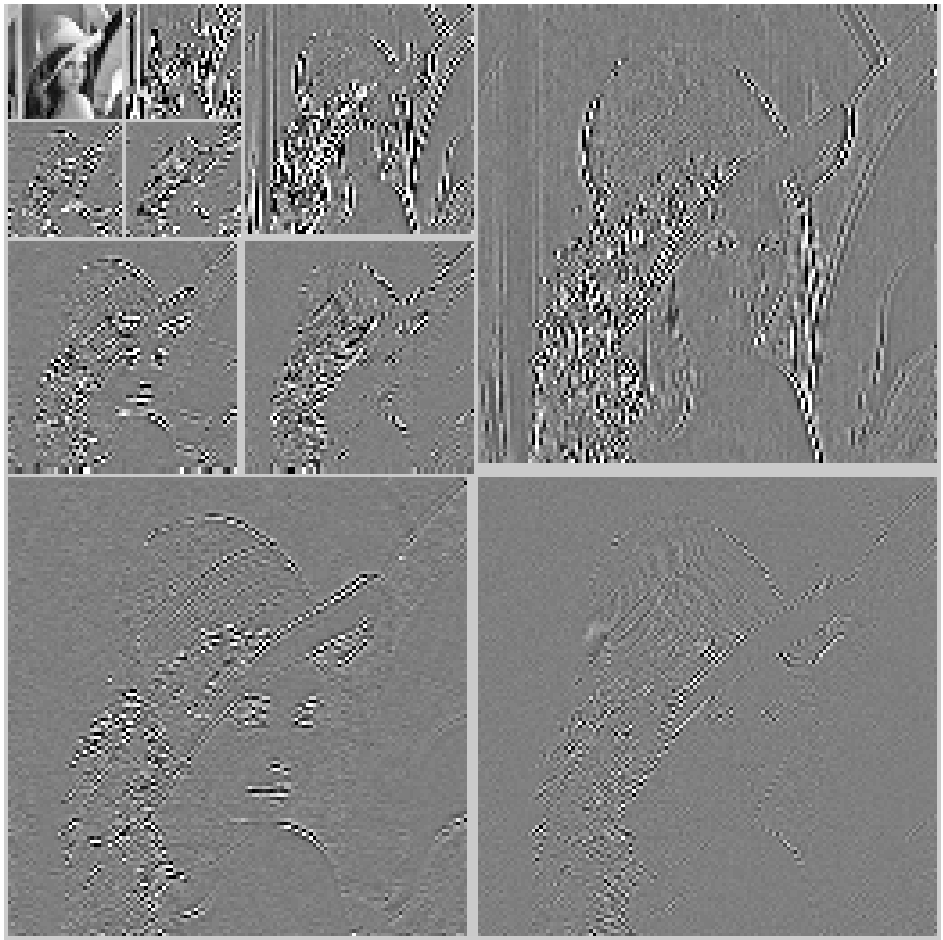
$$\beta_j^\star = 1_{|\alpha_j| \geq \sqrt{2\lambda}} \alpha_j.$$

Trick: start with a high value for λ, and gradually decrease it.

Part IV: Structured Sparsity

Wavelet coefficients

- Zero-tree wavelets coding [Shapiro, 1993];
- block thresholding [Cai, 1999].



Sparse linear models for natural image patches

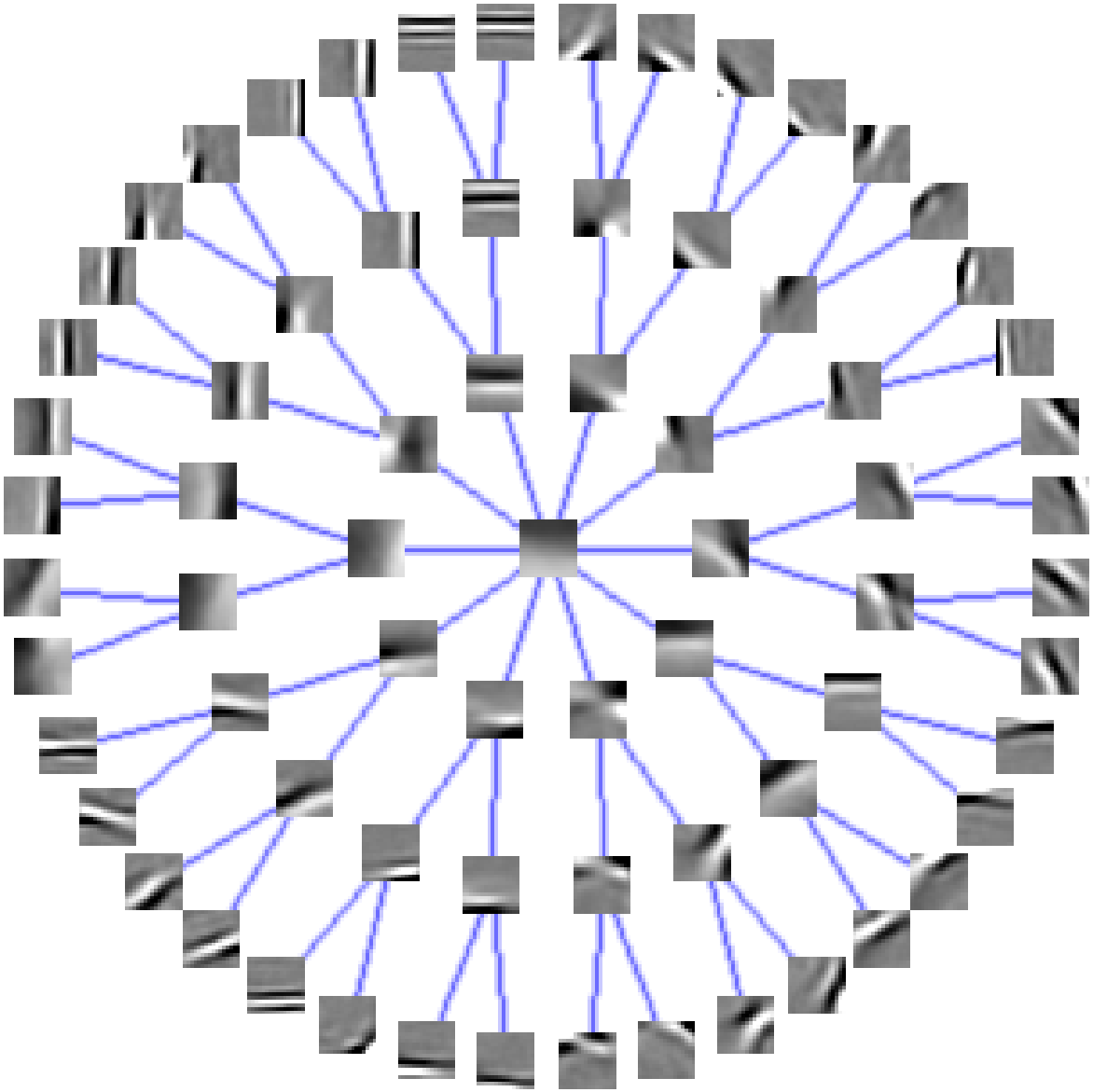
Image restoration

Sparse linear models for natural image patches

Image restoration

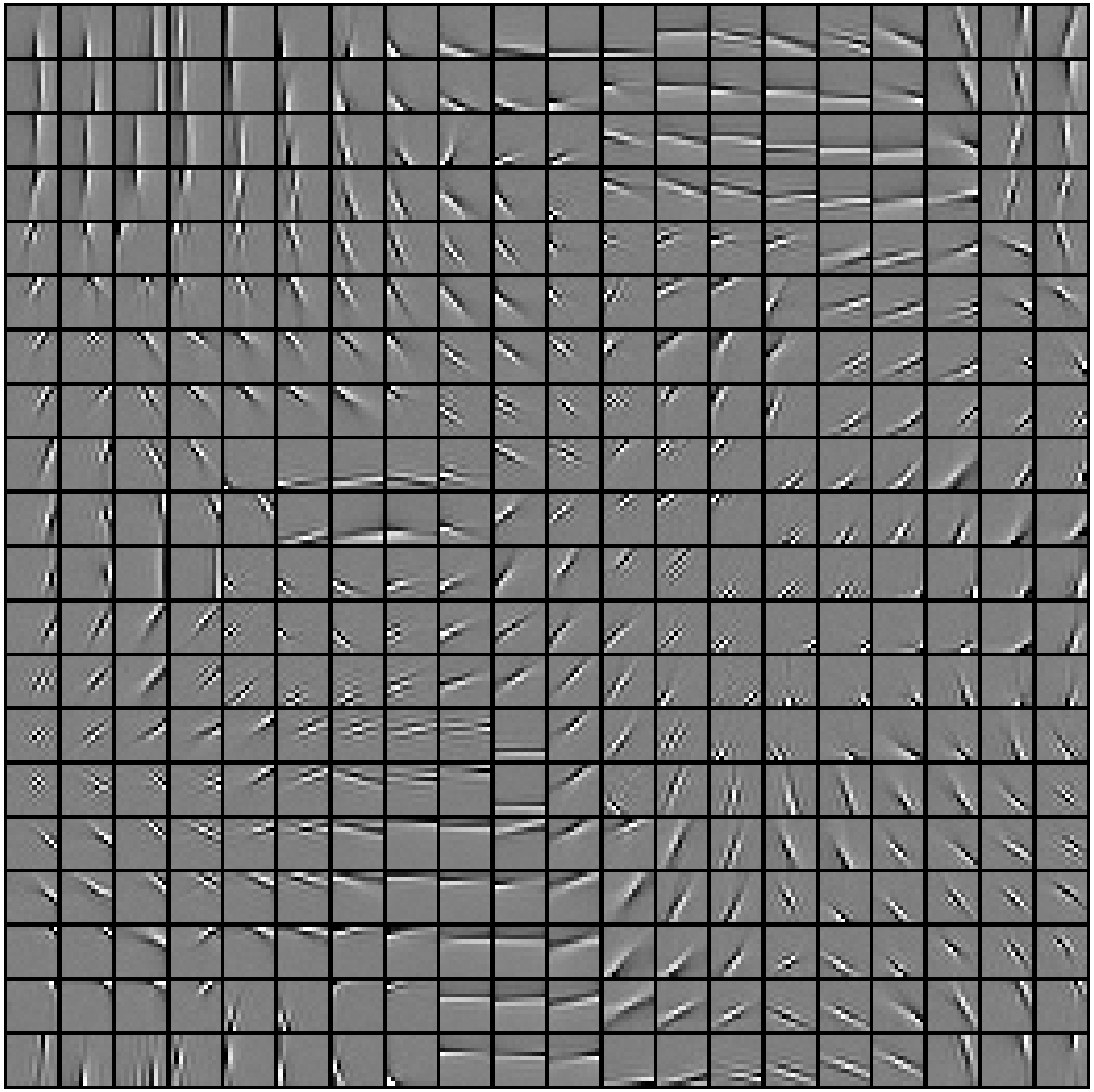
Structured dictionary for natural image patches

[Jenatton, Mairal, Obozinski, and Bach, 2010]



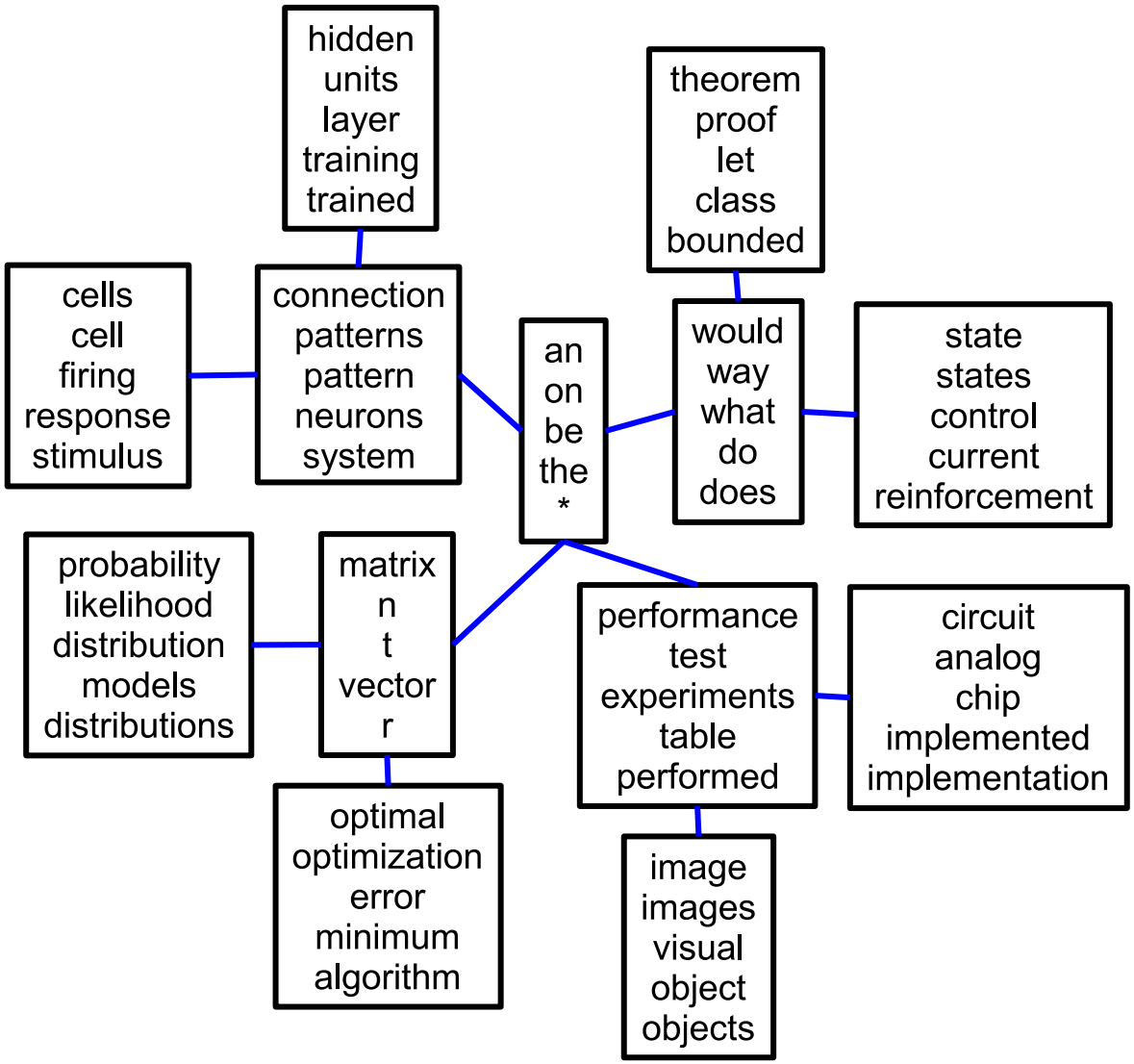
Structured dictionary for natural image patches

[Mairal, Jenatton, Obozinski, and Bach, 2011]



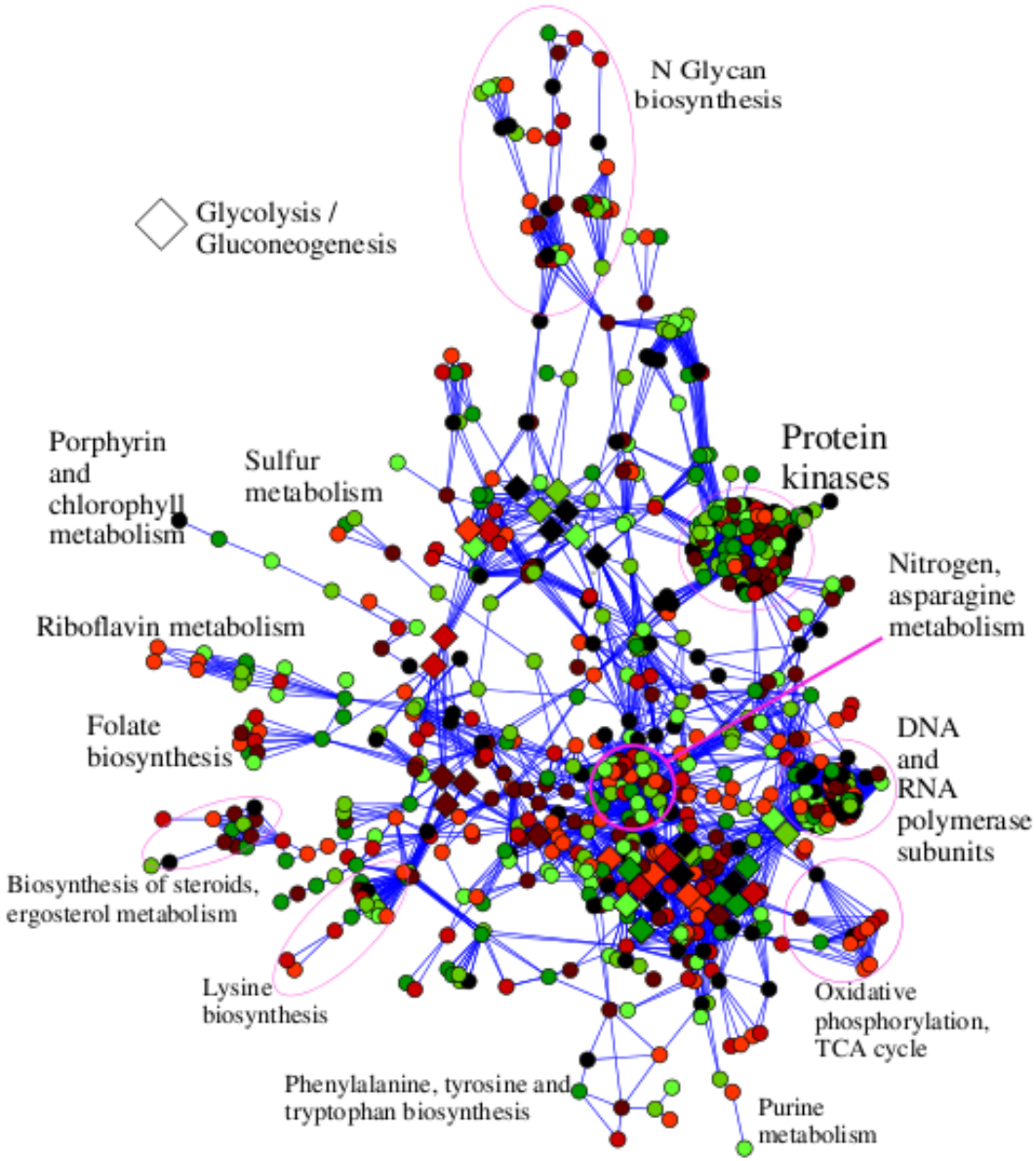
Tree of topics

[Jenatton, Mairal, Obozinski, and Bach, 2010]



Metabolic network of the budding yeast

from Rapaport, Zinovyev, Dutreix, Barillot, and Vert [2007]



Metabolic network of the budding yeast

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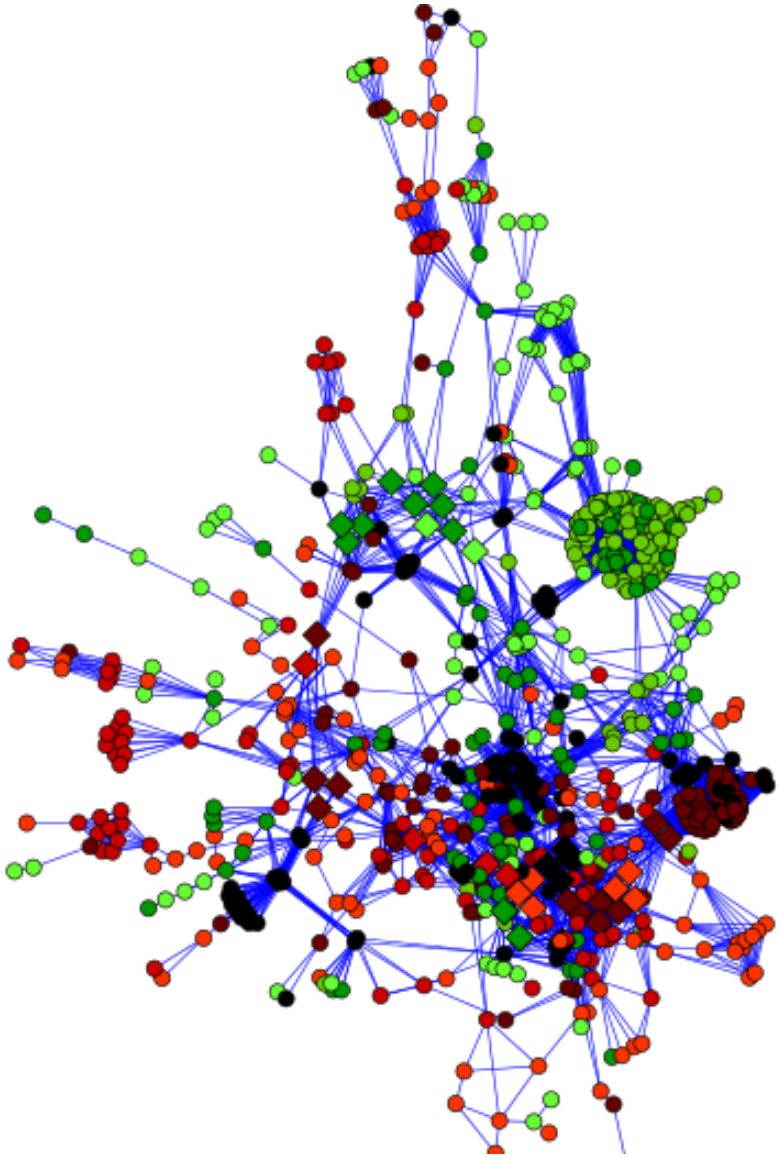

Questions about structured sparsity

$$\min_{\beta \in \mathbb{R}^p} \underbrace{f(\beta)}_{\text{convex, smooth}} + \underbrace{\lambda \Omega(\beta)}_{\text{regularization}},$$

Ω should encode some a priori knowledge about β.

☺ In this part, we will see

- how to design structured sparsity-inducing functions Ω;
- How to solve the corresponding estimation/inverse problems.

☹ out of the scope of this part:

- consistency, recovery, theoretical properties (statistics...)

In 3D.

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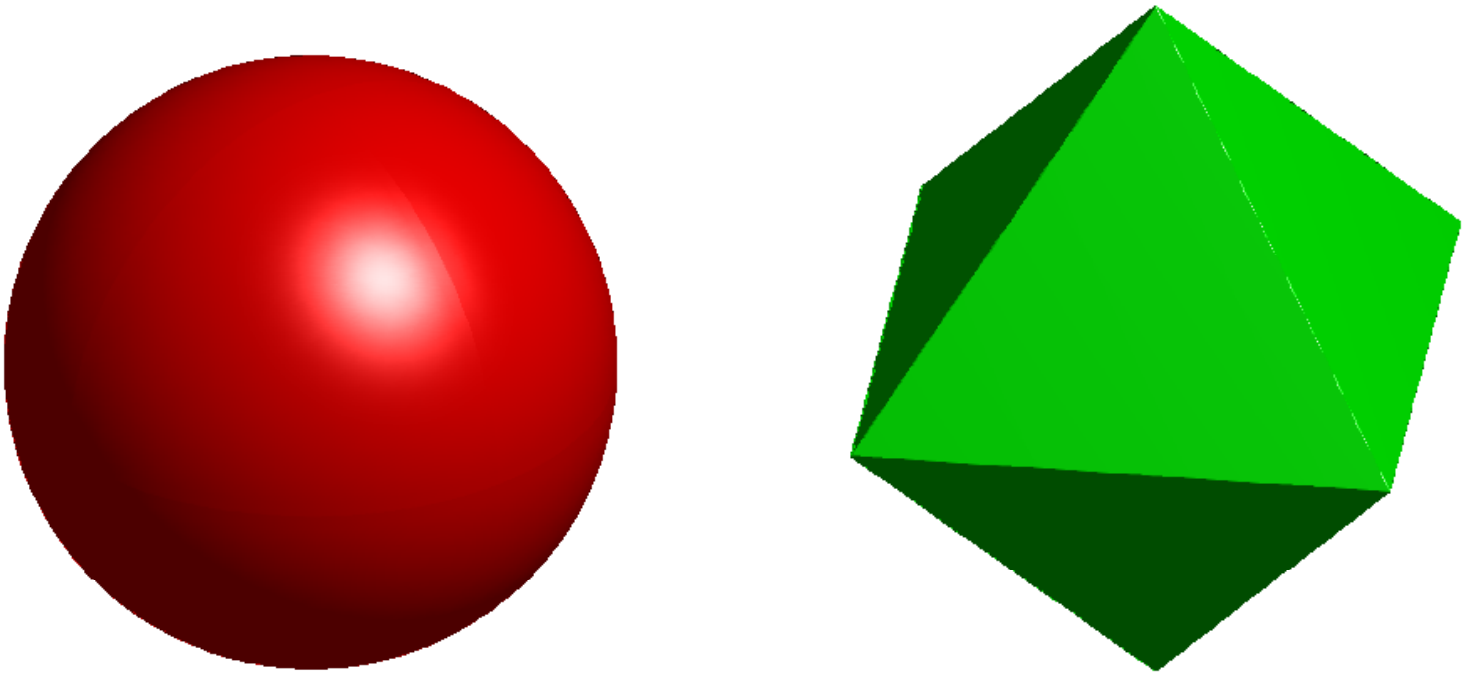

What about more complicated norms?

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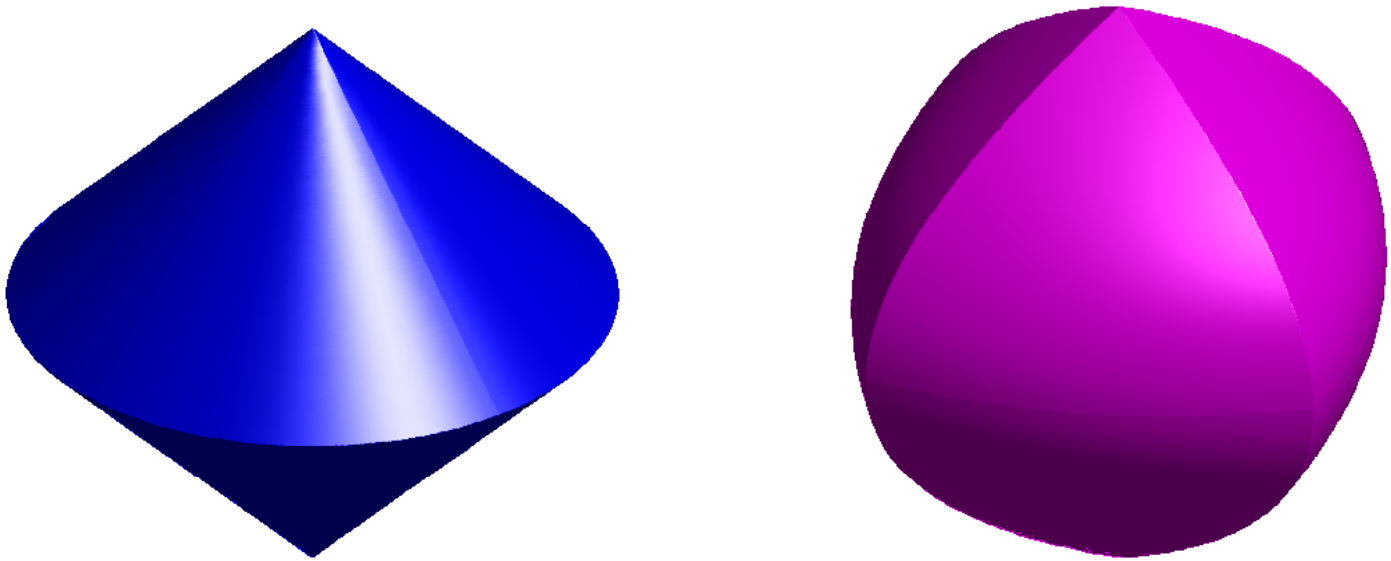

What about more complicated norms?

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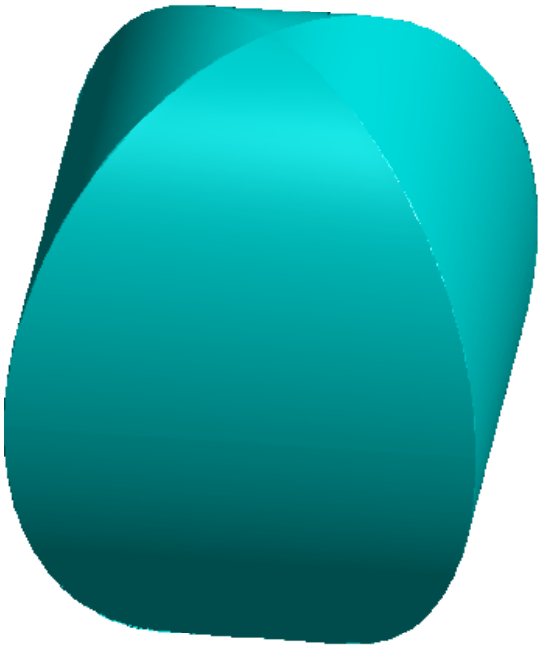
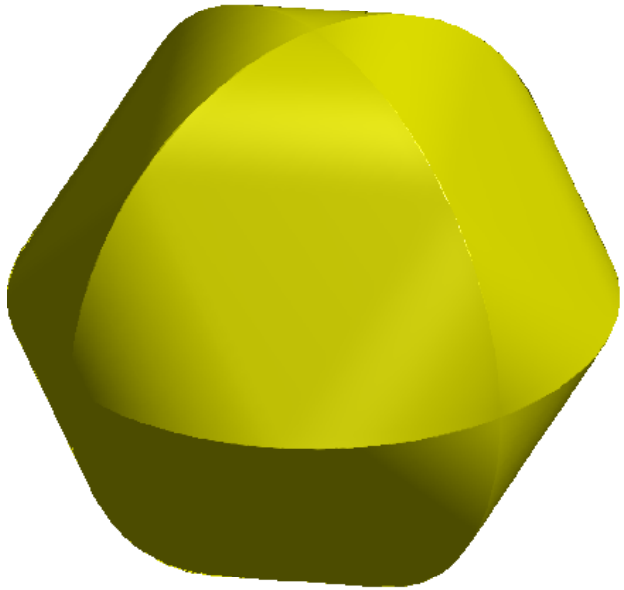


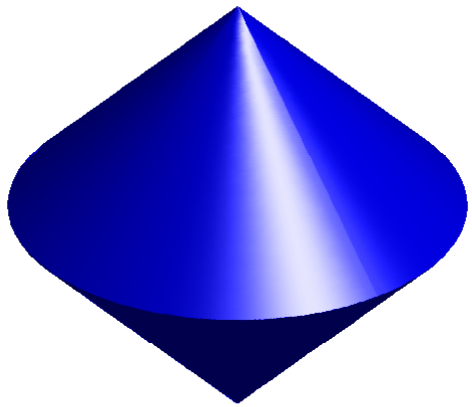


Group Lasso

Turlach et al. [2005], Yuan and Lin [2006], Zhao et al. [2009]

$$\text{the } \ell_1/\ell_q\text{-norm}: \qquad \Omega(\beta) = \sum_{g \in \mathcal{G}} \|\beta_g\|_q.$$

- $\mathcal{G}$ is a **partition** of $\{1, \ldots, p\}$;
- $q = 2$ or $q = \infty$ in practice;
- can be interpreted as the ℓ_1-norm of $[\|\beta_g\|_q]_{g \in \mathcal{G}}$.



$$\Omega(\beta) = \|\beta_{\{1,2\}}\|_2 + |\beta_3|.$$

Structured sparsity with overlapping groups

Warning: Under the name "structured sparsity" appear in fact significantly different formulations!

1. non-convex
   - zero-tree wavelets [Shapiro, 1993];
   - predefined collection of sparsity patterns: [Baraniuk et al., 2010];
   - **select a union of groups: [Huang et al., 2009]**;
   - structure via Markov Random Fields: [Cehver et al., 2008];
2. convex (norms)
   - **tree-structure: [Zhao et al., 2009]**;
   - **select a union of groups: [Jacob et al., 2009]**;
   - **zero-pattern is a union of groups: [Jenatton et al., 2009]**;
   - other norms: [Micchelli et al., 2011].

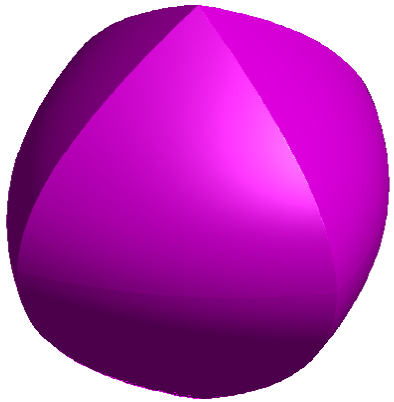
Group Lasso with overlapping groups

[Jenatton, Audibert, and Bach, 2009]

$$\Omega(\beta) = \sum_{g \in \mathcal{G}} \|\beta_g\|_q.$$

What happens when the groups overlap?

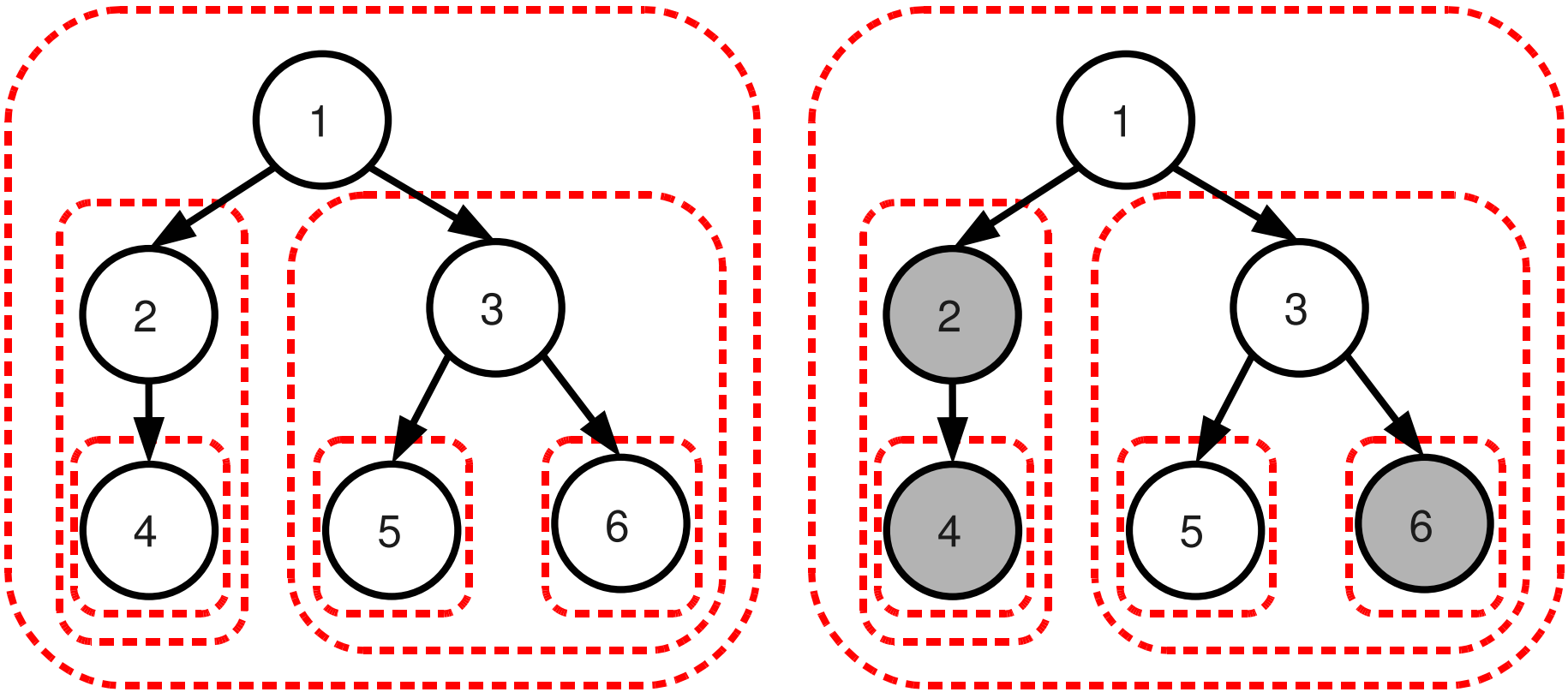
- the pattern of non-zero variables is an intersection of groups;
- the **zero pattern is a union of groups**.



$$\Omega(\beta) = \|\beta\|_2 + |\beta_2| + |\beta_3|.$$

Hierarchical Norms

[Zhao, Rocha, and Yu, 2009]



A node can be active only if its **ancestors are active**.

The selected patterns are **rooted subtrees.**

Proximal Gradient methods

A few proximal operators:

- ℓ_0-penalty: hard-thresholding;
- ℓ_1-norm: soft-thresholding;
- group-Lasso: group soft-thresholding;
- fused-lasso (1D total variation): [Hoefling, 2010];
- **hierarchical norms**: [Jenatton et al., 2010], $O(p)$ complexity;
- **overlapping group Lasso with ℓ_∞-norm**: [Mairal et al., 2010], (link with network flow optimization);

Modelling Patterns as Unions of Groups

the non-convex penalty of Huang, Zhang, and Metaxas [2009]

Warning: different point of view than in the two previous slides

$$\varphi(\boldsymbol{\beta}) \triangleq \min_{\mathcal{J} \subseteq \mathcal{G}} \left\{ \sum_{g \in \mathcal{J}} \eta_g \quad \text{s.t.} \quad \text{Supp}(\boldsymbol{\beta}) \subseteq \bigcup_{g \in \mathcal{J}} g \right\}.$$

- the penalty is **non-convex**.
- is **NP-hard** to compute (set cover problem).
- The pattern of non-zeroes in $\boldsymbol{\beta}$ is a **union** of (a few) groups.

It can be rewritten as a boolean linear program:

$$\varphi(\boldsymbol{\beta}) = \min_{\mathbf{x} \in \{0,1\}^{|\mathcal{G}|}} \left\{ \boldsymbol{\eta}^\top \mathbf{x} \quad \text{s.t.} \quad \mathbf{N}\mathbf{x} \geq \text{Supp}(\boldsymbol{\beta}) \right\}.$$

Modelling Patterns as Unions of Groups

convex relaxation and the penalty of Jacob, Obozinski, and Vert [2009]

The penalty of Huang et al. [2009]:

$$\varphi(\boldsymbol{\beta}) = \min_{\mathbf{x}\in\{0,1\}^{|\mathcal{G}|}} \left\{ \boldsymbol{\eta}^\top \mathbf{x} \;\text{ s.t. }\; \mathbf{N}\mathbf{x} \geq \text{Supp}(\boldsymbol{\beta}) \right\}.$$

A convex LP-relaxation:

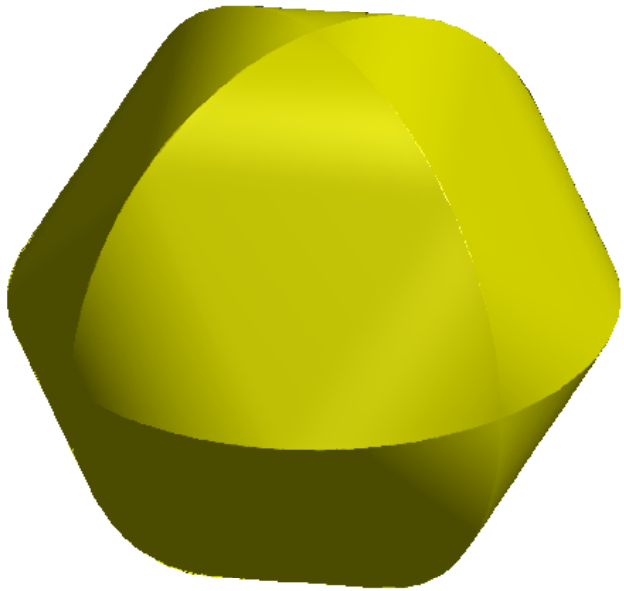
$$\psi(\boldsymbol{\beta}) \triangleq \min_{\mathbf{x}\in\mathbb{R}_+^{|\mathcal{G}|}} \left\{ \boldsymbol{\eta}^\top \mathbf{x} \;\text{ s.t. }\; \mathbf{N}\mathbf{x} \geq |\boldsymbol{\beta}| \right\}.$$

Lemma: ψ is the penalty of Jacob et al. [2009] with the ℓ_∞-norm:

$$\psi(\boldsymbol{\beta}) = \min_{(\boldsymbol{\xi}^g\in\mathbb{R}^p)_{g\in\mathcal{G}}} \sum_{g\in\mathcal{G}} \eta_g \|\boldsymbol{\xi}^g\|_\infty \;\text{ s.t. }\; \boldsymbol{\beta} = \sum_{g\in\mathcal{G}} \boldsymbol{\xi}^g \text{ and } \forall g,\ \text{Supp}(\boldsymbol{\xi}^g) \subseteq g,$$

Modelling Patterns as Unions of Groups

The norm of Jacob et al. [2009] in 3D



$\psi(\boldsymbol{\beta})$ with $\mathcal{G} = \{\{1,2\},\{2,3\},\{1,3\}\}$.

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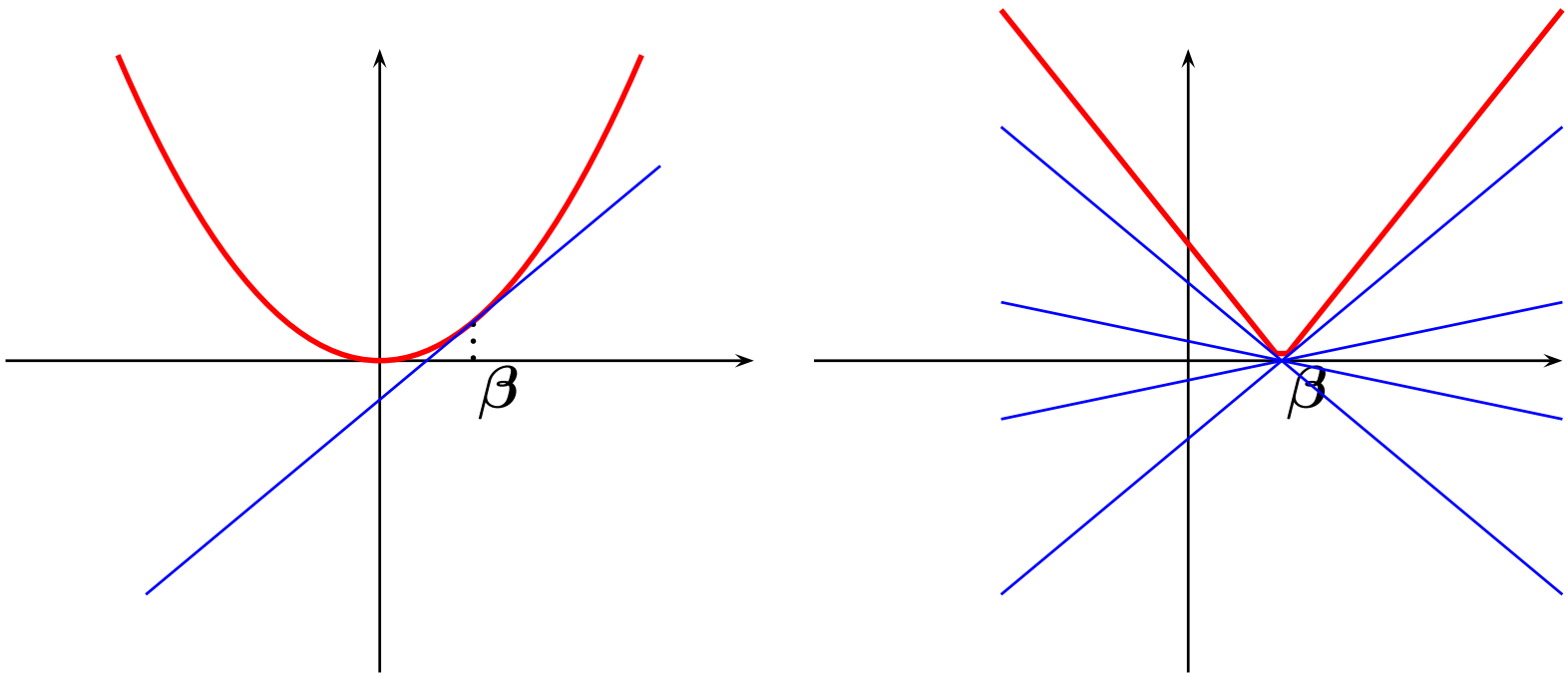
Appendix

Basic convex optimization tools: subgradients



(a) Smooth case (b) Non-smooth case

Figure: Gradients and subgradients for smooth and non-smooth functions.

$$\partial f(\beta) \triangleq \{\kappa \in \mathbb{R}^p \mid f(\beta) + \kappa^\top(\beta' - \beta) \leq f(\beta') \text{ for all } \beta' \in \mathbb{R}^p\}.$$

Basic convex optimization tools: subgradients

Some nice properties

- $\partial f(\beta) = \{g\}$ iff f differentiable at β and $g = \nabla f(\beta)$.
- many calculus rules: $\partial(\alpha f + \beta g) = \alpha \partial f + \beta \partial g$ for $\alpha, \beta > 0$.

for more details, see Boyd and Vandenberghe [2004], Bertsekas [1999], Borwein and Lewis [2006] and S. Boyd's course at Stanford.

Optimality conditions

For $g : \mathbb{R}^p \to \mathbb{R}$ convex,

- g differentiable: $\beta^\star$ minimizes g iff $\nabla g(\beta^\star) = 0$.
- g nondifferentiable: $\beta^\star$ minimizes g iff $0 \in \partial g(\beta^\star)$.

Careful: the concept of subgradient requires a function to be above its tangents. It does only make sense for convex functions!

Basic convex optimization tools: dual-norm

Definition

Let $\boldsymbol{\kappa}$ be in $\mathbb{R}^p$,

$$\|\boldsymbol{\kappa}\|_* \triangleq \max_{\boldsymbol{\beta}\in\mathbb{R}^p:\|\boldsymbol{\beta}\|\leq 1} \boldsymbol{\beta}^\top \boldsymbol{\kappa}.$$

Exercises

- $\|\boldsymbol{\beta}\|_{**} = \|\boldsymbol{\beta}\|$ (true in finite dimension)
- ℓ_2 is dual to itself.
- ℓ_1 and ℓ_∞ are dual to each other.
- ℓ_q and ℓ'_q are dual to each other if $\frac{1}{q} + \frac{1}{q'} = 1$.
- similar relations for spectral norms on matrices.
- $\partial\|\boldsymbol{\beta}\| = \{\boldsymbol{\kappa} \in \mathbb{R}^p \text{ s.t. } \|\boldsymbol{\kappa}\|_* \leq 1 \text{ and } \boldsymbol{\kappa}^\top\boldsymbol{\beta} = \|\boldsymbol{\beta}\|\}$.

Optimality conditions

Let $f : \mathbb{R}^p \to \mathbb{R}$ be convex differentiable and $\|.\|$ be any norm.

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} f(\boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|.$$

$\boldsymbol{\beta}$ is solution if and only if

$$0 \in \partial(f(\boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|) = \nabla f(\boldsymbol{\beta}) + \lambda \partial \|\boldsymbol{\beta}\|$$

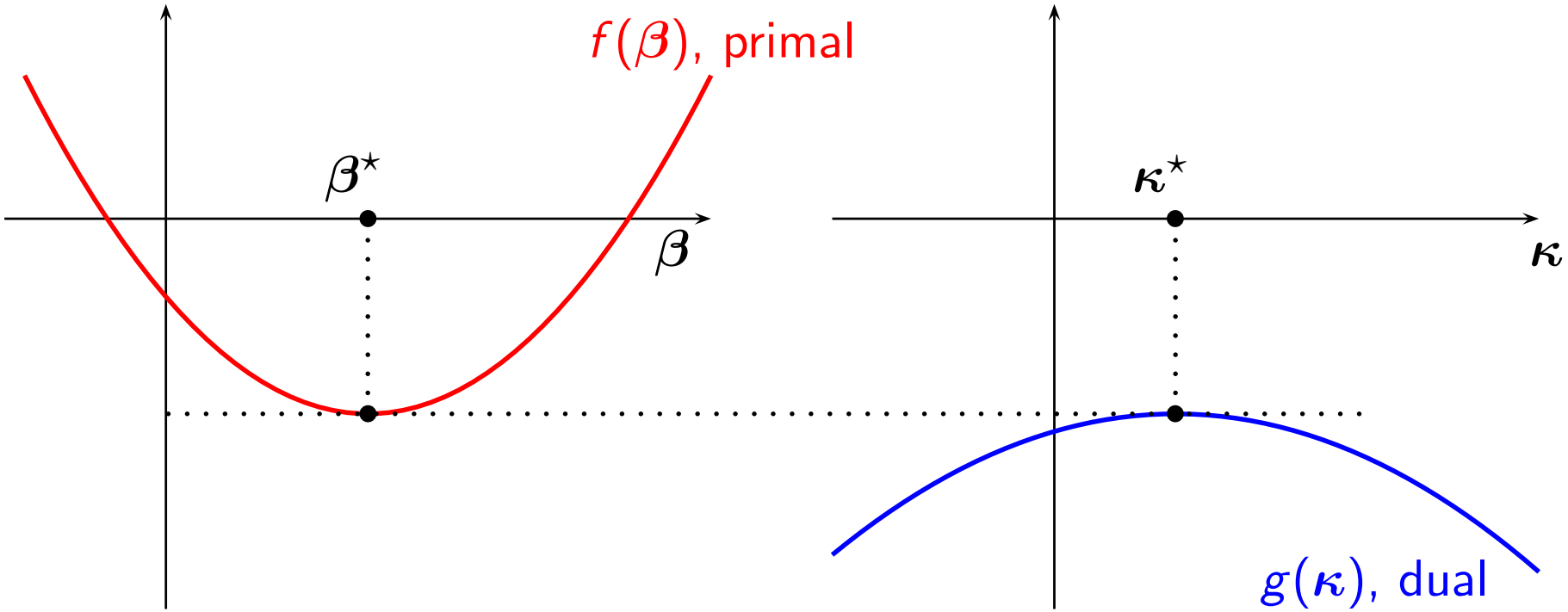
Since $\partial \|\boldsymbol{\beta}\| = \{\boldsymbol{\kappa} \in \mathbb{R}^p \text{ s.t. } \|\boldsymbol{\kappa}\|_* \leq 1 \text{ and } \boldsymbol{\kappa}^\top \boldsymbol{\beta} = \|\boldsymbol{\beta}\|\}$,

General optimality conditions:

$$\|\nabla f(\boldsymbol{\beta})\|_* \leq \lambda \quad \text{and} \quad -\nabla f(\boldsymbol{\beta})^\top \boldsymbol{\beta} = \lambda \|\boldsymbol{\beta}\|.$$

Convex Duality

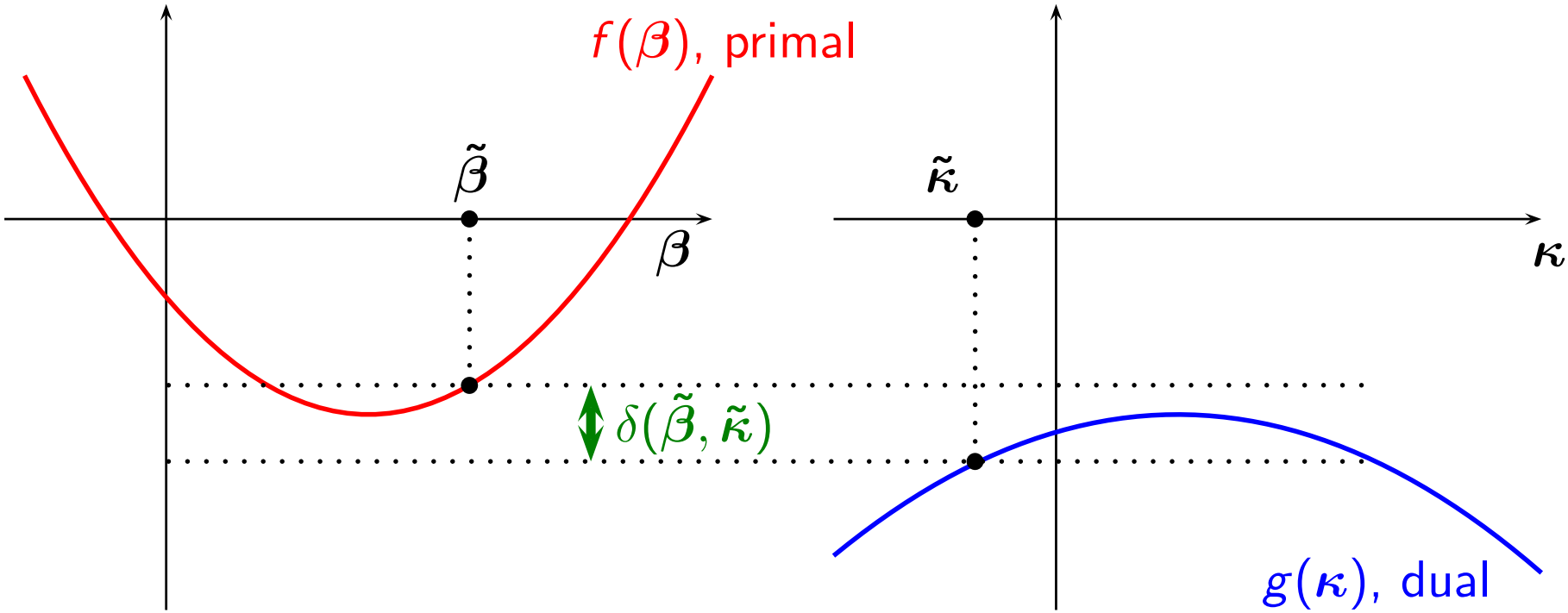
Strong Duality



Strong duality means that $\max_\kappa g(\kappa) = \min_\beta f(\beta)$

Convex Duality

Duality Gaps



Strong duality means that $\max_{\kappa} g(\kappa) = \min_{\beta} f(\beta)$

The duality gap guarantees us that $0 \leq f(\tilde{\beta}) - f(\beta^\star) \leq \delta(\tilde{\beta}, \tilde{\kappa})$.

Part V (Bonus): Dictionary Learning and Matrix Factorization

Matrix Factorization and Clustering

Let us cluster some training vectors $\mathbf{y}^1, \ldots, \mathbf{y}^m$ into p clusters using K-means:

$$\min_{(\mathbf{x}^j)_{j=1}^p, (l_i)_{i=1}^m} \sum_{i=1}^m \|\mathbf{y}^i - \mathbf{x}^{l_i}\|_2^2.$$

It can be equivalently formulated as

$$\min_{\mathbf{X}\in\mathbb{R}^{n\times p}, \mathbf{B}\in\{0,1\}^{p\times m}} \sum_{i=1}^m \|\mathbf{y}^i - \mathbf{X}\boldsymbol{\beta}^i\|_F^2 \quad \text{s.t.} \quad \boldsymbol{\beta}^i \geq 0 \text{ and } \sum_{j=1}^p \boldsymbol{\beta}_j^i = 1,$$

which is a **matrix factorization** problem:

$$\min_{\mathbf{X}\in\mathbb{R}^{n\times p}, \mathbf{B}\in\{0,1\}^{p\times m}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2 \quad \text{s.t.} \quad \mathbf{B} \geq 0 \text{ and } \sum_{j=1}^p \boldsymbol{\beta}_j^i = 1,$$

Matrix Factorization and Clustering

Hard clustering

$$\min_{\mathbf{X}\in\mathbb{R}^{n\times p},\mathbf{B}\in\{0,1\}^{p\times m}} \|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2 \quad \text{s.t.} \quad \mathbf{B}\geq 0 \text{ and } \sum_{j=1}^{p}\beta_j^i = 1,$$

$\mathbf{X} = [\mathbf{x}_1,\ldots,\mathbf{x}_p]$ are the centroids of the p clusters.

Soft clustering

$$\min_{\mathbf{X}\in\mathbb{R}^{n\times p},\mathbf{B}\in\mathbb{R}^{p\times m}} \|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2 \quad \text{s.t.} \quad \mathbf{B}\geq 0 \text{ and } \sum_{j=1}^{p}\beta_j^i = 1,$$

$\mathbf{X} = [\mathbf{x}_1,\ldots,\mathbf{x}_p]$ are the centroids of the p clusters.

Other Matrix Factorization Problems

PCA

$$\min_{\substack{\mathbf{B}\in\mathbb{R}^{p\times n}\\ \mathbf{X}\in\mathbb{R}^{m\times p}}} \frac{1}{2}\|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2 \quad \text{s.t.} \quad \mathbf{X}^\top\mathbf{X}=\mathbf{I} \text{ and } \mathbf{B}\mathbf{B}^\top \text{ is diagonal.}$$

$\mathbf{X}=[\mathbf{x}_1,\ldots,\mathbf{x}_p]$ are the principal components.

Other Matrix Factorization Problems

Non-negative matrix factorization [Lee and Seung, 2001]

$$\min_{\substack{\mathbf{B}\in\mathbb{R}^{p\times n}\\ \mathbf{X}\in\mathbb{R}^{m\times p}}} \frac{1}{2}\|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2 \quad \text{s.t.} \quad \mathbf{B}\geq 0 \text{ and } \mathbf{X}\geq 0.$$

Dictionary Learning and Matrix Factorization

[Olshausen and Field, 1997]

$$\min_{\mathbf{X}\in\mathcal{X},\mathbf{B}\in\mathbb{R}^{p\times m}} \sum_{i=1}^{n} \frac{1}{2}\|\mathbf{y}^i - \mathbf{X}\boldsymbol{\beta}^i\|_F^2 + \lambda\|\boldsymbol{\beta}^i\|_1,$$

which is again a matrix factorization problem

$$\min_{\substack{\mathbf{B}\in\mathbb{R}^{p\times n}\\ \mathbf{X}\in\mathcal{X}}} \frac{1}{2}\|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2 + \lambda\|\mathbf{B}\|_1.$$

Why having a unified point of view?

$$\min_{\substack{\mathbf{B}\in\mathcal{B}\\ \mathbf{X}\in\mathcal{X}}} \frac{1}{2}\|\mathbf{Y}-\mathbf{X}\mathbf{B}\|_F^2 + \lambda\psi(\mathbf{B}).$$

- same framework for NMF, sparse PCA, dictionary learning, clustering, topic modelling;
- can play with various constraints/penalties on $\mathbf{B}$ (coefficients) and on $\mathbf{X}$ (loadings, dictionary, centroids);
- same algorithms (no need to reinvent the wheel): alternate minimization, online learning [Mairal et al., 2009].

The Image Denoising Problem

$$\underbrace{\mathbf{y}}_{\text{measurements}} = \underbrace{\mathbf{x}_{orig}}_{\text{original image}} + \underbrace{\varepsilon}_{\text{noise}}$$

Sparse representations for image restoration

$$\underbrace{\mathbf{y}}_{\text{measurements}} = \underbrace{\mathbf{x}_{orig}}_{\text{original image}} + \underbrace{\varepsilon}_{\text{noise}}$$

Energy minimization problem - MAP estimation

$$E(\mathbf{x}) = \underbrace{\frac{1}{2}\|\mathbf{y}-\mathbf{x}\|_2^2}_{\text{relation to measurements}} + \underbrace{\psi(\mathbf{x})}_{\text{image model (-log prior)}}$$

Some classical priors

- Smoothness $\lambda\|\mathcal{L}\mathbf{x}\|_2^2$
- Total variation $\lambda\|\nabla\mathbf{x}\|_1^2$
- MRF priors
- ...

Sparse representations for image restoration

Designed dictionaries

[Haar, 1910], [Zweig, Morlet, Grossman ∼70s], [Meyer, Mallat, Daubechies, Coifman, Donoho, Candes ∼80s-today]. . . (see [Mallat, 1999])
Wavelets, Curvelets, Wedgelets, Bandlets, . . . lets

Learned dictionaries of patches

[Olshausen and Field, 1997], [Engan et al., 1999], [Lewicki and Sejnowski, 2000], [Aharon et al., 2006]

$$\min_{\boldsymbol{\beta}_i, \mathbf{X} \in \mathcal{C}} \sum_i \underbrace{\frac{1}{2}\|\mathbf{y}_i - \mathbf{X}\boldsymbol{\beta}_i\|_2^2}_{\text{reconstruction}} + \underbrace{\lambda\psi(\boldsymbol{\beta}_i)}_{\text{sparsity}}$$

- $\psi(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_0$ ("ℓ_0 pseudo-norm")
- $\psi(\boldsymbol{\beta}) = \|\boldsymbol{\beta}\|_1$ (ℓ_1 norm)

Sparse representations for image restoration

Solving the denoising problem

[Elad and Aharon, 2006]

- Extract all overlapping 8×8 patches $\mathbf{y}_i$.
- Solve a matrix factorization problem:

$$\min_{\boldsymbol{\beta}_i, \mathbf{X} \in \mathcal{C}} \sum_{i=1}^{n} \underbrace{\frac{1}{2}\|\mathbf{y}_i - \mathbf{X}\boldsymbol{\beta}_i\|_2^2}_{\text{reconstruction}} + \underbrace{\lambda\psi(\boldsymbol{\beta}_i)}_{\text{sparsity}},$$

  with $n > 100,000$

- Average the reconstruction of each patch.

Sparse representations for image restoration

K-SVD: [Elad and Aharon, 2006]

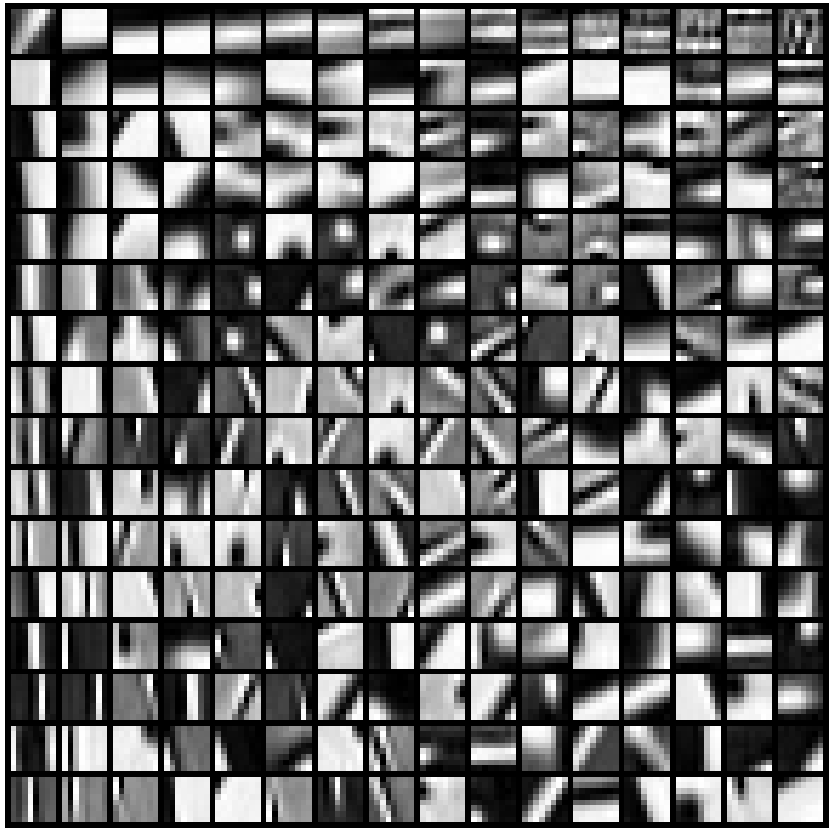
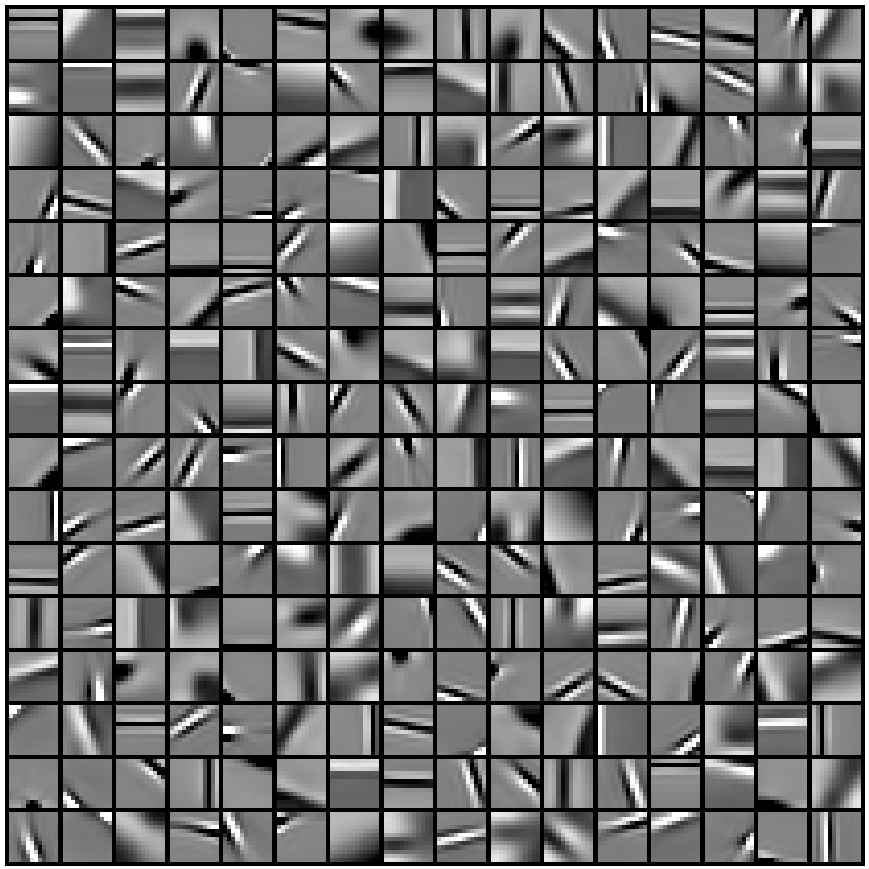
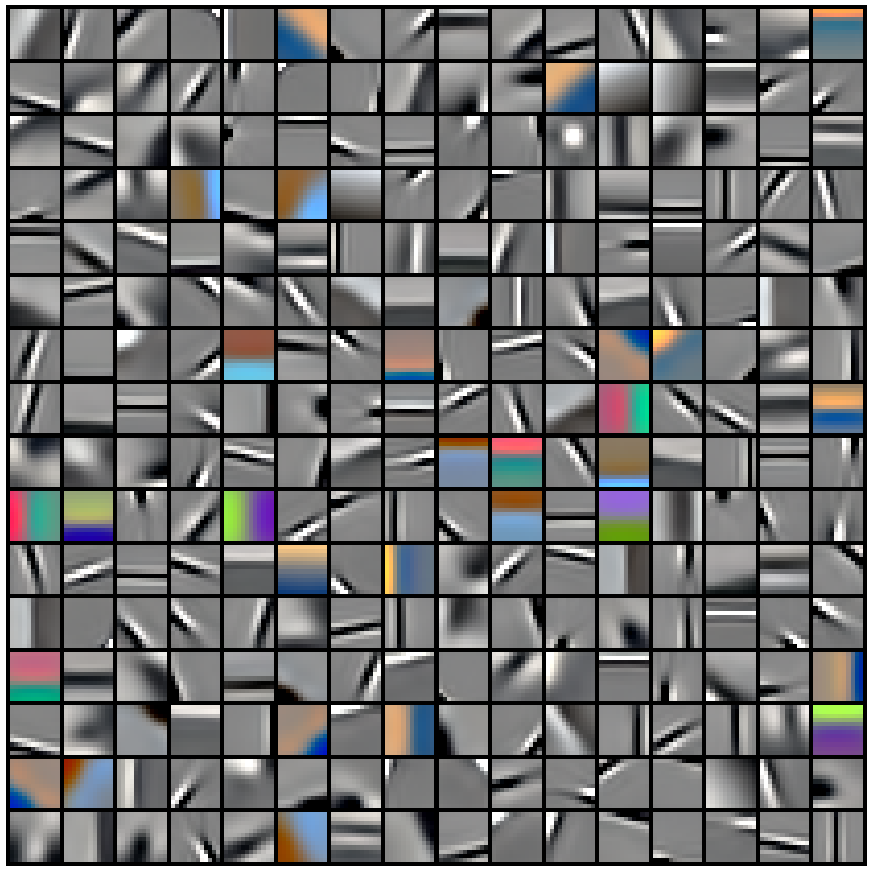


Figure: Dictionary trained on a noisy version of the image boat.

Sparse representations for image restoration

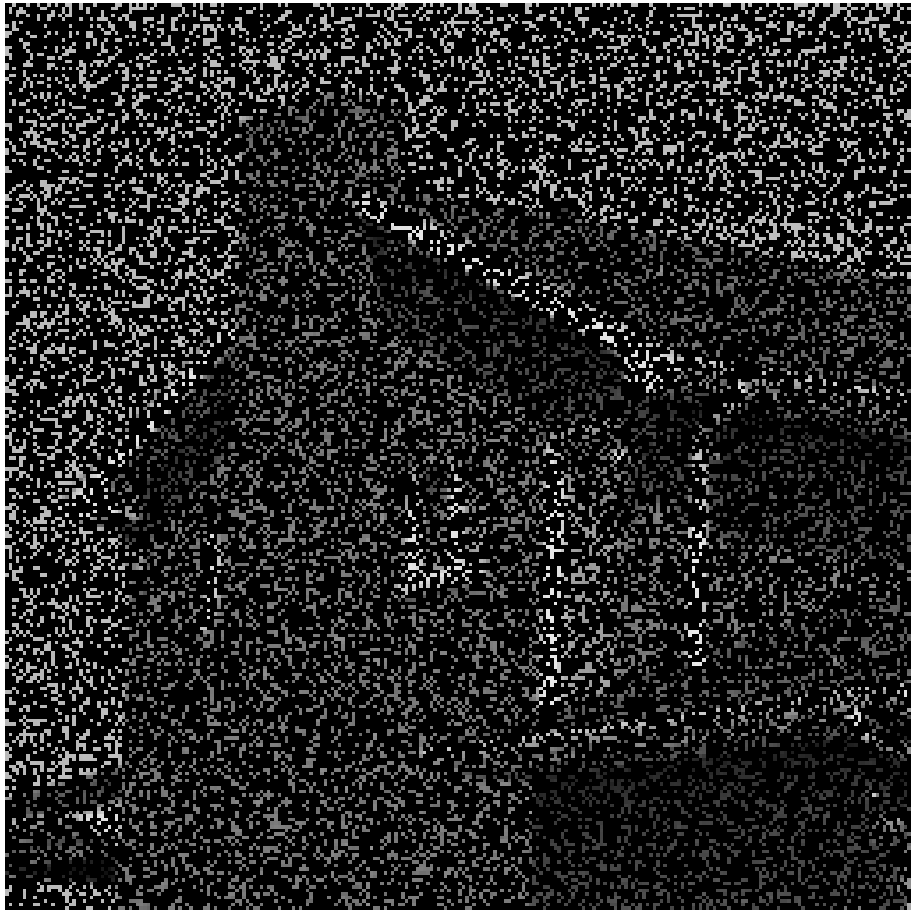
Grayscale vs color image patches





Sparse representations for image restoration

[Mairal, Sapiro, and Elad, 2008b]



Sparse representations for image restoration

Inpainting, [Mairal, Elad, and Sapiro, 2008a]

Sparse representations for image restoration

Inpainting, [Mairal, Elad, and Sapiro, 2008a]

Sparse representations for video restoration

Key ideas for video processing

[Protter and Elad, 2009]

- Using a 3D dictionary.
- Processing of many frames at the same time.
- Dictionary propagation.

Sparse representations for image restoration

Inpainting, [Mairal, Sapiro, and Elad, 2008b]

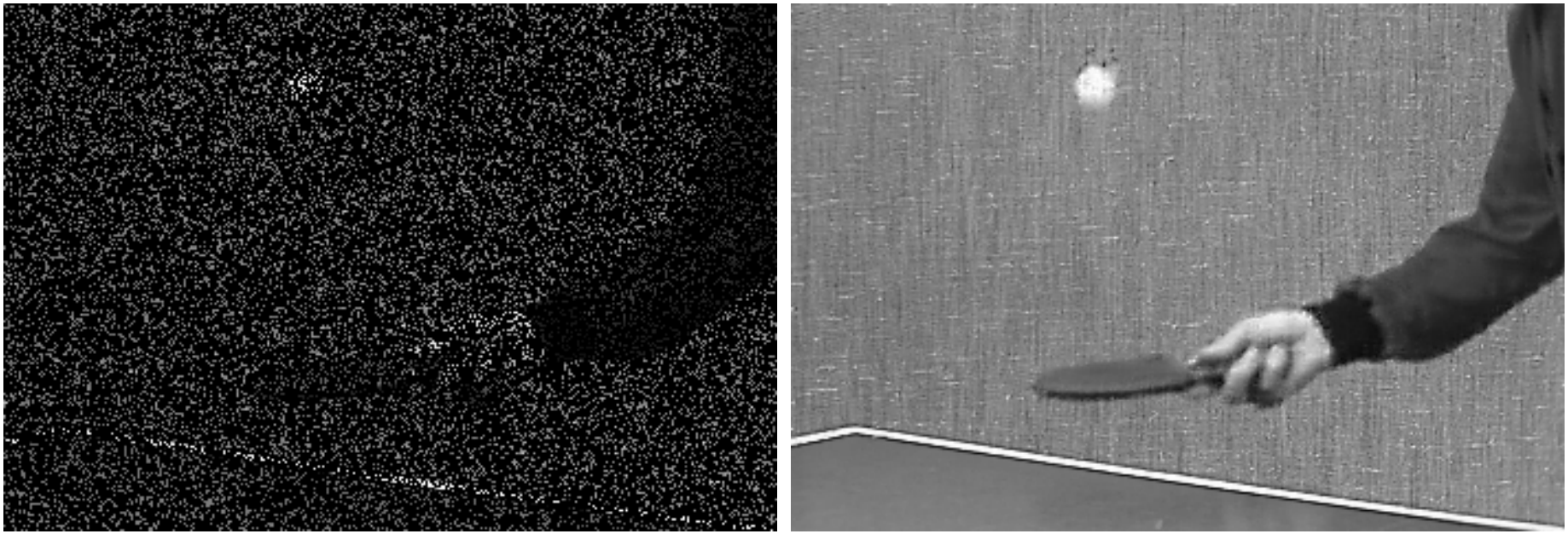


Figure: Inpainting results.

Sparse representations for image restoration

Inpainting, [Mairal, Sapiro, and Elad, 2008b]

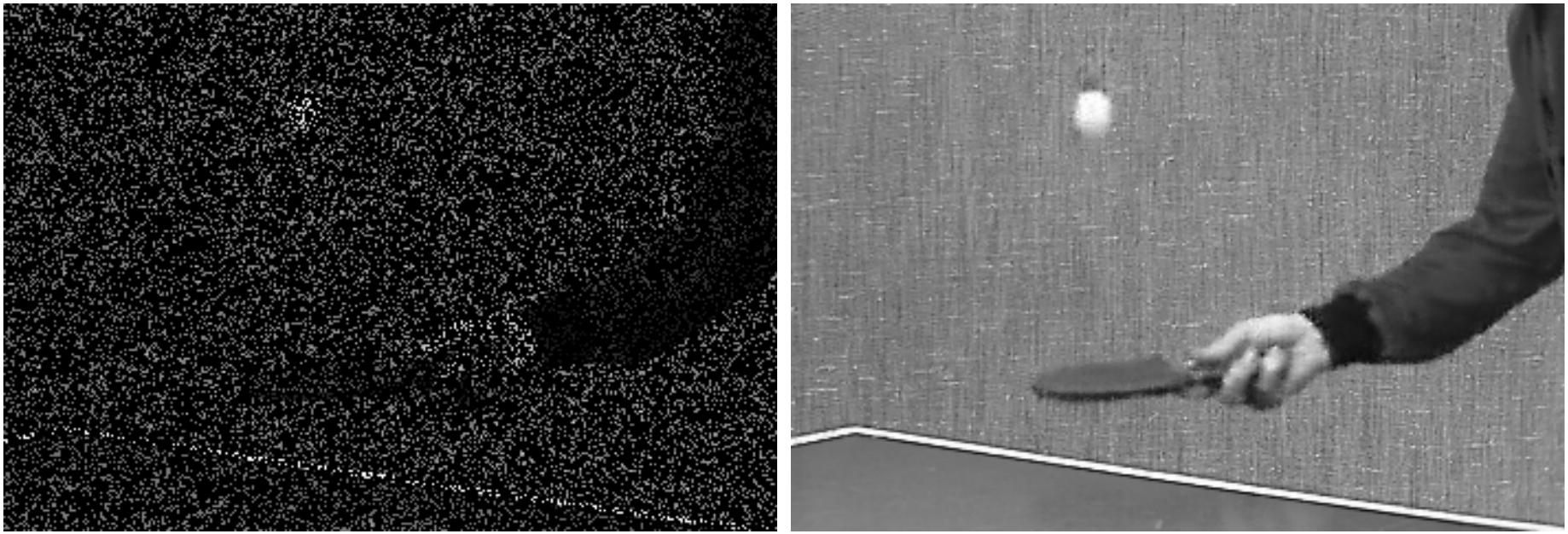


Figure: Inpainting results.

Sparse representations for image restoration

Inpainting, [Mairal, Sapiro, and Elad, 2008b]

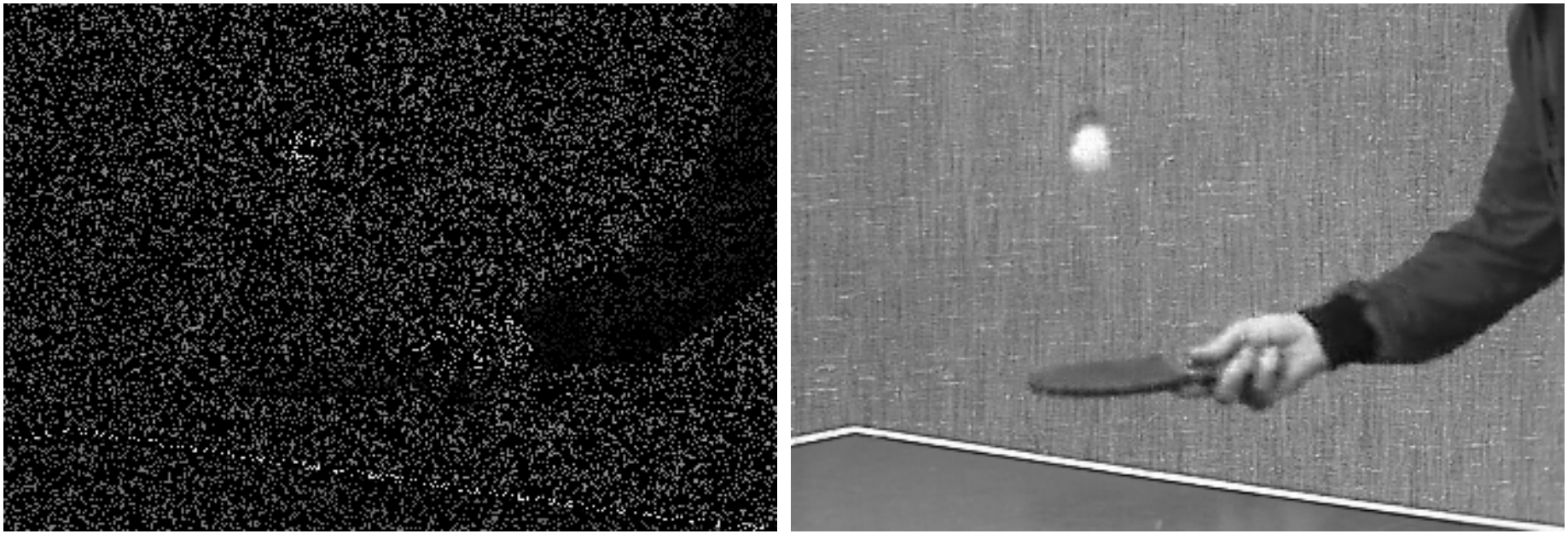


Figure: Inpainting results.

Sparse representations for image restoration

Inpainting, [Mairal, Sapiro, and Elad, 2008b]

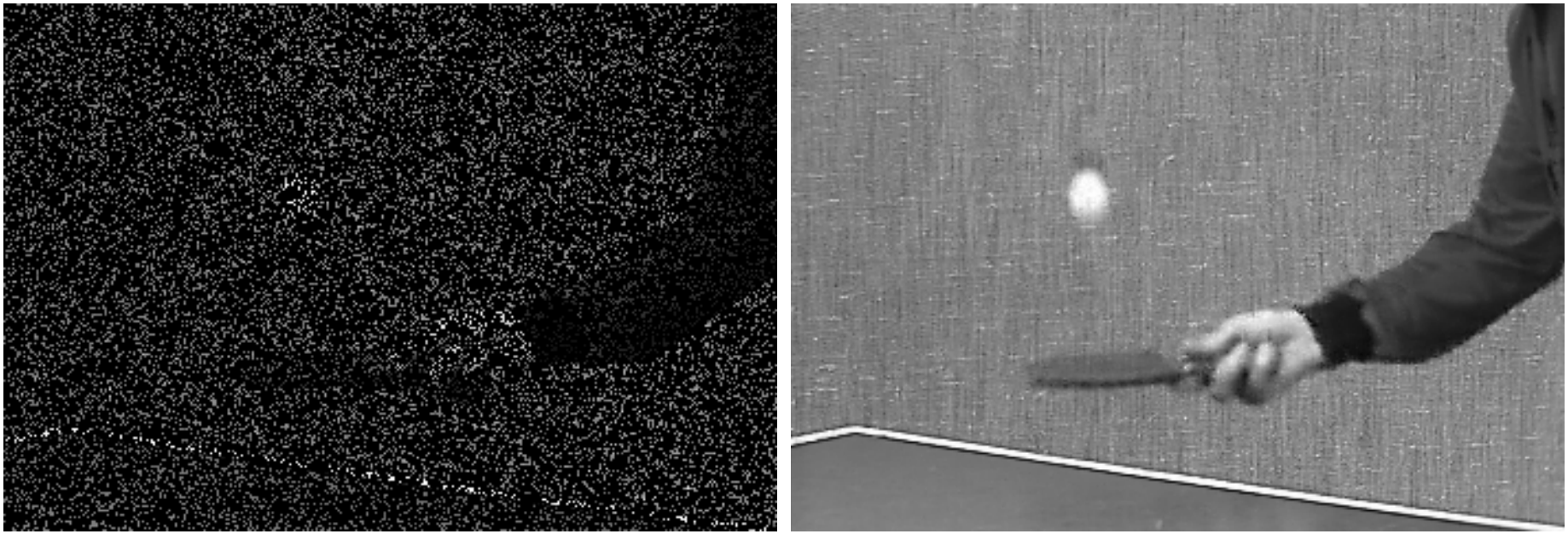


Figure: Inpainting results.

Sparse representations for image restoration

Inpainting, [Mairal, Sapiro, and Elad, 2008b]

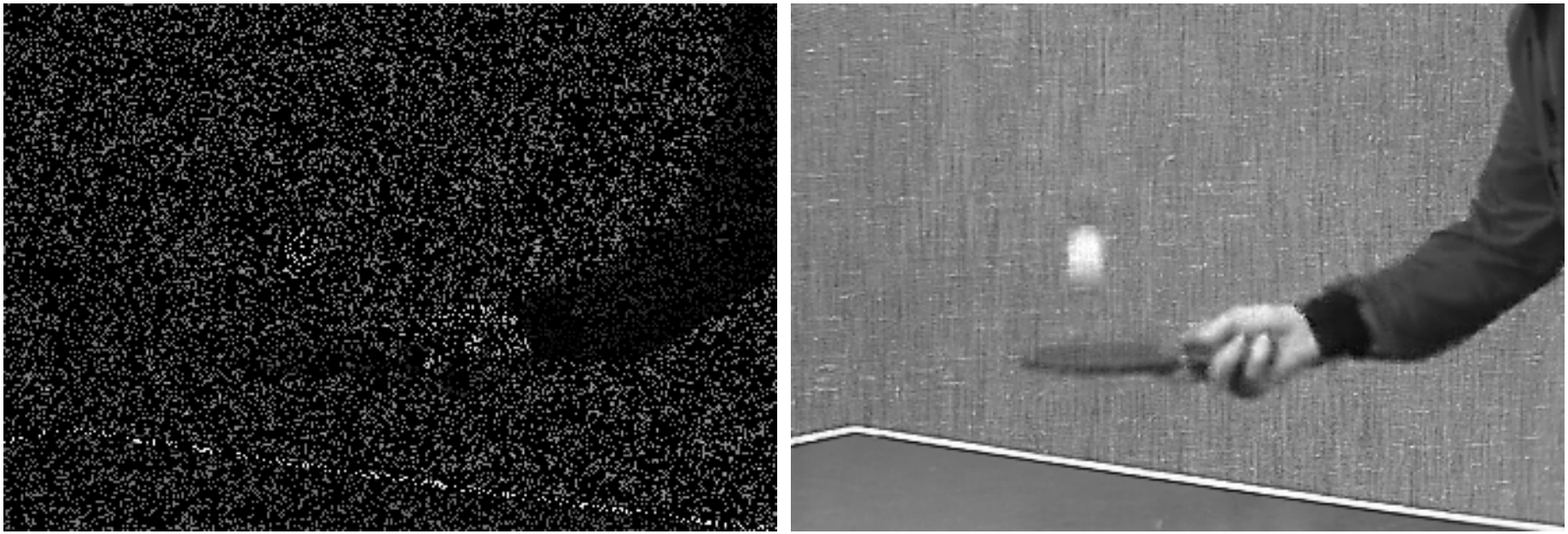


Figure: Inpainting results.

Sparse representations for image restoration

Color video denoising, [Mairal, Sapiro, and Elad, 2008b]

Figure: Denoising results. $\sigma = 25$

Sparse representations for image restoration

Color video denoising, [Mairal, Sapiro, and Elad, 2008b]

Figure: Denoising results. $\sigma = 25$

Sparse representations for image restoration

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Sparse representations for image restoration

Color video denoising, [Mairal, Sapiro, and Elad, 2008b]

Figure: Denoising results. $\sigma = 25$

Digital Zooming

[Couzinie-Devy et al., 2011], Original

Digital Zooming

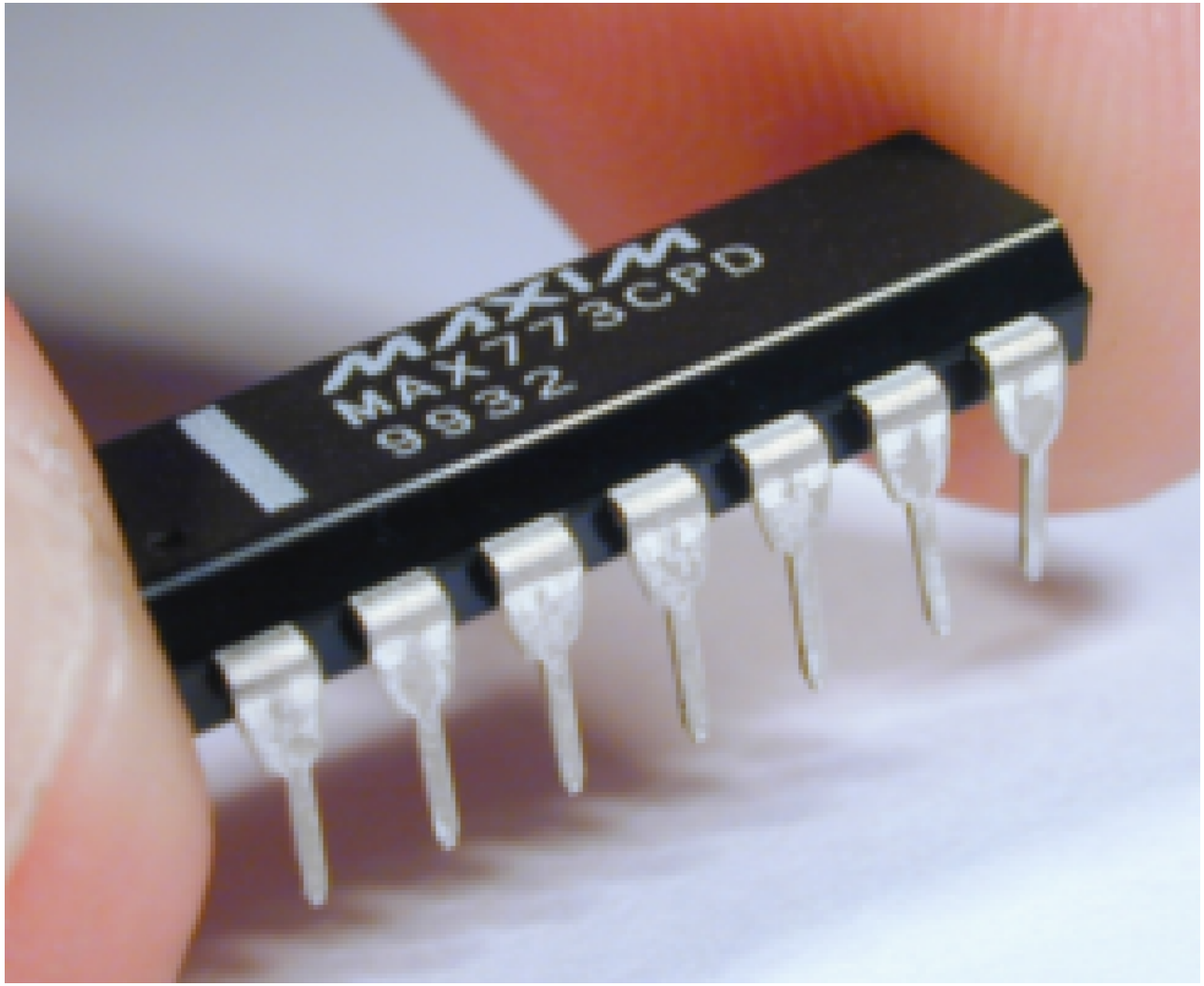
[Couzinie-Devy et al., 2011], Bicubic

Digital Zooming

[Couzinie-Devy et al., 2011], Proposed method

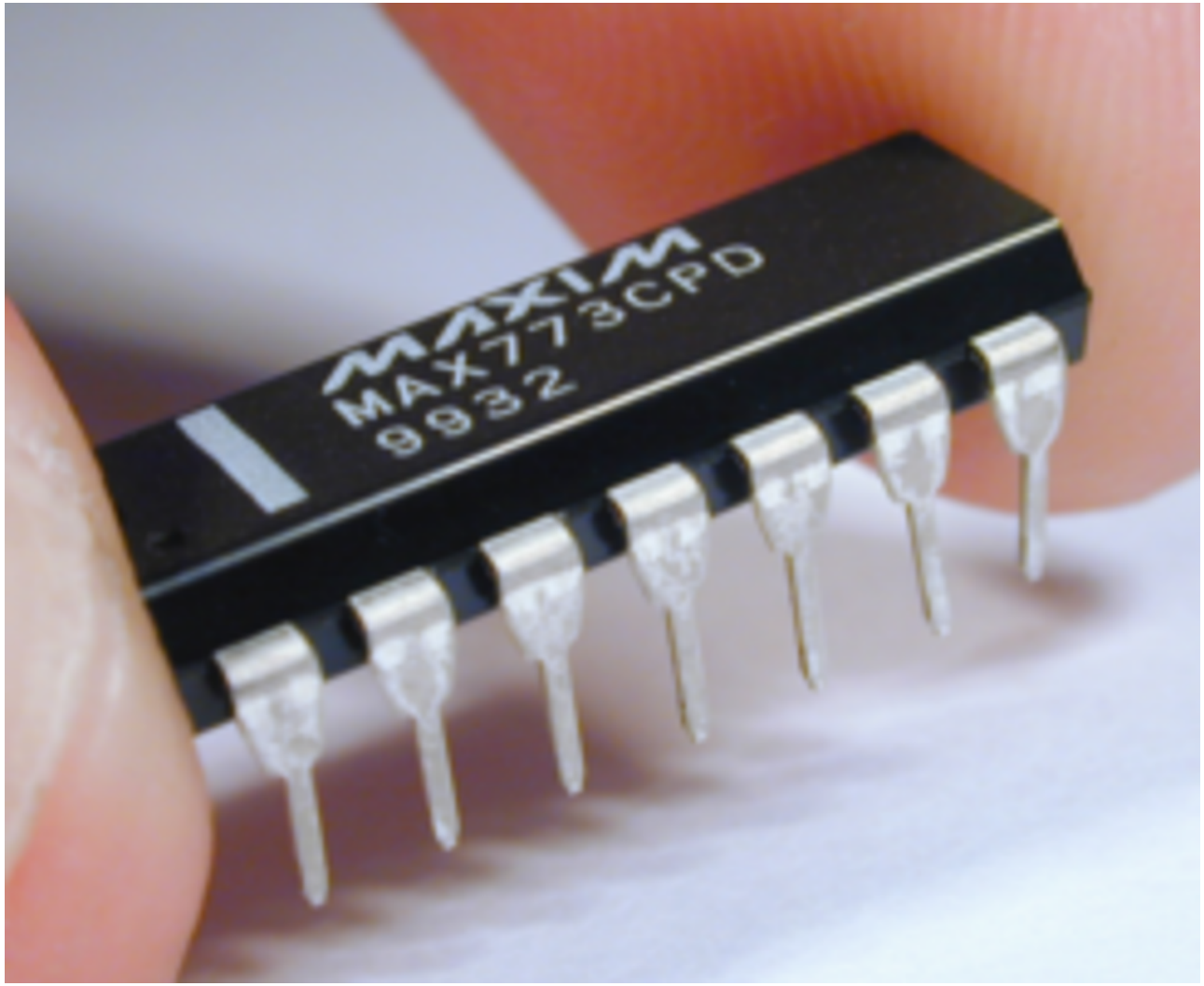
Digital Zooming

[Couzinie-Devy et al., 2011], Original



Digital Zooming

[Couzinie-Devy et al., 2011], Bicubic



Digital Zooming

[Couzinie-Devy et al., 2011], Proposed approach

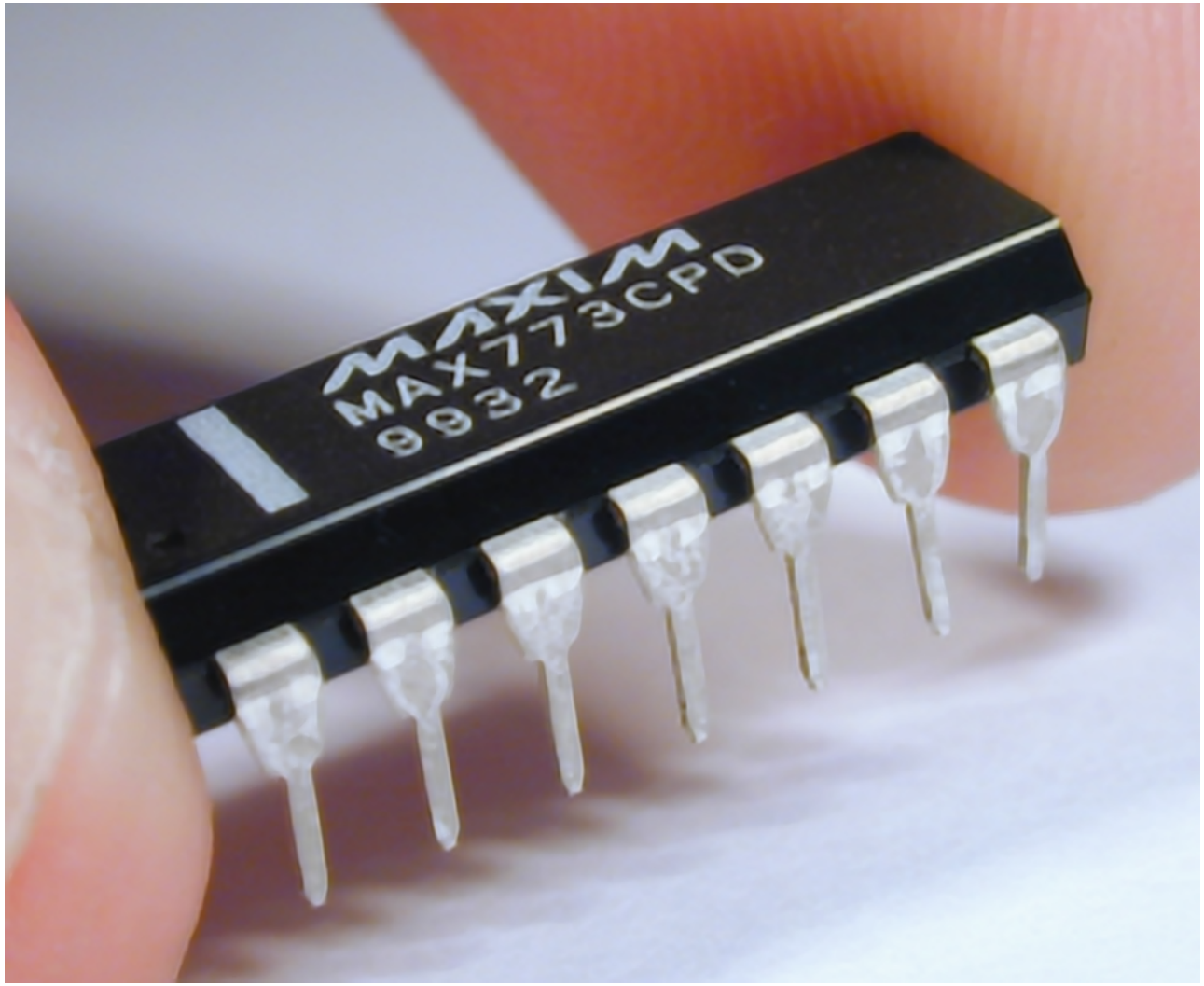


Image Deblurring

[Couzinie-Devy et al., 2011], Original

Image Deblurring

[Couzinie-Devy et al., 2011], Blurry and Noisy

Image Deblurring

[Couzinie-Devy et al., 2011], Result

Image Deblurring

[Couzinie-Devy et al., 2011], Original

Image Deblurring

[Couzinie-Devy et al., 2011], Blurry and Noisy

Image Deblurring

[Couzinie-Devy et al., 2011], Result

Inverse half-toning

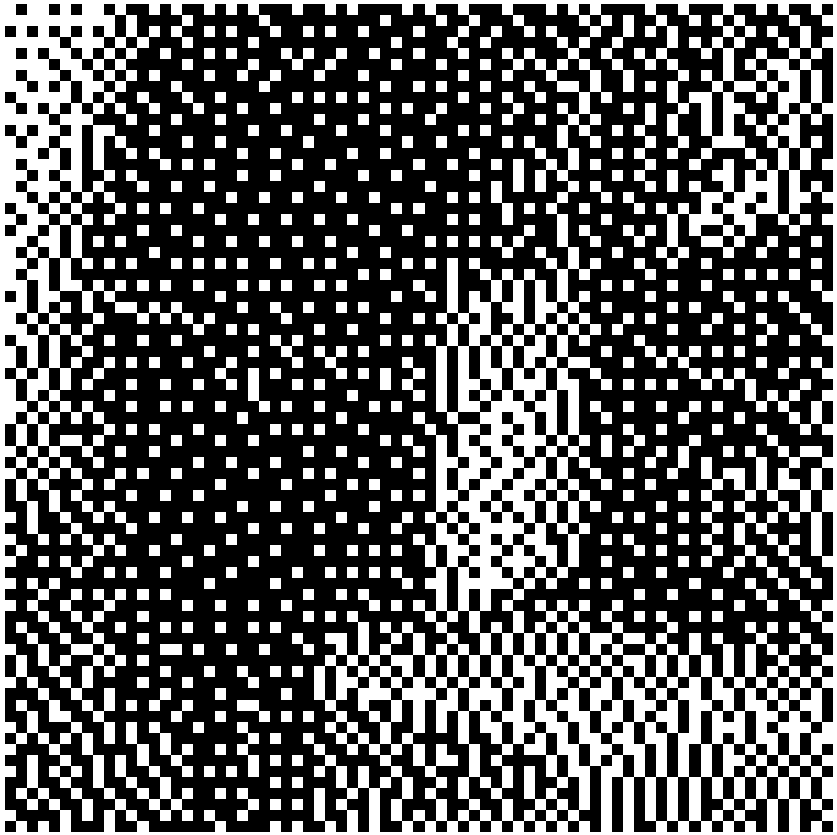
Original

Inverse half-toning

Reconstructed image

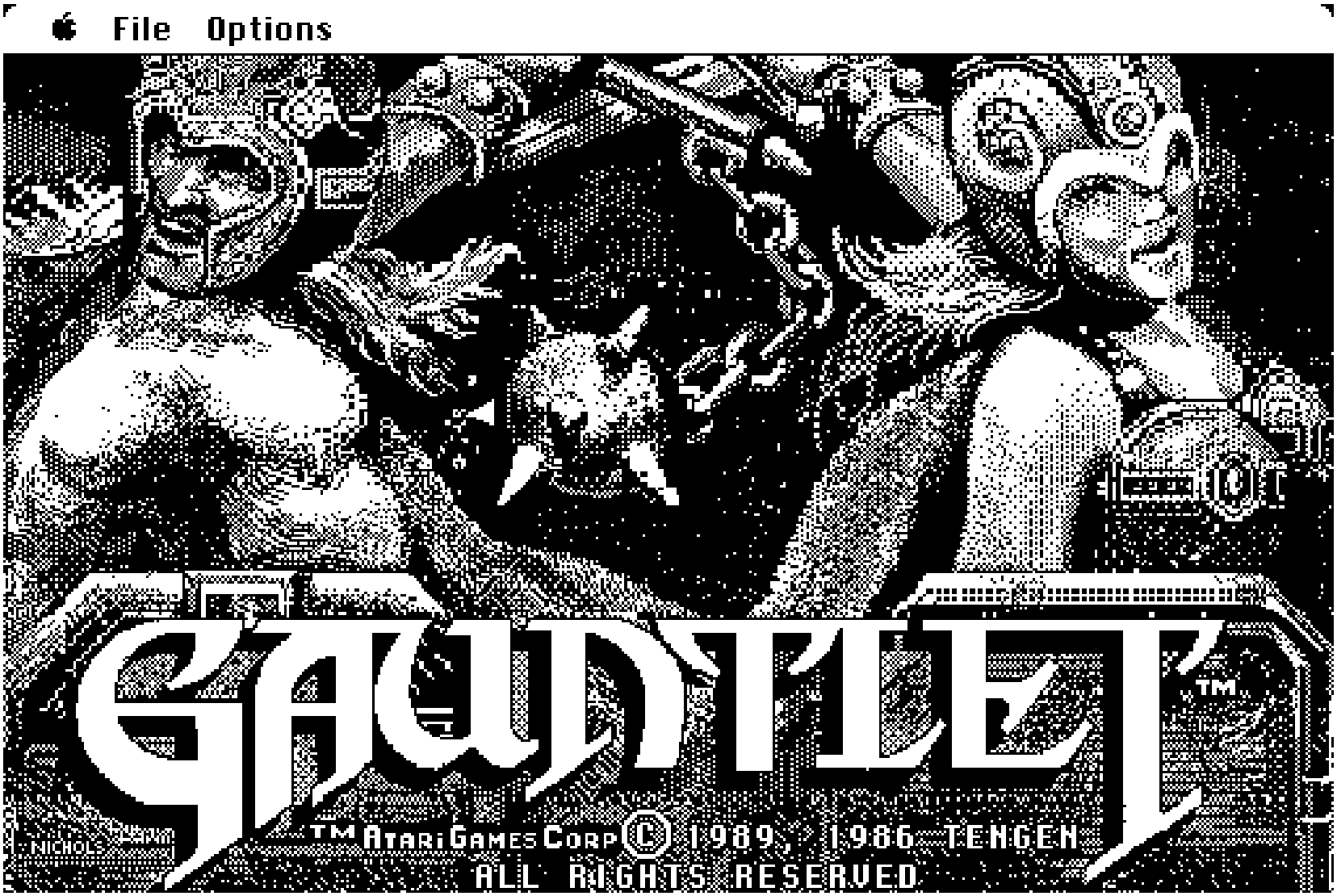
Inverse half-toning

Reconstructed image



Inverse half-toning

Original



Inverse half-toning

Reconstructed image

Inverse half-toning

Original

Inverse half-toning

Reconstructed image

Inverse half-toning

Original

Inverse half-toning

Reconstructed image

Inverse half-toning

Original

Inverse half-toning

Reconstructed image